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AN EXPLICIT AND SYMMETRIC EXPONENTIAL WAVE INTEGRATOR FOR THE NONLINEAR SCHRÖDINGER EQUATION WITH LOW REGULARITY POTENTIAL AND NONLINEARITY*

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Abstract. We propose and analyze a novel symmetric Gautschi-type exponential wave integrator (sEWI) for the nonlinear Schrödinger equation (NLSE) with low regularity potential and typical power-type nonlinearity of the form $|\psi|^{2\sigma}\psi$ with ψ being the wave function and $\sigma > 0$ being the exponent of the nonlinearity. The sEWI is explicit and stable under a time step size restriction independent of the mesh size. We rigorously establish error estimates of the sEWI under various regularity assumptions on potential and nonlinearity. For "good" potential and nonlinearity (H^2-potential and $\sigma \geq 1$), we establish an optimal second-order error bound in the L^2-norm. For low regularity potential and nonlinearity (L^∞-potential and $\sigma > 0$), we obtain a first-order L^2-norm error bound accompanied with a uniform H^2-norm bound of the numerical solution. Moreover, adopting a new technique of *regularity compensation oscillation* to analyze error cancellation, for some nonresonant time steps, the optimal second-order L^2-norm error bound is proved under a weaker assumption on the nonlinearity: $\sigma \geq 1/2$. For all the cases, we also present corresponding fractional order error bounds in the H^1-norm, which is the natural norm in terms of energy. Extensive numerical results are reported to confirm our error estimates and to demonstrate the superiority of the sEWI, including much weaker regularity requirements on potential and nonlinearity, and excellent long-time behavior with near-conservation of mass and energy.

Key words. nonlinear Schrödinger equation, symmetric exponential wave integrator, low regularity potential, low regularity nonlinearity, error estimate

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1. Introduction.

The nonlinear Schrödinger equation (NLSE) arises in various physical applications such as quantum physics and chemistry, Bose–Einstein condensation, laser beam propagation, plasma and particle physics [7, 28, 46, 40]. In this paper, we consider the following NLSE on a bounded domain $\Omega = \Pi_{i=1}^d (a_i, b_i) \subset \mathbb{R}^d$ ($d = 1, 2, 3$) equipped with the periodic boundary condition

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

where t is time, $\mathbf{x} \in \mathbb{R}^d$ is the spatial coordinate, and $\psi := \psi(\mathbf{x}, t)$ is a complex-valued wave function. Here, $V := V(\mathbf{x}) \in L^\infty(\Omega)$ is a given real-valued external potential, and f is assumed to be the power-type nonlinearity given by

$$f(\rho) = \beta\rho^\sigma, \quad \rho := |\psi|^2 \geq 0, \tag{1.2}$$

where $\beta \in \mathbb{R}$ is a given constant and $\sigma > 0$ is the exponent of the nonlinearity.

There are many important dynamical properties of the solution ψ to the NLSE (1.1) [6]. The NLSE (1.1) is time reversible or symmetric, i.e., it is unchanged under

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the change of variable in time as $t \to -t$ and complex conjugating the equation. It is also time transverse or gauge invariant, i.e., the equation still holds under the transformation $V \to V + \alpha$ with α a given constant and $\psi \to \psi e^{-i\alpha t}$, which immediately implies that the density $\rho = |\psi|^2$ is unchanged. Moreover, the NLSE (1.1) conserves the mass

$$M(\psi(\cdot,t)) = \int_\Omega |\psi(\mathbf{x},t)|^2 \mathrm{d}\mathbf{x} \equiv M(\psi_0), \quad t \geq 0, \tag{1.3}$$

and the energy

$$E(\psi(\cdot,t)) = \int_\Omega \left[|\nabla\psi(\mathbf{x},t)|^2 + V(\mathbf{x})|\psi(\mathbf{x},t)|^2 + F(|\psi(\mathbf{x},t)|^2)\right] \mathrm{d}\mathbf{x} \equiv E(\psi_0), \tag{1.4}$$

where the interaction energy density $F(\rho) = \frac{\beta}{\sigma+1}\rho^{\sigma+1}$.

When the nonlinearity is chosen as the cubic nonlinearity (i.e., $\sigma = 1$ in (1.2)) and the potential is chosen as the harmonic trapping potential (namely, $V(\mathbf{x}) = |\mathbf{x}|^2/2$), the NLSE (1.1) reduces to the cubic NLSE with smooth potential, which is also known as the Gross–Pitaevskii equation (GPE), especially in the context of Bose–Einstein condensation. In this case, both V and f are smooth functions. While the NLSE with smooth potential and nonlinearity, such as the GPE, is prevalent, diverse physics applications require the incorporation of low regularity potential and/or nonlinearity, including discontinuous potential, disorder potential, and noninteger power nonlinearity (see [18, 19, 32, 48] and references therein for the applications).

For the cubic NLSE with sufficiently smooth initial data, many accurate and efficient numerical methods have been proposed and analyzed in the last two decades, including the finite difference time domain (FDTD) method [1, 8, 7, 6, 32], the exponential wave integrator (EWI) [9, 35, 24, 19], and the time-splitting method [16, 20, 41, 7, 27, 6, 42, 10, 22, 18]. Among these methods, the Strang time-splitting method is widely used due to its efficient implementation and the preservation of many dynamical properties including the time symmetry, time transverse invariance, dispersion relation, and mass conservation at the discrete level [6]. Recently, some low regularity integrators (LRIs) have also been designed for the cubic NLSE with low regularity initial data and with/without potential [44, 39, 43, 3, 21, 5, 4].

Most of the aforementioned numerical methods can be extended straightforwardly to solve the NLSE (1.1) with low regularity potential and/or nonlinearity, e.g., the FDTD method [32], the time-splitting method [36, 25, 18, 48, 17], the EWI [19], and the LRI [48, 5, 3] (different from some singular nonlinearities [12, 13, 14, 15, 47], where regularization may be needed). However, their performances deviate considerably when compared to the smooth setting. As demonstrated in [19], compared with FDTD methods, time-splitting methods, and LRIs, in the presence of low regularity potential and/or nonlinearity, the EWI outperforms all of them (at least at the semidiscrete level). Nevertheless, the EWI presented in [19] remains a first-order method and fails to preserve either the time symmetry or the conservation of mass and energy. It is of great interest to devise numerical schemes of high order that are capable of preserving the dynamical properties at a discrete level. Based on the discussion above, we focus on designing and analyzing structure-preserving EWIs, especially time symmetric EWIs.

In fact, extensive efforts have been made in the literature to design symmetric exponential integrators for the cubic NLSE, motivated by the structure-preserving properties and favorable long-time behavior of these symmetric schemes [24, 30, 31, 2, 29, 4].

However, most of them are fully implicit, which necessitates solving a fully nonlinear system at each time step. Usually, the nonlinear system is solved by a fixed point iteration, which is time consuming, especially in two dimensions (2D) and three dimensions (3D) [24, 2, 29]. Actually, if the nonlinear system is not solved up to sufficient accuracy (e.g., machine accuracy), the symmetric property of the scheme may be destroyed. Moreover, although there are some explicit symmetric schemes in the literature [34, 30], they are different from ours when applied to the NLSE and they are only conditionally stable under certain CFL-type time step size restrictions. Additionally, all those schemes lack error estimates under low regularity assumptions on potential and nonlinearity.

In this work, we introduce a second-order explicit and symmetric Gautschi-type EWI (sEWI), which possesses two main advantages: (i) it is explicit and symmetric while it remains stable under a time step size restriction independent of the mesh size; (ii) it is rigorously proved to be advantageous for the NLSE with low regularity potential and nonlinearity. Note that, despite sharing a similar spirit in the construction, the sEWI is a completely new method and it differs from the first-order EWI introduced in [19] in that it is a symmetric two-step method and is of second order. In fact, any symmetric method is at least second order [31]. In addition, a similar idea was employed in [37] but for a different purpose.

To show the merit of our new sEWI for the NLSE with low regularity potential and nonlinearity, we rigorously establish error estimates under varying regularity assumptions on potential and nonlinearity. The analysis is carried out in the one dimensional setting; however, it remains essentially the same in 2D and 3D. Main results are stated in sections 3.1 and 4.1, and we also summarize them here:

(i) under the assumption of the H^2-potential, $\sigma \geq 1$, and the H^4-solution, we derive an optimal second-order error bound in the L^2-norm at both semidiscrete (Theorem 3.1) and fully discrete (Theorem 4.1) levels;

(ii) under more general assumptions of the L^∞-potential, $\sigma > 0$, and H^2-solution, we establish a first-order error bound in the L^2-norm along with a uniform H^2-bound of the numerical solution at both semidiscrete (Theorem 3.2) and fully discrete (Theorem 4.2) levels;

(iii) for the full-discretization scheme, the assumption on the nonlinearity in (i) can be relaxed to $\sigma \geq 1/2$ for certain nonresonant time steps (Theorem 4.3).

For the first-order L^2-norm error bound in time, (ii) mirrors the first-order EWI in [19], which, to our best knowledge, requires the weakest regularity of both potential and nonlinearity, among FDTD methods [32], time-splitting methods [18, 17, 36, 25], and LRIs [3, 5]. In terms of the optimal second-order error bound, the assumption of the sEWI in (i) is significantly weaker than the requirement of the Strang time-splitting method which requires the H^4-potential and $\sigma \geq 3/2$ (or $\sigma = 1$) [20, 41, 7]. Although recent results in [17] show that, for the full discretization of the Strang time-splitting method, it can obtain an optimal L^2-norm error bound under the same assumption as the sEWI in (i), a CFL-type time step size restriction is necessary. Actually, if imposing the same time step size restriction, the regularity requirement on nonlinearity for the sEWI can be further relaxed as in (iii). It should be noted the concept of "low regularity" includes two aspects: one is, given low regularity potential and nonlinearity, determining the highest convergence order that can be achieved (corresponding to (ii)); and the other is identifying the lowest regularity required to obtain a given convergence order (corresponding to (i) and (iii)).

The rest of the paper is organized as follows. In section 2, we present the sEWI and its spatial discretization by the Fourier spectral method. Sections 3–4 are devoted to the error estimates of the sEWI at a semidiscrete level and the fully discrete level, respectively. Numerical results are reported in section 5 to confirm our error estimates. Finally, some conclusions are drawn in section 6. Throughout the paper, we adopt standard notations of vector-valued Sobolev spaces as well as their corresponding norms. The bold letters are always used for vector-valued functions or operators. We 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. An explicit and symmetric EWI. In this section, we introduce sEWI and its spatial discretization to solve the NLSE (1.1). For simplicity of the presentation and to avoid heavy notations, we only carry out the analysis in one dimension (1D) and take $\Omega=(a,b)$. Generalizations to 2D and 3D are straightforward. In fact, main dimension sensitive estimates are the Sobolev embeddings. Throughout this paper, we only use embeddings $H^1(\Omega)\hookrightarrow L^4(\Omega)$, $H^{\frac{7}{4}}(\Omega)\hookrightarrow L^\infty(\Omega)$, and $H^2(\Omega)\hookrightarrow L^\infty(\Omega)$, which are valid in 1D, 2D and 3D. We define the periodic Sobolev spaces as (see, e.g., [3], for the definition in the phase space)

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

2.1. A semidiscretization in time. For simplicity, define an operator B as

$$B(v)(x) := V(x)v(x) + f(|v(x)|^2)v(x), \quad v\in L^2(\Omega). \tag{2.1}$$

Choose a time step size $\tau>0$ and denote time steps as $t_n = n\tau$ for $n=0,1,\ldots$. In the following, we shall always abbreviate $\psi(\cdot,t)$ by $\psi(t)$ for simplicity when there is no confusion. By Duhamel's formula, the exact solution ψ satisfies

$$\psi(t_n+\zeta) = e^{i\zeta\Delta}\psi(t_n) - i\int_0^\zeta e^{i(\zeta-s)\Delta}B(\psi(t_n+s))\mathrm{d}s, \quad \zeta\in\mathbb{R}. \tag{2.2}$$

Multiplying both sides of (2.2) by $e^{-i\zeta\Delta}$, we obtain

$$e^{-i\zeta\Delta}\psi(t_n+\zeta) = \psi(t_n) - i\int_0^\zeta e^{-is\Delta}B(\psi(t_n+s))\mathrm{d}s. \tag{2.3}$$

Taking $\zeta=\tau$ in (2.3), we get

$$e^{-i\tau\Delta}\psi(t_{n+1}) = \psi(t_n) - i\int_0^\tau e^{-is\Delta}B(\psi(t_n+s))\mathrm{d}s. \tag{2.4}$$

Taking $\zeta=-\tau$ in (2.3), we get

$$\begin{aligned} e^{i\tau\Delta}\psi(t_{n-1}) &= \psi(t_n) - i\int_0^{-\tau} e^{-is\Delta}B(\psi(t_n+s))\mathrm{d}s \\ &= \psi(t_n) + i\int_{-\tau}^0 e^{-is\Delta}B(\psi(t_n+s))\mathrm{d}s. \end{aligned} \tag{2.5}$$

Subtracting (2.5) from (2.4), we obtain

$$e^{-i\tau\Delta}\psi(t_{n+1}) - e^{i\tau\Delta}\psi(t_{n-1}) = -i\int_{-\tau}^\tau e^{-is\Delta}B(\psi(t_n+s))\mathrm{d}s. \tag{2.6}$$

Multiplying by $e^{i\tau\Delta}$ on both sides of (2.6) yields

$$\psi(t_{n+1}) = e^{2i\tau\Delta}\psi(t_{n-1}) - i\int_{-\tau}^{\tau} e^{i(\tau-s)\Delta}B(\psi(t_n+s))\mathrm{d}s. \tag{2.7}$$

Applying the Gautschi-type rule to approximate the integral in (2.7), i.e., approximating $\psi(t_n+s)$ by $\psi(t_n)$ and integrating out $e^{i(\tau-s)\Delta}$ exactly, we get

$$\begin{aligned}\int_{-\tau}^{\tau} e^{i(\tau-s)\Delta}B(\psi(t_n+s))\mathrm{d}s &\approx \int_{-\tau}^{\tau} e^{i(\tau-s)\Delta}B(\psi(t_n))\mathrm{d}s\\ &= 2\tau e^{i\tau\Delta}\varphi_{\mathrm{s}}(\tau\Delta)B(\psi(t_n)),\end{aligned} \tag{2.8}$$

where $\varphi_{\mathrm{s}}:\mathbb{R}\to\mathbb{R}$ is an analytic and even function defined as

$$\varphi_{\mathrm{s}}(\theta) = \mathrm{sinc}(\theta) = \frac{\sin(\theta)}{\theta}, \qquad \theta\in\mathbb{R}. \tag{2.9}$$

Plugging (2.8) into (2.7) yields

$$\psi(t_{n+1}) \approx e^{2i\tau\Delta}\psi(t_{n-1}) - 2i\tau e^{i\tau\Delta}\varphi_{\mathrm{s}}(\tau\Delta)B(\psi(t_n)). \tag{2.10}$$

For the first step, we apply a first-order approximation as

$$\begin{aligned}\psi(t_1) &= e^{i\tau\Delta}\psi(t_0) - i\int_0^{\tau} e^{i(\tau-s)\Delta}B(\psi(t_0+s))\mathrm{d}s\\ &\approx e^{i\tau\Delta}\psi(t_0) - i\int_0^{\tau} e^{i(\tau-s)\Delta}B(\psi(t_0))\mathrm{d}s = e^{i\tau\Delta}\psi(t_0) - i\tau\varphi_1(i\tau\Delta)B(\psi(t_0)),\end{aligned} \tag{2.11}$$

where $\varphi_1:\mathbb{C}\to\mathbb{C}$ is an entire function defined as

$$\varphi_1(z) = \frac{e^z-1}{z}, \qquad z\in\mathbb{C}. \tag{2.12}$$

The operators $\varphi_1(i\tau\Delta)$ and $\varphi_s(\tau\Delta)$ are defined through their action in the Fourier space, and they satisfy $\varphi_1(i\tau\Delta)v, \varphi_s(\tau\Delta)v\in H^2_{\mathrm{per}}(\Omega)$ for all $v\in L^2(\Omega)$ (see (2.3) and (2.5) in [19]).

Let $\psi^n(\cdot)$ be the approximation of $\psi(\cdot,t_n)$ for $n\geq 0$. Applying the approximations (2.10) and (2.11), we obtain the sEWI as

$$\begin{aligned}&\psi^{n+1} = e^{2i\tau\Delta}\psi^{n-1} - 2i\tau e^{i\tau\Delta}\varphi_{\mathrm{s}}(\tau\Delta)B(\psi^n), \quad n\geq 1,\\ &\psi^1 = e^{i\tau\Delta}\psi^0 - i\tau\varphi_1(i\tau\Delta)B(\psi^0),\\ &\psi^0 = \psi_0.\end{aligned} \tag{2.13}$$

One can check that the scheme is unchanged for $n\geq 1$ when exchanging $n-1$ and $n+1$ and replacing τ with $-\tau$, which implies that the scheme (2.13) is symmetric in time.

Remark 2.1. For the computation of the first step ψ^1, instead of the first-order EWI we present here, one may choose other methods such as the Strang time-splitting method to guarantee time symmetry in the first step, which would be beneficial in the smooth setting. However, according to the analysis in [18, 19, 17], time-splitting methods cannot give accurate approximations in the presence of low regularity potential and/or nonlinearity, and it may totally destroy the regularity of the numerical solution even for one step. Hence, if one wants a better approximation of the first step under the low regularity setting, we suggest computing ψ^1 "accurately" by using the first-order EWI a few times with a small time step.

2.2. A full discretization by using the Fourier spectral method in space. In this subsection, we further discretize the sEWI (2.13) in space by the Fourier spectral method to obtain a fully discrete scheme. Usually, the Fourier pseudospectral method is used for spatial discretization, which can be efficiently implemented with FFT. However, due to the low regularity of potential and/or nonlinearity, it is very hard to establish error estimates of the Fourier pseudospectral method, and it is impossible to obtain optimal error bounds in space as order reduction can be observed numerically [19, 26].

Choose a mesh size $h = (b-a)/N$ with N being a positive even integer. Define the index set

$$\mathcal{T}_N = \left\{-\frac{N}{2}, \ldots, \frac{N}{2}-1\right\},$$

and denote

$$X_N = \mathrm{span}\left\{e^{i\mu_l(x-a)} : l \in \mathcal{T}_N\right\}, \quad \mu_l = \frac{2\pi l}{b-a}. \tag{2.14}$$

Let $P_N : L^2(\Omega) \to X_N$ be the standard L^2-projection onto X_N as

$$(P_N u)(x) = \sum_{l\in\mathcal{T}_N} \widehat{u}_l e^{i\mu_l(x-a)}, \qquad x \in \overline{\Omega} = [a,b], \tag{2.15}$$

where $u \in L^2(\Omega)$ and $\widehat{u}_l$ are the Fourier coefficients of u defined as

$$\widehat{u}_l = \frac{1}{b-a}\int_a^b u(x)e^{-i\mu_l(x-a)}\mathrm{d}x, \qquad l \in \mathbb{Z}. \tag{2.16}$$

Let $\psi_N^n(\cdot)$ be the numerical approximations of $\psi(\cdot, t_n)$ for $n \geq 0$. Then the sEWI Fourier spectral method (sEWI-FS) reads

$$\begin{aligned} &\widehat{(\psi_N^{n+1})}_l = e^{-2i\tau\mu_l^2}\widehat{(\psi_N^{n-1})}_l - 2i\tau e^{-i\tau\mu_l^2}\varphi_s(\tau\mu_l^2)\widehat{(B(\psi_N^n))}_l, \quad l\in\mathcal{T}_N, \quad n\geq 1,\\ &\widehat{(\psi_N^1)}_l = e^{-i\tau\mu_l^2}\widehat{(\psi_N^0)}_l - i\tau\varphi_1(-i\tau\mu_l^2)\widehat{(B(\psi_N^0))}_l, \quad l\in\mathcal{T}_N,\\ &\widehat{(\psi_N^0)}_l = \widehat{(\psi_0)}_l, \quad l\in\mathcal{T}_N. \end{aligned} \tag{2.17}$$

Then the numerical solution ψ_N^n $(n \geq 0) \in X_N$ obtained from (2.17) satisfies

$$\begin{aligned} &\psi_N^{n+1} = e^{2i\tau\Delta}\psi_N^{n-1} - 2i\tau e^{i\tau\Delta}\varphi_s(\tau\Delta)P_N B(\psi_N^n), \quad n\geq 1,\\ &\psi_N^1 = e^{i\tau\Delta}\psi_N^0 - i\tau\varphi_1(i\tau\Delta)P_N B(\psi_N^0),\\ &\psi_N^0 = P_N\psi_0. \end{aligned} \tag{2.18}$$

One may check again that when exchanging $n+1$ and $n-1$ and replacing τ with $-\tau$ in the first equation of (2.18), the equation remains unchanged, which implies that the fully discrete scheme is still time symmetric. Note that the Fourier spectral discretization of the Strang time-splitting method (which is considered in [17]) is no longer symmetric in time.

By performing the standard Von Neumann analysis, we obtain the following linear stability of the sEWI-FS method: Assuming that $V(x) \equiv V_0 \in \mathbb{R}$ and $f(\rho) \equiv f_0 \in \mathbb{R}$, then the sEWI-FS method (2.17) is stable when $\tau|V_0 + f_0| \leq 1$. Note that this stability condition is independent of the mesh size! Moreover, it suggests that one shall choose the time step size τ satisfying $\tau \lesssim 1/(\sup_{x\in\Omega}|V(x)|)$ in practice.

3. Error estimates of the semidiscretization (2.13).

In this section, we shall prove error estimates for the semidiscrete scheme (2.13) under different regularity assumptions on the potential, nonlinearity, and exact solution as shown below.

Let $T_{\max}$ be the maximal existing time of the solution to (1.1) and take $0<T<T_{\max}$ be some fixed time. We shall work under the following three sets of assumptions:

(A) Assumptions for "good" potential and nonlinearity:

$$\begin{aligned}&V\in H^2_{\text{per}}(\Omega),\quad \sigma\geq 1,\\ &\psi\in C([0,T];H^4_{\text{per}}(\Omega))\cap C^1([0,T];H^2(\Omega))\cap C^2([0,T];L^2(\Omega)).\end{aligned}\tag{3.1}$$

(B) Assumptions for low regularity potential and/or nonlinearity:

$$V\in L^\infty(\Omega),\quad \sigma>0,\quad \psi\in C([0,T];H^2_{\text{per}}(\Omega))\cap C^1([0,T];L^2(\Omega)).\tag{3.2}$$

(C) Assumptions with relaxed requirement on nonlinearity compared to (3.1):

$$\begin{aligned}&V\in H^2_{\text{per}}(\Omega),\quad \sigma\geq 1/2,\\ &\psi\in C([0,T];H^4_{\text{per}}(\Omega))\cap C^1([0,T];H^2(\Omega))\cap C^2([0,T];L^2(\Omega)).\end{aligned}\tag{3.3}$$

3.1. Main results.

In this subsection, we present our main error estimates for the semidiscrete scheme under assumptions (3.1) and (3.2), respectively. Since optimal error bounds under (3.3) can only be proved at the fully discrete level with nonresonant time steps, the corresponding result is postponed to section 4.

Let $\psi^n (n\geq 0)$ be obtained from the semidiscretization (2.13). For sufficiently smooth potential and nonlinearity as well as the exact solution, we have the following optimal second-order L^2-norm error bound.

THEOREM 3.1 (optimal error bounds for good potential and nonlinearity). *Under the assumptions* (3.1)*, there exists $\tau_0>0$ sufficiently small such that when $0<\tau<\tau_0$, we have*

$$\|\psi(\cdot,t_n)-\psi^n\|_{L^2}\lesssim\tau^2,\quad \|\psi(\cdot,t_n)-\psi^n\|_{H^1}\lesssim\tau^{\frac{3}{2}},\quad 0\leq n\leq T/\tau.\tag{3.4}$$

For a more general low regularity potential and/or nonlinearity, which inevitably results in low regularity of the exact solution, we have the following first-order L^2-norm error bound.

THEOREM 3.2 (error bounds for low regularity potential and/or nonlinearity). *Under the assumptions* (3.2)*, there exists $\tau_0>0$ sufficiently small such that when $0<\tau<\tau_0$, we have*

$$\|\psi(\cdot,t_n)-\psi^n\|_{L^2}\lesssim\tau,\ \|\psi(\cdot,t_n)-\psi^n\|_{H^1}\lesssim\tau^{\frac{1}{2}},\ \|\psi^n\|_{H^2}\lesssim 1,\quad 0\leq n\leq T/\tau.\tag{3.5}$$

Remark 3.3. Recall the results in [20, 41, 7], to obtain the second-order L^2-norm error bound of the Strang time-splitting method at a semidiscrete level, it is required that $V\in H^4_{\text{per}}(\Omega)$ and $\sigma\geq 3/2$ (or $\sigma=1$), which is much stronger than the requirement in Theorem 3.1 of the sEWI. Similarly, in terms of the first-order L^2-norm error bound at a semidiscrete level, as is already discussed in [19], the sEWI also needs significantly weaker regularity than the Lie–Trotter splitting method analyzed in [18].

Remark 3.4. Regarding the assumption of Theorem 3.2, according to the results in [23, 38] (see also [18, 19, 17]), when $V\in L^\infty(\Omega)$ and $\sigma>0$ ($\sigma<2$ if in 3D), it can be expected that there exists a unique exact solution $\psi\in C([0,T];H^2_{\text{per}}(\Omega))\cap$

$C^1([0,T];L^2(\Omega))$ if $\psi_0\in H^2_{\rm per}(\Omega)$ in the NLSE (1.1). The assumption of Theorem 3.1 is compatible with this assumption in the sense that the increment of differentiability orders of potential and nonlinearity are the same as the exact solution. In other words, when $V\in H^2_{\rm per}(\Omega)$ and $\sigma\geq 1$, if $\psi_0\in H^4_{\rm per}(\Omega)$, one could expect $\psi\in C([0,T];H^4_{\rm per}(\Omega))\cap C^1([0,T];H^2(\Omega))\cap C^2([0,T];L^2(\Omega))$.

In the rest of this section, we shall prove Theorems 3.1 and 3.2. Note that the assumption of Theorem 3.2 is more general than that of Theorem 3.1. Hence, we start with the proof of Theorem 3.2, and the uniform H^2-norm bound of the numerical solution established in Theorem 3.2 will be used to simplify the proof of Theorem 3.1.

3.2. Proof of Theorem 3.2 for low regularity potential and/or nonlinearity. In this subsection, we will establish a first-order error bound for the sEWI under low regularity assumptions (3.2) made in Theorem 3.2.

Under similar assumptions, a first-order error bound has recently been shown for the first-order EWI in [19]. Here, following a similar idea, we can prove the same first-order error bound for the sEWI.

To follow the proof for the one-step method, we first rewrite the sEWI scheme (2.13) in matrix form. We define $\Phi^\tau:[H^2_{\rm per}(\Omega)]^2\to H^2_{\rm per}(\Omega)$ as

$$\Phi^\tau(\phi_1,\phi_0)=e^{2i\tau\Delta}\phi_0-2i\tau e^{i\tau\Delta}\varphi_{\rm s}(\tau\Delta)B(\phi_1),\quad \phi_0,\phi_1\in H^2_{\rm per}(\Omega). \tag{3.6}$$

Recalling (2.13), one immediately has

$$\psi^{n+1}=\Phi^\tau(\psi^n,\psi^{n-1}),\qquad n\geq 1.$$

We introduce a semidiscrete numerical flow $\mathbf{\Phi}^\tau:[H^2_{\rm per}(\Omega)]^2\to[H^2_{\rm per}(\Omega)]^2$ as

$$\mathbf{\Phi}^\tau\begin{pmatrix}\phi_1\\ \phi_0\end{pmatrix}=\mathbf{A}(\tau)\begin{pmatrix}\phi_1\\ \phi_0\end{pmatrix}+\tau\mathbf{H}(\phi_1)=\begin{pmatrix}\Phi^\tau(\phi_1,\phi_0)\\ \phi_1\end{pmatrix},\quad \phi_0,\phi_1\in H^2_{\rm per}(\Omega), \tag{3.7}$$

where Φ^τ is defined in (3.6) and

$$\mathbf{A}(t):=\begin{pmatrix}0 & e^{2it\Delta}\\ I & 0\end{pmatrix},\quad \mathbf{H}(\phi):=\begin{pmatrix}-2ie^{i\tau\Delta}\varphi_{\rm s}(\tau\Delta)B(\phi)\\ 0\end{pmatrix},\quad \phi\in H^2_{\rm per}(\Omega). \tag{3.8}$$

Define the semidiscrete solution vector $\mathbf{\Psi}^n(1\leq n\leq T/\tau)\in[H^2_{\rm per}(\Omega)]^2$ as

$$\mathbf{\Psi}^n:=(\psi^n,\psi^{n-1})^T,\qquad 1\leq n\leq T/\tau. \tag{3.9}$$

Then the sEWI scheme (2.13) can be equivalently written in matrix form as

$$\begin{aligned}&\mathbf{\Psi}^{n+1}=\mathbf{\Phi}^\tau(\mathbf{\Psi}^n)=\mathbf{A}(\tau)\begin{pmatrix}\psi^n\\ \psi^{n-1}\end{pmatrix}+\tau\mathbf{H}(\psi^n),\quad n\geq 1,\\ &\mathbf{\Psi}^1=\begin{pmatrix}\psi^1\\ \psi^0\end{pmatrix}=\begin{pmatrix}e^{i\tau\Delta}\psi_0-i\tau\varphi_1(i\tau\Delta)B(\psi_0)\\ \psi_0\end{pmatrix}.\end{aligned} \tag{3.10}$$

For $1\leq n\leq T/\tau$, we also define the exact solution vector $\mathbf{\Psi}(t_n)$ as

$$\mathbf{\Psi}(t_n):=(\psi(t_n),\psi(t_{n-1}))^T. \tag{3.11}$$

We first present some estimates of the operator B (2.1) from [17].

LEMMA 3.5. *Under the assumptions $V\in L^\infty(\Omega)$ and $\sigma>0$, for any $v,w\in L^\infty(\Omega)$ satisfying $\|v\|_{L^\infty}\le M$ and $\|w\|_{L^\infty}\le M$, we have*

$$\|B(v)-B(w)\|_{L^2}\le C(\|V\|_{L^\infty},M)\|v-w\|_{L^2}.$$

Let $dB(\cdot)[\cdot]$ be the Gâteaux derivative defined as (see also [18])

$$dB(v)[w]:=\lim_{\varepsilon\to 0}\frac{B(v+\varepsilon w)-B(v)}{\varepsilon}, \tag{3.12}$$

where the limit is taken for real ε. Introduce a continuous function $G:\mathbb{C}\to\mathbb{C}$ as

$$G(z)=\begin{cases} f'(|z|^2)z^2=\beta\sigma|z|^{2\sigma-2}z^2, & z\neq 0,\\ 0, & z=0,\end{cases}\qquad z\in\mathbb{C}. \tag{3.13}$$

Plugging the expression of B (2.1) into (3.12), we obtain

$$dB(v)[w]=-i\left[Vw+f(|v|^2)w+f'(|v|^2)|v|^2w+G(v)\overline{w}\right], \tag{3.14}$$

where $G(v)(x)=G(v(x))$ for $x\in\Omega$. Then we have the following.

LEMMA 3.6. *Under the assumptions $V\in L^\infty(\Omega)$ and $\sigma>0$, for any $v,w\in L^2(\Omega)$ satisfying $\|v\|_{L^\infty}\le M$, we have*

$$\|dB(v)[w]\|_{L^2}\le C(\|V\|_{L^\infty},M)\|w\|_{L^2}.$$

By Lemma 3.5, for $\mathbf{H}$ in (3.8), using the boundedness of $e^{it\Delta}$ and $\varphi_{\mathrm{s}}(t\Delta)$, we have

$$\|\mathbf{H}(v)-\mathbf{H}(w)\|_{L^2}\le 2\|B(v)-B(w)\|_{L^2}\le C(\|V\|_{L^\infty},M)\|v-w\|_{L^2}. \tag{3.15}$$

Then we shall prove Theorem 3.2. By Proposition 3.7 of [19] with $n=0$, noting

$$\mathbf{\Psi}(t_1)-\mathbf{\Psi}^1=(\psi(t_1),\psi(t_0))^T-(\psi^1,\psi_0)^T=(\psi(t_1)-\psi^1,0)^T,$$

we have the following error estimate of the first step.

PROPOSITION 3.7. *Under the assumptions* (3.2), *we have*

$$\left\|\mathbf{\Psi}(t_1)-\mathbf{\Psi}^1\right\|_{H^\alpha}\lesssim\tau^{2-\alpha/2},\quad 0\le\alpha\le 2.$$

By Lemma 3.6 in [19], for $v\in C([0,\tau];L^2(\Omega))\cap W^{1,\infty}([0,\tau];L^2(\Omega))$ and

$$u_1=-i\int_0^\tau e^{i(\tau-s)\Delta}v(s)\mathrm{d}s,$$

we have

$$\|\Delta u_1\|_{L^2}\le 2\|v\|_{L^\infty([0,\tau];L^2)}+\tau\|\partial_t v\|_{L^\infty([0,\tau];L^2)}. \tag{3.16}$$

As an immediate corollary, if $v\in C([-\tau,\tau];L^2(\Omega))\cap W^{1,\infty}([-\tau,\tau];L^2(\Omega))$ and

$$u_2=-i\int_{-\tau}^\tau e^{i(\tau-s)\Delta}v(s)\mathrm{d}s,$$

we have

$$\|\Delta u_2\|_{L^2}\le 4\|v\|_{L^\infty([-\tau,\tau];L^2)}+2\tau\|\partial_t v\|_{L^\infty([-\tau,\tau];L^2)}. \tag{3.17}$$

PROPOSITION 3.8. *Under the assumptions* (3.2), *we have*

$$\|\mathbf{\Psi}(t_{n+1}) - \mathbf{\Phi}^\tau(\mathbf{\Psi}(t_n))\|_{H^\alpha} \lesssim \tau^{2-\alpha/2}, \quad 0 \le \alpha \le 2, \quad 1 \le n \le T/\tau - 1.$$

Proof. Recalling (3.7) and (3.11), we have, for $1 \le n \le T/\tau - 1$,

$$\mathbf{\Psi}(t_{n+1}) - \mathbf{\Phi}^\tau(\mathbf{\Psi}(t_n)) = \begin{pmatrix} \psi(t_{n+1}) - \Phi^\tau(\psi(t_n), \psi(t_{n-1})) \\ 0 \end{pmatrix} =: \begin{pmatrix} \mathcal{L}^n \\ 0 \end{pmatrix}. \tag{3.18}$$

Recalling (2.8) and (3.6), we have

$$\begin{aligned} \Phi^\tau(\psi(t_n), \psi(t_{n-1})) &= e^{2i\tau\Delta}\psi(t_{n-1}) - 2i\tau e^{i\tau\Delta}\varphi_{\mathrm{s}}(\tau\Delta)B(\psi(t_n)) \\ &= e^{2i\tau\Delta}\psi(t_{n-1}) - i\int_{-\tau}^{\tau} e^{i(\tau-s)\Delta}B(\psi(t_n))\mathrm{d}s. \end{aligned} \tag{3.19}$$

From the definition of $\mathcal{L}^n$ in (3.18), subtracting (3.19) from (2.7), we have

$$\mathcal{L}^n = -i\int_{-\tau}^{\tau} e^{i(\tau-s)\Delta}\left[B(\psi(t_n+s)) - B(\psi(t_n))\right]\mathrm{d}s, \quad 1 \le n \le T/\tau - 1. \tag{3.20}$$

By Lemmas 3.5 and 3.6, noting that $\partial_t B(\psi(t)) = dB(\psi(t))[\partial_t\psi(t)]$, we have, for $g(s) := B(\psi(t_n+s)) - B(\psi(t_n))$ with $-\tau \le s \le \tau$,

$$\|g\|_{L^\infty([-\tau,\tau];L^2)} \lesssim \tau, \quad \|\partial_t g\|_{L^\infty([-\tau,\tau];L^2)} \lesssim 1. \tag{3.21}$$

From (3.20), using (3.17), noting (3.21), we obtain

$$\|\Delta\mathcal{L}^n\|_{L^2} \lesssim \tau. \tag{3.22}$$

From (3.20), using the isometry property of $e^{it\Delta}$ and (3.21), we have

$$\|\mathcal{L}^n\|_{L^2} \le \int_{-\tau}^{\tau} \|g(s)\|_{L^2}\mathrm{d}s \le 2\tau\|g\|_{L^\infty([-\tau,\tau];L^2)} \lesssim \tau^2. \tag{3.23}$$

The conclusion then follows from (3.22) and (3.23) and the standard interpolation inequalities immediately. ∎

For the operator $\mathbf{A}(t)$ defined in (3.8), we have the following estimate, which shall be compared with the isometry property of the free Schrödinger group $e^{it\Delta}$.

LEMMA 3.9. *Let* $\mathbf{v} = (v_1, v_2)^T \in [H^2_{\mathrm{per}}(\Omega)]^2$. *For any* $t \ge 0$, *we have*

$$\|\mathbf{A}(t)\mathbf{v}\|_{H^\alpha} = \|\mathbf{v}\|_{H^\alpha}, \quad 0 \le \alpha \le 2.$$

Proof. Recalling (3.8) and using the isometry property of $e^{it\Delta}$, we have

$$\|\mathbf{A}(t)\mathbf{v}\|^2_{H^\alpha} = \|e^{2it\Delta}v_2\|^2_{H^\alpha} + \|v_1\|^2_{H^\alpha} = \|v_2\|^2_{H^\alpha} + \|v_1\|^2_{H^\alpha} = \|\mathbf{v}\|^2_{H^\alpha},$$

which completes the proof. ∎

By Parseval's identity, noting that $|\varphi_{\mathrm{s}}(\theta)| \le 1$ for $\theta \in \mathbb{R}$, we immediately have $\varphi_{\mathrm{s}}(\tau\Delta)$ is bounded from $H^m_{\mathrm{per}}(\Omega)$ to $H^m_{\mathrm{per}}(\Omega)$ for all $m \in \mathbb{Z}^+$ and $\tau > 0$. Besides, we have the following analogs of Lemma 3.8 in [19].

LEMMA 3.10. *Let* $v \in L^2(\Omega)$. *For any* $0 < \tau < 1$, *we have*

$$\|\varphi_s(\tau\Delta)v\|_{H^\alpha} \lesssim \tau^{-\alpha/2}\|v\|_{L^2}, \quad 0 \le \alpha \le 2.$$

With Lemmas 3.9 and 3.10, we can establish the L^∞-conditional stability estimate of $\mathbf{\Phi}^\tau$ defined in (3.7). The proof is similar to that of Proposition 3.10 in [19] and thus is omitted.

PROPOSITION 3.11 (L^∞-conditional H^α-stability). *Assume that $V\in L^\infty(\Omega)$. Let $\mathbf{v}=(v_1,v_0)^T,\mathbf{w}=(w_1,w_0)^T$ such that $v_j,w_j\in H^2_{\rm per}(\Omega)$ for $j=0,1$ with $\|v_1\|_{L^\infty}\le M$ and $\|w_1\|_{L^\infty}\le M$. For any $\tau>0$, we have, for $0\le\alpha\le 2$,*

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

With Propositions 3.7, 3.8, and 3.11, the proof of Theorem 3.2 can be obtained by following the coupled induction argument used in the proof of (3.2) in Theorem 3.1 of [19]. We sketch the proof here for the convenience of the reader.

Proof of Theorem 3.2. Define the error function $e^n:=\psi(t_n)-\psi^n$ for $0\le n\le T/\tau$ and let

$$\mathbf{e}^n:=\mathbf{\Psi}(t_n)-\mathbf{\Psi}^n=(e^n,e^{n-1})^T,\quad 1\le n\le T/\tau. \tag{3.24}$$

Recalling (3.10), by the triangle inequality, we get, for $0\le\alpha\le 2$ and $1\le n\le T/\tau-1$,

$$\|\mathbf{e}^{n+1}\|_{H^\alpha}\le\|\mathbf{\Psi}(t_{n+1})-\mathbf{\Phi}^\tau(\mathbf{\Psi}(t_n))\|_{H^\alpha}+\|\mathbf{\Phi}^\tau(\mathbf{\Psi}(t_n))-\mathbf{\Phi}^\tau(\mathbf{\Psi}^n)\|_{H^\alpha}. \tag{3.25}$$

We shall show that, when $\tau<\tau_0$ with $\tau_0>0$ sufficiently small, for $1\le n\le T/\tau-1$,

$$\|\mathbf{e}^n\|_{L^2}\lesssim\tau,\quad \|\mathbf{e}^n\|_{H^{\frac{7}{4}}}\lesssim\tau^{\frac{1}{8}}. \tag{3.26}$$

We shall use an induction argument to prove it. Note that (3.26) holds for $n=1$ by Proposition 3.7. We assume that (3.26) holds for $1\le n\le m\le T/\tau-1$. To proceed, choosing $\alpha=0$ and $\alpha=7/4$ in (3.25) and using Propositions 3.8 and 3.11, we get

$$\|\mathbf{e}^{n+1}\|_{L^2}\le(1+C_0\tau)\|\mathbf{e}^n\|_{L^2}+C_1\tau^2, \tag{3.27}$$

$$\|\mathbf{e}^{n+1}\|_{H^{\frac{7}{4}}}\le\|\mathbf{e}^n\|_{H^{\frac{7}{4}}}+C_0\tau^{\frac{1}{8}}\|\mathbf{e}^n\|_{L^2}+C_1\tau^{1+\frac{1}{8}}, \tag{3.28}$$

where, under the given regularity assumptions and the assumption for the induction, by the Sobolev embedding $H^{\frac{7}{4}}\hookrightarrow L^\infty$, C_0 and C_1 are uniformly bounded. Applying the discrete Gronwall's inequality to (3.27), we have $\|\mathbf{e}^{m+1}\|_{L^2}\lesssim\tau$. Summing over n from 1 to m in (3.28) yields, by the assumption for the induction, $\|\mathbf{e}^{m+1}\|_{H^{\frac{7}{4}}}\lesssim\tau^{\frac{1}{8}}$. Then we prove (3.26) for $n=m+1$ and, thus, for all $1\le n\le T/\tau$ by the induction. The rest of the proof follows immediately. More details can be found in [19]. ∎

3.3. Proof of Theorem 3.1 for good potential and nonlinearity. In this subsection, we shall prove an optimal second-order error bound for the sEWI under the assumptions (3.1).

We first recall some additional estimates for the operator B, which will be frequently used in the proof.

LEMMA 3.12 (see [18, Lemma 4.2]). *Under the assumptions that $V\in W^{1,4}(\Omega)$ and $\sigma\ge 1/2$, for any $v,w\in H^2(\Omega)$ such that $\|v\|_{H^2}\le M$, $\|w\|_{H^2}\le M$, we have*

$$\|B(v)-B(w)\|_{H^1}\le C(\|V\|_{W^{1,4}},M)\|v-w\|_{H^1}.$$

LEMMA 3.13 (see [17, Lemma 4.3]). *Under the assumptions $V\in L^\infty(\Omega)$ and $\sigma\ge 1/2$, for any $v_j,w_j\in L^\infty(\Omega)$ satisfying $\|v_j\|_{L^\infty}\le M$ and $\|w_j\|_{L^\infty}\le M$ with $j=1,2$, we have*

$$\|dB(v_1)[w_1]-dB(v_2)[w_2]\|_{L^2}\le C(\|V\|_{L^\infty},M)\left(\|v_1-v_2\|_{L^2}+\|w_1-w_2\|_{L^2}\right).$$

LEMMA 3.14 (see [17, Lemma 4.4]). *Under the assumptions $V \in H^2(\Omega)$ and $\sigma \geq 1$, for any $v, w \in H^2(\Omega)$ satisfying $\|v\|_{H^2} \leq M$, $\|w\|_{H^2} \leq M$, we have*

$$\|dB(v)[w]\|_{H^2} \leq C(\|V\|_{H^2}, M).$$

Then we shall prove Theorem 3.1 under the assumptions (3.1). We start with establishing higher-order estimates of the local truncation error.

Define an even analytic function φ_{c} as

$$\varphi_{\mathrm{c}}(\theta) = \frac{\theta \cos(\theta) - \sin(\theta)}{\theta^3}, \qquad \theta \in \mathbb{R}. \tag{3.29}$$

Note that φ_{c} defined in (3.29) is bounded on $\mathbb{R}$, and thus the operator $\varphi_{\mathrm{c}}(\tau\Delta)$ is bounded from $H^m_{\mathrm{per}}(\Omega)$ to $H^m_{\mathrm{per}}(\Omega)$ for all $m \in \mathbb{Z}^+$ and $\tau > 0$. Moreover, similarly to Lemma 3.10, we have the following.

LEMMA 3.15. *Let $\phi \in L^2(\Omega)$. For any $0 < \tau < 1$, we have*

$$\|\varphi_c(\tau\Delta)\phi\|_{H^\alpha} \lesssim \tau^{-\alpha/2}\|\phi\|_{L^2}, \quad 0 \leq \alpha \leq 2.$$

Then we can obtain the following estimate of the local truncation error.

PROPOSITION 3.16. *Under the assumptions* (3.1), *we have*

$$\|\boldsymbol{\Psi}(t_{n+1}) - \boldsymbol{\Phi}^\tau(\boldsymbol{\Psi}(t_n))\|_{H^\alpha} \lesssim \tau^{3-\alpha/2}, \quad 0 \leq \alpha \leq 2, \quad 1 \leq n \leq T/\tau - 1.$$

Proof. Recalling (3.18), it suffices to establish the estimate of $\mathcal{L}^n$. By (3.20),

$$\begin{aligned} \mathcal{L}^n &= -i\int_{-\tau}^{\tau} e^{i(\tau-s)\Delta}\left[B(\psi(t_n+s)) - B(\psi(t_n))\right] \mathrm{d}s \\ &= -i\int_{-\tau}^{\tau} e^{i(\tau-s)\Delta}\big[B(\psi(t_n+s)) - B(\psi(t_n)) - s dB(\psi(t_n))[\partial_t\psi(t_n)]\big] \mathrm{d}s \\ &\quad - i\int_{-\tau}^{\tau} s e^{i(\tau-s)\Delta}\big(dB(\psi(t_n))[\partial_t\psi(t_n)]\big) \mathrm{d}s =: r_1^n + r_2^n. \end{aligned} \tag{3.30}$$

For r_1^n in (3.30), recalling that $\partial_t B(\psi(t)) = dB(\psi(t))[\partial_t\psi(t)]$, we have

$$\begin{aligned} &B(\psi(t_n+s)) - B(\psi(t_n)) - s dB(\psi(t_n))[\partial_t\psi(t_n)] \\ &\quad = \int_0^s \big[\partial_w[B(\psi(t_n+w)] - dB(\psi(t_n))[\partial_t\psi(t_n)]\big] \mathrm{d}w \\ &\quad = \int_0^s \big[dB(\psi(t_n+w))[\partial_t\psi(t_n+w)] - dB(\psi(t_n))[\partial_t\psi(t_n)]\big] \mathrm{d}w. \end{aligned} \tag{3.31}$$

From (3.31), using Lemma 3.13, we obtain, for $-\tau \leq s \leq \tau$,

$$\begin{aligned} &\|B(\psi(t_n+s)) - B(\psi(t_n)) - s dB(\psi(t_n))[\partial_t\psi(t_n)]\|_{L^2} \\ &\quad \leq \left|\int_0^s \|dB(\psi(t_n+w))[\partial_t\psi(t_n+w)] - dB(\psi(t_n))[\partial_t\psi(t_n)]\|_{L^2} \mathrm{d}w\right| \\ &\quad \lesssim \left|\int_0^s (\|\psi(t_n+w) - \psi(t_n)\|_{L^2} + \|\partial_t\psi(t_n+w) - \partial_t\psi(t_n)\|_{L^2}) \,\mathrm{d}w\right| \\ &\quad \lesssim s^2 \left(\|\partial_t\psi\|_{L^\infty([t_{n-1},t_{n+1}];L^2)} + \|\partial_{tt}\psi\|_{L^\infty([t_{n-1},t_{n+1}];L^2)}\right) \lesssim s^2. \end{aligned} \tag{3.32}$$

Recalling the definition of r_1^n in (3.30), using (3.32) and the isometry property of $e^{it\Delta}$, we get

$$\|r_1^n\|_{L^2} \leq \int_{-\tau}^{\tau} \|B(\psi(t_n+s)) - B(\psi(t_n)) - sdB(\psi(t_n))[\partial_t\psi(t_n)]\|_{L^2}\mathrm{d}s \lesssim \tau^3. \tag{3.33}$$

On the other hand, applying (3.17) to r_1^n in (3.30), using the identity $\partial_t B(\psi(t)) = dB(\psi(t))[\partial_t\psi(t)]$, (3.32), and Lemma 3.13, we have

$$\begin{aligned}\|\Delta r_1^n\|_{L^2} &\lesssim \sup_{-\tau\leq s\leq\tau} \|B(\psi(t_n+s)) - B(\psi(t_n)) - sdB(\psi(t_n))[\partial_t\psi(t_n)]\|_{L^2} \\ &\quad + \tau \sup_{-\tau\leq s\leq\tau} \|\partial_t B(\psi(t_n+s)) - dB(\psi(t_n))[\partial_t\psi(t_n)]\|_{L^2} \\ &\lesssim \tau^2 + \tau \sup_{-\tau\leq s\leq\tau} \|dB(\psi(t_n+s))[\partial_t\psi(t_n+s)] - dB(\psi(t_n))[\partial_t\psi(t_n)]\|_{L^2} \\ &\lesssim \tau^2 + \tau\left(\|\psi(t_n+s)-\psi(t_n)\|_{L^2} + \|\partial_t\psi(t_n+s) - \partial_t\psi(t_n)\|_{L^2}\right) \lesssim \tau^2.\end{aligned} \tag{3.34}$$

Combining (3.33) and (3.34), and using the interpolation inequality, we get

$$\|r_1^n\|_{H^\alpha} \lesssim \tau^{3-\alpha/2}, \quad 0\leq\alpha\leq 2. \tag{3.35}$$

Then we shall estimate r_2^n in (3.30). Using the identity $e^{it\Delta} = \cos(t\Delta) + i\sin(t\Delta)$ and the symmetry of the integral domain, we have

$$\begin{aligned}-i\int_{-\tau}^{\tau} se^{-is\Delta}\mathrm{d}s &= -i\int_{-\tau}^{\tau} s\cos(s\Delta)\mathrm{d}s - \int_{-\tau}^{\tau} s\sin(s\Delta)\mathrm{d}s \\ &= -2\int_0^{\tau} s\sin(s\Delta)\mathrm{d}s = 2\tau^3\Delta\varphi_{\mathrm{c}}(\tau\Delta),\end{aligned} \tag{3.36}$$

where φ_{c} is defined in (3.29). Recalling (3.30), using (3.36), we have

$$\begin{aligned}r_2^n &= -i\int_{-\tau}^{\tau} se^{i(\tau-s)\Delta}\big(dB(\psi(t_n))[\partial_t\psi(t_n)]\big)\mathrm{d}s \\ &= -ie^{i\tau\Delta}\int_{-\tau}^{\tau} se^{-is\Delta}\mathrm{d}s\big(dB(\psi(t_n))[\partial_t\psi(t_n)]\big) \\ &= \tau^3 e^{i\tau\Delta}\Delta\varphi_{\mathrm{c}}(\tau\Delta)dB(\psi(t_n))[\partial_t\psi(t_n)].\end{aligned} \tag{3.37}$$

From (3.37), using Lemmas 3.14 and 3.15, noting that $dB(\psi(t_n))[\partial_t\psi(t_n)] \in H^2_{\mathrm{per}}(\Omega)$, and that $\varphi_{\mathrm{c}}(\tau\Delta)$, Δ, and $e^{i\tau\Delta}$ commute, by the isometry property of $e^{i\tau\Delta}$, we obtain

$$\|r_2^n\|_{H^\alpha} \lesssim \tau^{-\alpha/2}\tau^3\|\Delta dB(\psi(t_n))[\partial_t\psi(t_n)]\|_{L^2} \lesssim \tau^{3-\alpha/2}, \quad 0\leq\alpha\leq 2, \tag{3.38}$$

which, together with (3.35), yields from (3.30) that

$$\|\mathcal{L}^n\|_{H^\alpha} \lesssim \tau^{3-\alpha/2}, \quad 0\leq\alpha\leq 2, \quad 1\leq n\leq T/\tau - 1, \tag{3.39}$$

which completes the proof. ∎

PROPOSITION 3.17 (H^1-stability). *Assume that $V \in W^{1,4}(\Omega)\cap H^1_{\mathrm{per}}(\Omega)$ and $\sigma\geq 1$. Let $\mathbf{v} = (v_1,v_0)^T, \mathbf{w} = (w_1,w_0)^T$ such that $v_j, w_j \in H^2_{\mathrm{per}}(\Omega)$ for $j=0,1$ with $\|v_1\|_{H^2}\leq M$ and $\|w_1\|_{H^2}\leq M$. For $\tau>0$, we have*

$$\|\mathbf{\Phi}^\tau(\mathbf{v}) - \mathbf{\Phi}^\tau(\mathbf{w})\|_{H^1} \leq (1 + C(\|V\|_{W^{1,4}}, M)\tau)\|\mathbf{v}-\mathbf{w}\|_{H^1}.$$

Proof. Recalling (3.7), using Lemma 3.9, and the boundedness of $e^{it\Delta}$ and $\varphi_{\mathrm{s}}(\tau\Delta)$, we obtain

$$\begin{aligned}\|\mathbf{\Phi}^\tau(\mathbf{v})-\mathbf{\Phi}^\tau(\mathbf{w})\|_{H^1} &\le \|\mathbf{A}(\tau)(\mathbf{v}-\mathbf{w})\|_{H^1}+\tau\|\mathbf{H}(v_1)-\mathbf{H}(w_1)\|_{H^1}\\ &\le \|\mathbf{v}-\mathbf{w}\|_{H^1}+2\tau\|B(v_1)-B(w_1)\|_{H^1}.\end{aligned} \tag{3.40}$$

The conclusion follows from Lemma 3.12 immediately. ∎

Proof of Theorem 3.1. Recall that $e^n=\psi(t_n)-\psi^n$ and $\mathbf{e}^n=(e^n,e^{n-1})^T$ in the proof of Theorem 3.2. We start with the estimate of $\mathbf{e}^1=(e^1,0)^T$. Recalling (2.11) and (2.13), using the isometry property of $e^{it\Delta}$, Lemmas 3.5 and 3.12, we have

$$\|\mathbf{e}^1\|_{H^\alpha}=\|e^1\|_{H^\alpha}\lesssim \tau^2,\quad \alpha=0,1. \tag{3.41}$$

From (3.25), using Proposition 3.11 with $\alpha=0$, and Propositions 3.16 and 3.17, we obtain

$$\|\mathbf{e}^{n+1}\|_{H^\alpha}\le (1+C_2\tau)\|\mathbf{e}^n\|_{H^\alpha}+C_3\tau^{3-\alpha/2},\quad \alpha=0,1, \tag{3.42}$$

where C_2 depends, in particular, on $\|\psi^n\|_{H^2}$. By the uniform H^2-norm bound of ψ^n established in Theorem 3.2 and given regularity assumptions, the constants C_2 and C_3 in (3.42) are uniformly bounded. From (3.42), using the discrete Gronwall's inequality, noting (3.41), we can obtain the desired result. ∎

4. Error estimates of the full discretization (2.17). In this section, we first extend the error estimates of the semidiscretization (2.13) to the full discretization (2.17). Then we present an improved error estimate which holds only at the fully discrete level for certain nonresonant time steps.

4.1. Main results. Let $\psi_N^n(0\le n\le T/\tau)$ be obtained from the full discretization sEWI-FS scheme (2.17). We first present the fully discrete counterparts of Theorems 3.1 and 3.2.

THEOREM 4.1 (optimal error bounds for good potential and nonlinearity). *Under the assumptions* (3.1), *there exists* $\tau_0>0, h_0>0$ *sufficiently small such that when* $0<\tau<\tau_0$ *and* $0<h<h_0$, *we have*

$$\|\psi(\cdot,t_n)-\psi_N^n\|_{L^2}\lesssim\tau^2+h^4,\quad \|\psi(\cdot,t_n)-\psi_N^n\|_{H^1}\lesssim\tau^{\frac32}+h^3,\quad 0\le n\le T/\tau.$$

THEOREM 4.2 (error bounds for low regularity potential and/or nonlinearity). *Under the assumptions* (3.2), *there exists* $\tau_0>0, h_0>0$ *sufficiently small such that when* $0<\tau<\tau_0$ *and* $0<h<h_0$, *we have*

$$\begin{aligned}&\|\psi(\cdot,t_n)-\psi_N^n\|_{L^2}\lesssim\tau+h^2,\quad \|\psi_N^n\|_{H^2}\lesssim 1,\\ &\|\psi(\cdot,t_n)-\psi_N^n\|_{H^1}\lesssim\tau^{\frac12}+h,\qquad 0\le n\le T/\tau.\end{aligned}$$

Recall that time-splitting methods require stronger regularity on potential and nonlinearity than the sEWI at a semidiscrete level as discussed in Remark 3.3. Although recent results in [17] indicate that the regularity requirement can be relaxed at the fully discrete level for time-splitting methods, however, a time step size restriction still needs to be imposed, which is not required by the sEWI. Moreover, under the same time step size restriction, the regularity requirement of the sEWI can be further relaxed to cover $\sigma\ge 1/2$. These demonstrate the superiority of the sEWI over time-splitting methods.

THEOREM 4.3 (improved optimal error bounds). *Under the assumptions* (3.3), *there exists* $\tau_0 > 0, h_0 > 0$ *sufficiently small such that when* $0 < \tau < \tau_0$, $0 < h < h_0$, *and* $\tau \leq \frac{h^2}{2\pi}$, *we have*

$$\|\psi(\cdot,t_n) - \psi_N^n\|_{L^2} \lesssim \tau^2 + h^4, \quad \|\psi(\cdot,t_n) - \psi_N^n\|_{H^1} \lesssim \tau^{\frac{3}{2}} + h^3, \quad 0 \leq n \leq T/\tau.$$

Remark 4.4. According to the numerical results in section 5 (see also [18]), when $V \in H^2_{\text{per}}(\Omega)$ and $\sigma \geq 1/2$, the regularity requirement of the exact solution in Theorem 4.3 (i.e., $\psi \in C([0,T]; H^4_{\text{per}}(\Omega)) \cap C^1([0,T]; H^2(\Omega)) \cap C^2([0,T]; L^2(\Omega))$) is possible for an H^4-initial datum. Besides, the time step size restriction $\tau \leq h^2/(2\pi)$ in Theorem 4.3 is natural for the balance of temporal and spatial errors.

Similarly to what we have done in the previous section, we shall start with the proof of Theorem 4.2 since the assumption of it is more general, and the uniform H^2-norm bound established in it will be useful to prove Theorems 4.1 and 4.3.

4.2. Proof of Theorem 4.2 for low regularity potential and/or nonlinearity. In this subsection, we shall prove Theorem 4.2 under the assumptions (3.2).

Again, we first rewrite the sEWI-FS scheme (2.17) in matrix form. Similarly to (3.6), we define $\Phi_h^\tau : (X_N)^2 \to X_N$ as

$$\Phi_h^\tau(\phi_1, \phi_0) = e^{2i\tau\Delta}\phi_0 - 2i\tau e^{i\tau\Delta}\varphi_{\text{s}}(\tau\Delta)P_N B(\phi_1), \quad \phi_0, \phi_1 \in X_N, \tag{4.1}$$

and one has, from (2.18),

$$\psi_N^{n+1} = \Phi_h^\tau(\psi_N^n, \psi_N^{n-1}), \quad n \geq 1. \tag{4.2}$$

Introducing a fully discrete numerical flow $\mathbf{\Phi}_h^\tau : (X_N)^2 \to (X_N)^2$ as

$$\mathbf{\Phi}_h^\tau \begin{pmatrix} \phi_1 \\ \phi_0 \end{pmatrix} = \mathbf{A}(\tau) \begin{pmatrix} \phi_1 \\ \phi_0 \end{pmatrix} + \tau P_N \mathbf{H}(\phi_1) = \begin{pmatrix} \Phi_h^\tau(\phi_1, \phi_0) \\ \phi_1 \end{pmatrix}, \quad \phi_0, \phi_1 \in X_N, \tag{4.3}$$

where $\mathbf{A}(\tau)$ and $\mathbf{H}$ are defined in (3.8), and P_N is understood as acting on each component. Define the fully discrete solution vector $\mathbf{\Psi}_N^n (1 \leq n \leq T/\tau) \in (X_N)^2$ as

$$\mathbf{\Psi}_N^n := (\psi_N^n, \psi_N^{n-1})^T, \qquad 1 \leq n \leq T/\tau. \tag{4.4}$$

Then (2.18) can be equivalently written in matrix form as

$$\begin{aligned} \mathbf{\Psi}_N^{n+1} &= \mathbf{\Phi}_h^\tau(\mathbf{\Psi}_N^n) = \mathbf{A}(\tau) \begin{pmatrix} \psi_N^n \\ \psi_N^{n-1} \end{pmatrix} + \tau P_N \mathbf{H}(\psi_N^n), \quad n \geq 1, \\ \mathbf{\Psi}_N^1 &= \begin{pmatrix} \psi_N^1 \\ \psi_N^0 \end{pmatrix} = \begin{pmatrix} e^{i\tau\Delta} P_N \psi_0 - i\tau\varphi_1(i\tau\Delta) P_N B(P_N \psi_0) \\ P_N \psi_0 \end{pmatrix}. \end{aligned} \tag{4.5}$$

To prove Theorem 4.2, we shall first estimate the error between the semidiscrete solution obtained from the sEWI (2.13) and the fully discrete solution obtained from the sEWI-FS (2.17).

PROPOSITION 4.5. *Under the assumptions* (3.2), *when* $0 < \tau < 1$, *we have*

$$\|P_N \mathbf{\Psi}^n - \mathbf{\Psi}_N^n\|_{L^2} \lesssim h^2, \quad 1 \leq n \leq T/\tau.$$

Proof. For the first step, recalling (3.10) and (4.5), by Lemma 3.5, the boundedness of $\varphi_{\rm s}(t\Delta)$ and P_N, and the standard projection error estimates of P_N, noting that P_N commutes with $e^{it\Delta}$ and $\varphi_{\rm s}(\tau\Delta)$, we have

$$\begin{aligned}\|P_N\mathbf{\Psi}^1-\mathbf{\Psi}^1_N\|_{L^2}&=\tau\|\varphi_{\rm s}(\tau\Delta)P_N(B(\psi_0)-B(P_N\psi_0))\|_{L^2}\le\tau\|B(\psi_0)-B(P_N\psi_0)\|_{L^2}\\&\lesssim\tau\|\psi_0-P_N\psi_0\|_{L^2}\lesssim\tau h^2.\end{aligned}\tag{4.6}$$

Recalling (3.7) and (4.3), using (3.15) and the standard projection error estimates, and noting that $\mathbf{A}(\tau)$ and P_N commute, we have, for $\mathbf{v}=(v_1,v_0)^T\in[H^2_{\rm per}(\Omega)]^2$,

$$\begin{aligned}&\|P_N\mathbf{\Phi}^\tau(\mathbf{v})-\mathbf{\Phi}^\tau_h(P_N\mathbf{v})\|_{L^2}\\&\quad=\|\mathbf{A}(\tau)P_N\mathbf{v}+\tau P_N\mathbf{H}(v_1)-\mathbf{A}(\tau)P_N\mathbf{v}-\tau P_N\mathbf{H}(P_Nv_1)\|_{L^2}\\&\quad=\tau\|P_N\mathbf{H}(v_1)-P_N\mathbf{H}(P_Nv_1)\|_{L^2}\lesssim\tau\|v_1-P_Nv_1\|_{L^2}\lesssim\tau h^2.\end{aligned}\tag{4.7}$$

Moreover, for any $\mathbf{v}=(v_1,v_0)^T,\mathbf{w}=(w_1,w_0)^T\in(X_N)^2$ such that $\|v_1\|_{L^\infty}\le M$ and $\|w_1\|_{L^\infty}\le M$, by using Lemma 3.9 and (3.15), and the boundedness of P_N, we have

$$\|\mathbf{\Phi}^\tau_h(\mathbf{v})-\mathbf{\Phi}^\tau_h(\mathbf{w})\|_{L^2}\le(1+C(\|V\|_{L^\infty},M)\tau)\|\mathbf{v}-\mathbf{w}\|_{L^2}.\tag{4.8}$$

By the triangle inequality, (4.7) and (4.8), noting that $\mathbf{\Psi}^{n+1}=\mathbf{\Phi}^\tau(\mathbf{\Psi}^n)$ and $\mathbf{\Psi}^{n+1}_N=\mathbf{\Phi}^\tau_h(\mathbf{\Psi}^n_N)$, recalling the uniform H^2-norm bound of ψ^n in Theorem 3.2, we have

$$\begin{aligned}&\|P_N\mathbf{\Psi}^{n+1}-\mathbf{\Psi}^{n+1}_N\|_{L^2}\\&\quad\le\|P_N\mathbf{\Psi}^{n+1}-\mathbf{\Phi}^\tau_h(P_N\mathbf{\Psi}^n)\|_{L^2}+\|\mathbf{\Phi}^\tau_h(P_N\mathbf{\Psi}^n)-\mathbf{\Phi}^\tau_h(\mathbf{\Psi}^n_N)\|_{L^2}\\&\quad\le C_5\tau h^2+(1+C_4\tau)\|P_N\mathbf{\Psi}^n-\mathbf{\Psi}^n_N\|_{L^2},\quad 1\le n\le T/\tau-1,\end{aligned}\tag{4.9}$$

where C_4 depends, in particular, on $\|\psi^n_N\|_{L^\infty}$. From (4.9), using the discrete Gronwall's inequality and (4.6), along with the induction argument and inverse estimates $\|\phi\|_{L^\infty}\lesssim h^{-1/2}\|\phi\|_{L^2}$ for $\phi\in X_N$ [45] to control the L^∞-norm of $\mathbf{\Psi}^n_N$ (and thus control C_4), we can prove the desired result (see Proposition 4.3 in [19] for details). ∎

Proof of Theorem 4.2. By Proposition 4.5 and Theorem 3.2, error estimates of P_N, and the inverse inequality $\|\phi\|_{H^\alpha}\lesssim h^{-\alpha}\|\phi\|_{L^2}$ for $\phi\in X_N$ [45], we get

$$\begin{aligned}\|\psi(\cdot,t_n)-\psi^n_N\|_{H^\alpha}&\le\|\psi(\cdot,t_n)-\psi^n\|_{H^\alpha}+\|\psi^n-P_N\psi^n\|_{H^\alpha}+\|P_N\psi^n-\psi^n_N\|_{H^\alpha}\\&\lesssim\tau^{1-\alpha/2}+h^{2-\alpha}+h^{-\alpha}\|P_N\mathbf{\Psi}^n-\mathbf{\Psi}^n_N\|_{L^2}\lesssim\tau^{1-\alpha/2}+h^{2-\alpha},\end{aligned}\tag{4.10}$$

which proves Theorem 4.2 by taking $\alpha=0,1,2$. ∎

4.3. Proof of Theorem 4.1 for good potential and nonlinearity. We define the fully discrete counterpart of $\mathcal{L}^n$ in (3.18) as

$$\mathcal{E}^n:=P_N\psi(t_{n+1})-\Phi^\tau_h(P_N\psi(t_n),P_N\psi(t_{n-1})),\quad 1\le n\le T/\tau-1,\tag{4.11}$$

where Φ^τ_h is defined in (4.1). We first decompose $\mathcal{E}^n$ into two parts, where the optimal error bound of one part can be obtained under weaker regularity assumptions than the other part. This decomposition will also be useful in the proof of Theorem 4.3 to obtain the improved optimal error bound for nonresonant time steps.

PROPOSITION 4.6. *Under the assumptions that $V\in H^2_{\rm per}(\Omega)$, $\sigma\ge1/2$, and $\psi\in C([0,T];H^4_{\rm per}(\Omega))\cap C^1([0,T];H^2(\Omega))\cap C^2([0,T];L^2(\Omega))$, we have, for $\mathcal{E}^n$ in* (4.11),

$$\mathcal{E}^n=\mathcal{E}^n_{\rm dom}+\mathcal{E}^n_2,\quad 1\le n\le T/\tau-1,\tag{4.12}$$

where $\|\mathcal{E}^n_2\|_{H^\alpha}\lesssim\tau^{3-\alpha/2}+\tau h^{4-\alpha}$ for $0\le\alpha\le2$ and

$$\mathcal{E}^n_{\rm dom}=2\tau^3\Delta e^{i\tau\Delta}\varphi_c(\tau\Delta)P_N dB(\psi(t_n))[\partial_t\psi(t_n)]\tag{4.13}$$

with $\varphi_c:\mathbb{R}\to\mathbb{R}$ defined in (3.29).

Proof. Applying P_N on both sides of (2.7), noting P_N and $e^{it\Delta}$ commute, we get

$$P_N\psi(t_{n+1}) = e^{2i\tau\Delta}P_N\psi(t_{n-1}) - i\int_{-\tau}^{\tau} e^{i(\tau-s)\Delta}P_N B(\psi(t_n+s))\mathrm{d}s. \tag{4.14}$$

Recalling (2.8) and (4.1), similarly to (3.19), we have

$$\begin{aligned}\Phi_h^\tau(P_N\psi(t_n), P_N\psi(t_{n-1})) &= e^{2i\tau\Delta}P_N\psi(t_{n-1}) - 2i\tau\varphi_s(\tau\Delta)P_N B(P_N\psi(t_n))\\ &= e^{2i\tau\Delta}P_N\psi(t_{n-1}) - i\int_{-\tau}^{\tau} e^{i(\tau-s)\Delta}P_N B(P_N\psi(t_n))\mathrm{d}s.\end{aligned} \tag{4.15}$$

Subtracting (4.15) from (4.14), and recalling (4.11), we obtain

$$\begin{aligned}\mathcal{E}^n &= P_N\psi(t_{n+1}) - \Phi_h^\tau(P_N\psi(t_n), P_N\psi(t_{n-1}))\\ &= -i\int_{-\tau}^{\tau} e^{i(\tau-s)\Delta}\left[P_N B(\psi(t_n+s)) - P_N B(P_N\psi(t_n))\right]\mathrm{d}s.\end{aligned} \tag{4.16}$$

From (4.16), we have

$$\begin{aligned}\mathcal{E}^n = &-i\int_{-\tau}^{\tau} e^{i(\tau-s)\Delta}\big[P_N B(\psi(t_n+s)) - P_N B(\psi(t_n))\big]\mathrm{d}s\\ &- i\int_{-\tau}^{\tau} e^{i(\tau-s)\Delta}\big[P_N B(\psi(t_n)) - P_N B(P_N\psi(t_n))\big]\mathrm{d}s =: r^n + r_h^n.\end{aligned} \tag{4.17}$$

By Lemma 3.5, the boundedness of $e^{it\Delta}$ and P_N, and the standard projection error estimates of P_N, we get

$$\|r_h^n\|_{L^2} \leq \int_{-\tau}^{\tau}\|B(\psi(t_n)) - B(P_N\psi(t_n))\|_{L^2}\mathrm{d}s \lesssim \tau\|\psi(t_n) - P_N\psi(t_n)\|_{L^2} \lesssim \tau h^4. \tag{4.18}$$

Note that the definition of r_h^n in (4.17) implies $r_h^n \in X_N$. Hence, by the inverse inequality and (4.18), we obtain

$$\|r_h^n\|_{H^\alpha} \lesssim \tau h^{4-\alpha}, \quad 0 \leq \alpha \leq 2. \tag{4.19}$$

For r^n defined in (4.17), recalling (3.30), (3.37), and (4.13), we have

$$r^n = P_N\mathcal{L}^n = P_N r_1^n + P_N r_2^n = P_N r_1^n + \mathcal{E}_{\mathrm{dom}}^n. \tag{4.20}$$

Moreover, one may check that to obtain the estimate of r_1^n in (3.35), it suffices to assume that $\sigma \geq 1/2$ instead of $\sigma \geq 1$. Hence, (3.35) is also valid here. By (3.35) and the boundedness of P_N, noting that $r_1^n \in H_{\mathrm{per}}^2(\Omega)$, we have

$$\|P_N r_1^n\|_{H^\alpha} \leq \|r_1^n\|_{H^\alpha} \lesssim \tau^{3-\alpha/2}, \quad 0 \leq \alpha \leq 2. \tag{4.21}$$

The proof can be completed by taking $\mathcal{E}_2^n = P_N r_1^n + r_h^n$ and noting that $\mathcal{E}^n = P_N r_1^n + r_h^n + \mathcal{E}_{\mathrm{dom}}^n$. ∎

As a corollary of Proposition 4.6, we have the following.

COROLLARY 4.7 (local truncation error). *Under the assumptions* (3.1)*, we have, for* $1 \leq n \leq T/\tau - 1$,

$$\|P_N\mathbf{\Psi}(t_{n+1}) - \mathbf{\Phi}_h^\tau(P_N\mathbf{\Psi}(t_n))\|_{H^\alpha} \lesssim \tau^{3-\alpha/2} + \tau h^{4-\alpha}, \quad 0 \leq \alpha \leq 2. \tag{4.22}$$

Proof. Recalling (3.11), (4.3), and (4.11), we have

$$\begin{aligned}&P_N\mathbf{\Psi}(t_{n+1})-\mathbf{\Phi}_h^\tau(P_N\mathbf{\Psi}(t_n))\\ &\quad=\begin{pmatrix}P_N\psi(t_{n+1})-\Phi_h^\tau(P_N\psi(t_{n+1}),P_N\psi(t_n))\\ P_N\psi(t_n)-P_N\psi(t_n)\end{pmatrix}=\begin{pmatrix}\mathcal{E}^n\\ 0\end{pmatrix}.\end{aligned}\tag{4.23}$$

It follows that

$$\|P_N\mathbf{\Psi}(t_{n+1})-\mathbf{\Phi}_h^\tau(P_N\mathbf{\Psi}(t_n))\|_{H^\alpha}=\|\mathcal{E}^n\|_{H^\alpha},\quad 0\le\alpha\le 2.\tag{4.24}$$

By Proposition 4.6, we have

$$\|\mathcal{E}^n\|_{H^\alpha}\lesssim\tau^{3-\alpha/2}+\tau h^{4-\alpha}+\|\mathcal{E}^n_{\rm dom}\|_{H^\alpha}.\tag{4.25}$$

Recalling that $\mathcal{E}^n_{\rm dom}=P_N r_2^n$, using (3.38) and the boundedness of P_N, we obtain

$$\|\mathcal{E}^n_{\rm dom}\|_{H^\alpha}\lesssim\|r_2^n\|_{H^\alpha}\lesssim\tau^{3-\alpha/2},\quad 0\le\alpha\le 2,\tag{4.26}$$

which, plugged into (4.25), completes the proof. ∎

Similarly to Proposition 3.17, we have the conditional H^1-stability estimate.

PROPOSITION 4.8 (H^1-stability). *Assume that $V\in W^{1,4}(\Omega)\cap H^1_{\rm per}(\Omega)$ and $\sigma\ge 1$. Let $\mathbf{v}=(v_1,v_0)^T,\mathbf{w}=(w_1,w_0)^T$ such that $v_j,w_j\in H^2_{\rm per}(\Omega)$ for $j=0,1$ with $\|v_1\|_{H^2}\le M$ and $\|w_1\|_{H^2}\le M$. Then we have*

$$\|\mathbf{\Phi}_h^\tau(\mathbf{v})-\mathbf{\Phi}_h^\tau(\mathbf{w})\|_{H^1}\le(1+C(\|V\|_{W^{1,4}},M)\tau)\|\mathbf{v}-\mathbf{w}\|_{H^1}.$$

With Corollary 4.7 and Proposition 4.8, we can prove Theorem 4.1 by using the standard argument as in the proof of Theorem 3.1.

Proof of Theorem 4.1. Let $e_N^n=P_N\psi(t_n)-\psi_N^n$ for $0\le n\le T/\tau$ and let

$$\mathbf{e}_N^n:=P_N\mathbf{\Psi}(t_n)-\mathbf{\Psi}_N^n=(e_N^n,e_N^{n-1})^T,\quad 1\le n\le T/\tau.\tag{4.27}$$

By the standard projection error estimates

$$\|\psi(t_n)-P_N\psi(t_n)\|_{H^\alpha}\lesssim h^{4-\alpha},\quad \alpha=0,1,\quad 0\le n\le T/\tau,\tag{4.28}$$

we only need to obtain the estimates of e_N^n.

We start with $\mathbf{e}_N^1=(e_N^1,e_N^0)^T=(e_N^1,0)^T$. Recalling the first equality in (2.11) and applying P_N on both sides, noting that P_N commutes with $e^{it\Delta}$, we have

$$P_N\psi(t_1)=e^{i\tau\Delta}P_N\psi_0-i\int_0^\tau e^{i(\tau-s)\Delta}P_NB(\psi(s))\mathrm{d}s.\tag{4.29}$$

Subtracting the second equation in (2.18) from (4.29), we get

$$e_N^1=P_N\psi(t_1)-\psi_N^1=-i\int_0^\tau e^{i(\tau-s)\Delta}P_N[B(\psi(s))-B(P_N\psi_0)]\mathrm{d}s.\tag{4.30}$$

From (4.30), using standard projection error estimates, the boundednss of $e^{it\Delta}$ and P_N, Lemmas 3.5 and 3.12, we obtain

$$\begin{aligned}\|\mathbf{e}_N^1\|_{H^\alpha}=\|e_N^1\|_{H^\alpha}&\le\int_0^\tau\|B(\psi(s))-B(P_N\psi_0)\|_{H^\alpha}\mathrm{d}s\\ &\le\int_0^\tau\left(\|B(\psi(s))-B(\psi_0)\|_{H^\alpha}+\|B(\psi_0)-B(P_N\psi_0)\|_{H^\alpha}\right)\mathrm{d}s\\ &\lesssim\tau^2+\tau h^{4-\alpha}\le\tau^{2-\alpha/2}+h^{4-\alpha},\qquad\alpha=0,1.\end{aligned}\tag{4.31}$$

Recalling (4.5) and (4.27), we have, for $1 \le n \le T/\tau - 1$,

$$\begin{aligned} \mathbf{e}_N^{n+1} &= P_N \mathbf{\Psi}(t_{n+1}) - \mathbf{\Psi}_N^{n+1} = P_N \mathbf{\Psi}(t_{n+1}) - \mathbf{\Phi}_h^\tau(\mathbf{\Psi}_N^n) \\ &= P_N \mathbf{\Psi}(t_{n+1}) - \mathbf{\Phi}_h^\tau(P_N \mathbf{\Psi}(t_n)) + \mathbf{\Phi}_h^\tau(P_N \mathbf{\Psi}(t_n)) - \mathbf{\Phi}_h^\tau(\mathbf{\Psi}_N^n), \end{aligned} \tag{4.32}$$

which implies, by using Corollary 4.7, (4.8), and Proposition 4.8,

$$\begin{aligned} \|\mathbf{e}_N^{n+1}\|_{H^\alpha} &\le \|P_N \mathbf{\Psi}(t_{n+1}) - \mathbf{\Phi}_h^\tau(P_N \mathbf{\Psi}(t_n))\|_{H^\alpha} + \|\mathbf{\Phi}_h^\tau(P_N \mathbf{\Psi}(t_n)) - \mathbf{\Phi}_h^\tau(\mathbf{\Psi}_N^n)\|_{H^\alpha} \\ &\le C_7 \left(\tau^{3-\alpha/2} + \tau h^{4-\alpha}\right) + (1 + C_6 \tau)\|\mathbf{e}_N^n\|_{H^\alpha}, \quad \alpha = 0, 1, \end{aligned} \tag{4.33}$$

where C_6 depends, in particular, on $\|\psi_N^n\|_{H^2}$. By the uniform H^2-norm bound of ψ_N^n established in Theorem 4.2 and the assumptions made in Theorem 4.1, the constants C_6 and C_7 in (4.33) are uniformly bounded. From (4.33), using the discrete Gronwall's inequality and noting (4.31), we can obtain the desired result. ∎

4.4. Proof of Theorem 4.3 for improved optimal error bound. In this subsection, we shall present the proof of Theorem 4.3. The key ingredient is to use the technique of regularity compensation oscillation [10, 11, 17] to analyze the error cancellation in the accumulation of local truncation errors (i.e., (4.40) below). Note that, under the assumptions (3.3), Proposition 4.6 still holds (while Corollary 4.7 does not).

Proof of Theorem 4.3. Recall $e_N^n = P_N \psi(t_n) - \psi_N^n$ and $\mathbf{e}_N^n = P_N \mathbf{\Psi}(t_n) - \mathbf{\Psi}_N^n = (e_N^n, e_N^{n-1})^T$ in the proof of Theorem 4.1. Similarly to (4.28), we only need to establish the L^2- and H^1-norm error bounds for e_N^n. From (4.32), by (4.23), we get

$$\begin{aligned} \mathbf{e}_N^{n+1} &= P_N \mathbf{\Psi}(t_{n+1}) - \mathbf{\Phi}_h^\tau(P_N \mathbf{\Psi}(t_n)) + \mathbf{\Phi}_h^\tau(P_N \mathbf{\Psi}(t_n)) - \mathbf{\Phi}_h^\tau(\mathbf{\Psi}_N^n) \\ &= \mathbf{A}\mathbf{e}_N^n + \begin{pmatrix} \mathcal{E}^n \\ 0 \end{pmatrix} + \tau P_N \left(\mathbf{H}(P_N \psi(t_n)) - \mathbf{H}(\psi_N^n)\right), \quad 1 \le n \le T/\tau - 1, \end{aligned} \tag{4.34}$$

where we abbreviate $\mathbf{A}(\tau)$ as $\mathbf{A}$. Iterating (4.34) and recalling (4.12), for $1 \le n \le T/\tau - 1$, we have

$$\mathbf{e}_N^{n+1} = \mathbf{A}^n \mathbf{e}_N^1 + \sum_{k=1}^n \mathbf{A}^{n-k} \begin{pmatrix} \mathcal{E}_{\mathrm{dom}}^k \\ 0 \end{pmatrix} + \sum_{k=1}^n \mathbf{A}^{n-k} \begin{pmatrix} \mathcal{E}_2^k \\ 0 \end{pmatrix} + \tau \sum_{k=1}^n \mathbf{A}^{n-k} \mathbf{Z}^k, \tag{4.35}$$

where

$$\mathbf{Z}^n = P_N \mathbf{H}(P_N \psi(t_n)) - P_N \mathbf{H}(\psi_N^n), \qquad 1 \le n \le T/\tau - 1. \tag{4.36}$$

In the following, we shall estimate the four terms on the right-hand side (RHS) of (4.35) in the L^2-norm, respectively. By Lemma 3.9 and (4.31) with $\alpha = 0$, we have

$$\|\mathbf{A}^n \mathbf{e}_N^1\|_{L^2} = \|\mathbf{e}_N^1\|_{L^2} = \|e_N^1\|_{L^2} \lesssim \tau^2 + h^4. \tag{4.37}$$

By Lemma 3.9 and Proposition 4.6 with $\alpha = 0$, we get

$$\left\| \sum_{k=1}^n \mathbf{A}^{n-k} \begin{pmatrix} \mathcal{E}_2^k \\ 0 \end{pmatrix} \right\|_{L^2} \le \sum_{k=1}^n \|\mathcal{E}_2^k\|_{L^2} \lesssim n(\tau^3 + \tau h^4) \lesssim \tau^2 + h^4. \tag{4.38}$$

Recalling (4.36), by Lemma 3.9, (3.15), and the boundedness of $\varphi_{\mathrm{s}}(t\Delta)$ and P_N, we have

$$\left\| \tau \sum_{k=1}^n \mathbf{A}^{n-k} \mathbf{Z}^k \right\|_{L^2} \le \tau \sum_{k=1}^n \|\mathbf{Z}^k\|_{L^2} \lesssim \tau \sum_{k=1}^n \|e_N^k\|_{L^2} \le \tau \sum_{k=1}^n \|\mathbf{e}_N^k\|_{L^2}, \tag{4.39}$$

where the constant depends on $\|V\|_{L^\infty}$, $\|P_N\psi(t_n)\|_{L^\infty}$ and $\|\psi_N^n\|_{L^\infty}$, and thus is uniformly bounded by the given assumptions and the uniform H^2-norm bound of ψ_N^n in Theorem 4.2.

It remains to estimate the second term on the RHS of (4.35), which is the accumulation of the dominant local truncation error:

$$\mathcal{J}^n := \sum_{k=1}^{n} \mathbf{A}^{n-k} \begin{pmatrix} \mathcal{E}_{\text{dom}}^k \\ 0 \end{pmatrix} = \sum_{k=0}^{n-1} \mathbf{A}^k \begin{pmatrix} \mathcal{E}_{\text{dom}}^{n-k} \\ 0 \end{pmatrix}, \quad 1 \le n \le T/\tau - 1. \tag{4.40}$$

Taking the Fourier transform of (4.40) componentwise, we obtain

$$\widehat{(\mathcal{J}^n)}_l = \sum_{k=0}^{n-1} (\mathbf{A}_l)^k \begin{pmatrix} \widehat{(\mathcal{E}_{\text{dom}}^{n-k})}_l \\ 0 \end{pmatrix}, \quad l \in \mathcal{T}_N, \quad 1 \le n \le T/\tau - 1, \tag{4.41}$$

where $\mathbf{A}_l$ is a unitary matrix defined as

$$\mathbf{A}_l := \begin{pmatrix} 0 & e^{-2i\tau\mu_l^2} \\ 1 & 0 \end{pmatrix}, \quad l \in \mathcal{T}_N. \tag{4.42}$$

Note that $\mathbf{A}_l$ can be decomposed as

$$\mathbf{A}_l = \mathbf{P}_l \mathbf{\Lambda}_l \mathbf{P}_l^*, \quad l \in \mathcal{T}_N, \tag{4.43}$$

where $\mathbf{P}_l^*$ is the complex conjugate transpose of $\mathbf{P}_l$ and

$$\mathbf{P}_l = \frac{1}{\sqrt{2}} \begin{pmatrix} \lambda_{+,l} & \lambda_{-,l} \\ 1 & 1 \end{pmatrix}, \quad \mathbf{\Lambda}_l = \begin{pmatrix} \lambda_{+,l} & 0 \\ 0 & \lambda_{-,l} \end{pmatrix}, \quad \lambda_{\pm,l} = \pm e^{-i\tau\mu_l^2}. \tag{4.44}$$

Define

$$\mathbf{S}_{l,n} := \sum_{k=0}^{n} (\mathbf{A}_l)^k = \mathbf{P}_l \begin{pmatrix} s_{l,n}^+ & 0 \\ 0 & s_{l,n}^- \end{pmatrix} \mathbf{P}_l^*, \qquad n \ge 0, \tag{4.45}$$

where

$$s_{l,n}^+ = \sum_{k=0}^{n} \lambda_{+,l}^k, \quad s_{l,n}^- = \sum_{k=0}^{n} \lambda_{-,l}^k. \tag{4.46}$$

From (4.46), recalling (4.44), noting that $\tau \le h^2/(2\pi)$ implies $\tau\mu_l^2 \le \pi/2$ for all $l \in \mathcal{T}_N$, we have

$$\left|s_{l,n}^+\right| = \left|\frac{1-\lambda_{+,l}^{n+1}}{1-\lambda_{+,l}}\right| \le \frac{2}{|1-e^{-i\tau\mu_l^2}|} = \frac{1}{|\sin(\tau\mu_l^2/2)|} \lesssim \frac{1}{\tau\mu_l^2}, \quad 0 \ne l \in \mathcal{T}_N, \tag{4.47}$$

$$\left|s_{l,n}^-\right| = \left|\frac{1-\lambda_{-,l}^{n+1}}{1-\lambda_{-,l}}\right| \le \frac{2}{|1+e^{-i\tau\mu_l^2}|} = \frac{1}{|\cos(\tau\mu_l^2/2)|} \lesssim 1, \quad l \in \mathcal{T}_N. \tag{4.48}$$

Using the summation by parts formula, we have, for $l \in \mathcal{T}_N$ and $1 \le n \le T/\tau - 1$,

$$\begin{aligned} \widehat{(\mathcal{J}^n)}_l &= \sum_{k=0}^{n-1} (\mathbf{A}_l)^k \begin{pmatrix} \widehat{(\mathcal{E}_{\text{dom}}^{n-k})}_l \\ 0 \end{pmatrix} \\ &= \mathbf{S}_{l,n-1} \begin{pmatrix} \widehat{(\mathcal{E}_{\text{dom}}^{1})}_l \\ 0 \end{pmatrix} - \sum_{k=0}^{n-2} \mathbf{S}_{l,k} \begin{pmatrix} \widehat{(\mathcal{E}_{\text{dom}}^{n-k-1})}_l - \widehat{(\mathcal{E}_{\text{dom}}^{n-k})}_l \\ 0 \end{pmatrix}. \end{aligned} \tag{4.49}$$

Recalling the definition of $\mathcal{E}^n_{\rm dom}$ in (4.13), setting $\phi^n := P_N dB(\psi(t_n))[\partial_t\psi(t_n)]$, we have

$$\widehat{(\mathcal{E}^n_{\rm dom})}_l = -2\tau^3\mu_l^2 e^{-i\tau\mu_l^2}\varphi_{\rm c}(\tau\mu_l^2)\widehat{\phi^n_l}, \quad l\in\mathcal{T}_N, \quad 1\le n\le T/\tau-1, \tag{4.50}$$

which implies, for $1\le n\le T/\tau-1$,

$$\left|\widehat{(\mathcal{E}^n_{\rm dom})}_l\right| \lesssim \tau^3 \sup_{x\in\mathbb{R}}|\varphi_{\rm c}(x)|\mu_l^2\left|\widehat{\phi^n_l}\right| \lesssim \tau^3\mu_l^2\left|\widehat{\phi^n_l}\right|, \quad l\in\mathcal{T}_N, \tag{4.51}$$

$$\left|\widehat{(\mathcal{E}^n_{\rm dom})}_l\right| \lesssim \tau^2 \sup_{x\in\mathbb{R}}|x\varphi_{\rm c}(x)|\left|\widehat{\phi^n_l}\right| \lesssim \tau^2\left|\widehat{\phi^n_l}\right|, \qquad l\in\mathcal{T}_N. \tag{4.52}$$

From (4.49), recalling (4.45) and (4.50), we have, for $l\in\mathcal{T}_N$,

$$\widehat{(\mathcal{J}^n)}_l = \frac{1}{\sqrt{2}}\mathbf{P}_l\begin{pmatrix} s^+_{l,n-1}\overline{\lambda_{+,l}} \\ s^-_{l,n-1}\overline{\lambda_{-,l}}\end{pmatrix}\widehat{(\mathcal{E}^1_{\rm dom})}_l - \frac{1}{\sqrt{2}}\mathbf{P}_l\sum_{k=0}^{n-2}\begin{pmatrix} s^+_{l,k}\overline{\lambda_{+,l}} \\ s^-_{l,k}\overline{\lambda_{-,l}}\end{pmatrix}\left[\widehat{(\mathcal{E}^{n-k-1}_{\rm dom})}_l - \widehat{(\mathcal{E}^{n-k}_{\rm dom})}_l\right]. \tag{4.53}$$

From (4.53), noting that $\|\mathbf{P}_l\|_2 = 1$ and $|\lambda_{\pm,l}|=1$, we have

$$\left|\widehat{(\mathcal{J}^n)}_l\right| \lesssim W^1_l + W^2_l + \sum_{k=0}^{n-2}\left(W^3_{k,l}+W^4_{k,l}\right), \quad l\in\mathcal{T}_N, \tag{4.54}$$

where

$$\begin{aligned} &W^1_l = \left|\widehat{(\mathcal{E}^1_{\rm dom})}_l\right|\left|s^+_{l,n-1}\right|, \qquad W^2_l = \left|\widehat{(\mathcal{E}^1_{\rm dom})}_l\right|\left|s^-_{l,n-1}\right|, \\ &W^3_{k,l} = \left|\widehat{(\mathcal{E}^{n-k}_{\rm dom})}_l - \widehat{(\mathcal{E}^{n-k-1}_{\rm dom})}_l\right|\left|s^+_{l,k}\right|, \\ &W^4_{k,l} = \left|\widehat{(\mathcal{E}^{n-k}_{\rm dom})}_l - \widehat{(\mathcal{E}^{n-k-1}_{\rm dom})}_l\right|\left|s^-_{l,k}\right|, \end{aligned} \quad k\in\left\{0,1,\ldots,\frac{T}{\tau}-3\right\}, \qquad l\in\mathcal{T}_N. \tag{4.55}$$

For W^1_l, using (4.47) and (4.51), when $\tau\le h^2/(2\pi)$, we have

$$|W^1_l| \lesssim \frac{\tau^3\mu_l^2}{\tau\mu_l^2}\left|\widehat{\phi^1_l}\right| \lesssim \tau^2\left|\widehat{\phi^1_l}\right|, \quad 0\ne l\in\mathcal{T}_N, \tag{4.56}$$

from which, noting that $|W^1_l|=0$ when $l=0$, we obtain

$$|W^1_l| \lesssim \tau^2\left|\widehat{\phi^1_l}\right|, \quad l\in\mathcal{T}_N. \tag{4.57}$$

For W^2_l, using (4.48) and (4.52), when $\tau\le h^2/(2\pi)$, we have

$$|W^2_l| \lesssim \tau^2\left|\widehat{\phi^1_l}\right|, \quad l\in\mathcal{T}_N. \tag{4.58}$$

Similarly, for $W^3_{k,l}$ and $W^4_{k,l}$, when $\tau\le h^2/(2\pi)$, we have

$$|W^3_{k,l}| \lesssim \tau^2\left|\widehat{\phi^{n-k}_l} - \widehat{\phi^{n-k-1}_l}\right|, \quad |W^4_{k,l}| \lesssim \tau^2\left|\widehat{\phi^{n-k}_l} - \widehat{\phi^{n-k-1}_l}\right|, \quad l\in\mathcal{T}_N. \tag{4.59}$$

From (4.54), using the Cauchy inequality, and noting (4.57)–(4.59), we get, for $\tau \leq h^2/(2\pi)$,

$$\begin{aligned}\left|\widehat{(\mathcal{J}^n)}_l\right|^2 &\lesssim \left|W_l^1\right|^2 + \left|W_l^2\right|^2 + n\sum_{k=0}^{n-2}\left(\left|W_{k,l}^3\right|^2 + \left|W_{k,l}^4\right|^2\right)\\ &\lesssim \tau^4\left|\widehat{\phi_l^1}\right|^2 + n\tau^4\sum_{k=1}^{n-1}\left|\widehat{\phi_l^{k+1}} - \widehat{\phi_l^k}\right|^2, \quad l\in\mathcal{T}_N, \quad 1\leq n\leq T/\tau - 1. \end{aligned}\tag{4.60}$$

Using Parseval's identity and (4.60), and changing the order of summation, we have

$$\begin{aligned}\|\mathcal{J}^n\|_{L^2}^2 &= (b-a)\sum_{l\in\mathcal{T}_N}\left|\widehat{(\mathcal{J}^n)}_l\right|^2 \lesssim \tau^4\sum_{l\in\mathcal{T}_N}\left|\widehat{\phi_l^1}\right|^2 + n\tau^4\sum_{l\in\mathcal{T}_N}\sum_{k=1}^{n-1}\left|\widehat{\phi_l^{k+1}} - \widehat{\phi_l^k}\right|^2\\ &\lesssim \tau^4\|\phi^1\|_{L^2}^2 + n\tau^4\sum_{k=1}^{n-1}\sum_{l\in\mathcal{T}_N}\left|\widehat{\phi_l^{k+1}} - \widehat{\phi_l^k}\right|^2\\ &\lesssim \tau^4\|\phi^1\|_{L^2}^2 + n\tau^4\sum_{k=1}^{n-1}\|\phi^{k+1}-\phi^k\|_{L^2}^2, \qquad 1\leq n\leq T/\tau-1.\end{aligned}\tag{4.61}$$

Recalling that $\phi_l^n = P_N dB(\psi(t_n))[\partial_t\psi(t_n)]$, by Lemma 3.13 and the boundedness of P_N, we have

$$\|\phi^1\|_{L^2} = \|P_N dB(\psi(t_1))[\partial_t\psi(t_1)]\|_{L^2} \leq \|dB(\psi(t_1))[\partial_t\psi(t_1)]\|_{L^2} \lesssim 1,$$

and

$$\begin{aligned}\|\phi^{k+1}-\phi^k\|_{L^2} &= \|P_N dB(\psi(t_{k+1}))[\partial_t\psi(t_{k+1})] - P_N dB(\psi(t_k))[\partial_t\psi(t_k)]\|_{L^2}\\ &\leq \|dB(\psi(t_{k+1}))[\partial_t\psi(t_{k+1})] - dB(\psi(t_k))[\partial_t\psi(t_k)]\|_{L^2}\\ &\lesssim \|\psi(t_{k+1})-\psi(t_k)\|_{L^2} + \|\partial_t\psi(t_{k+1}) - \partial_t\psi(t_k)\|_{L^2} \lesssim \tau,\end{aligned}$$

which, plugged into (4.61), yields

$$\|\mathcal{J}^n\|_{L^2}^2 \lesssim \tau^4 + n^2\tau^6 \lesssim \tau^4, \qquad 1\leq n\leq T/\tau - 1.\tag{4.62}$$

From (4.35), using (4.37)–(4.39) and (4.62), and recalling (4.40), we obtain

$$\|\mathbf{e}_N^{n+1}\|_{L^2} \lesssim \tau^2 + h^4 + \tau\sum_{k=1}^{n}\|\mathbf{e}_N^k\|_{L^2}, \qquad 0\leq n\leq T/\tau - 1,\tag{4.63}$$

where the case $n=0$ follows from $\|\mathbf{e}_N^1\|_{L^2} \lesssim \tau^2 + h^4$ established in (4.37). Then the proof of the L^2-norm error bound is completed by applying the discrete Gronwall's inequality to (4.63). The H^1-norm error bound can be obtained by directly applying the inverse inequality $\|\phi\|_{H^1} \lesssim h^{-1}\|\phi\|_{L^2}$ for $\phi\in X_N$ [45] as

$$\|e_N^n\|_{H^1} \lesssim h^{-1}\|e_N^n\|_{L^2} \lesssim \tau^2 h^{-1} + h^3 \lesssim \tau^{\frac{3}{2}} + h^3, \quad 0\leq n\leq T/\tau,\tag{4.64}$$

where we also use the fact that $\tau \leq h^2/(2\pi)$. The proof is then completed. ∎

5. Numerical results. In this section, we shall show some numerical results to validate our error estimates and to demonstrate the superiority of the sEWI. We first test the convergence of the sEWI under various potential, nonlinearity, and initial data. Then we perform some long-time simulation to show the near-conservation of mass and energy. To quantify the error, we introduce the following error functions:

$$e_{L^2}(t_n) := \|\psi(\cdot,t_n) - \psi_N^n\|_{L^2}, \quad e_{H^1}(t_n) := \|\psi(\cdot,t_n) - \psi_N^n\|_{H^1}, \quad 0 \le n \le T/\tau.$$

We start with good potential and nonlinearity and consider a 1 dimensional example. In the NLSE (1.1), we choose $\Omega = (-16,16)$, $\beta = 1$, $\sigma = 1.1$, and

$$V(x) = \left(\frac{x^2-4}{16}\right)^{1.51} \times \left(1 - \frac{x^2}{16^2}\right)^2, \quad \psi_0(x) = x|x|^{2.51} e^{-\frac{x^2}{2}}, \quad x \in \Omega. \tag{5.1}$$

Here in (5.1), the potential function V satisfies $V \in H^2_{\mathrm{per}}(\Omega)$ and the initial datum $\psi_0 \in H^4(\Omega)$ is intentionally chosen as an odd function. Note that, with an odd initial datum, the exact solution will remain an odd function for all time $t \ge 0$, and thus indeed suffer from the low regularity of nonlinearity at the origin.

In the numerical simulation, we choose $T = 1$. The "exact" solution is computed by the sEWI-FS method (2.17) with $\tau = 10^{-5}$ and $h = 2^{-9}$. The numerical results are presented in Figure 5.1, where we show temporal errors with respect to the time step size τ in (a) and spatial errors with respect to the mesh size h in (b). When computing temporal errors, we vary τ with fixed $h = 2^{-9}$, and when computing spatial errors, we vary h with fixed $\tau = 10^{-5}$.

From Figure 5.1, we can observe that under H^2-potential, $\sigma = 1.1$, and H^4-initial data, the temporal convergence is second order in the L^2-norm and 1.5-order in the H^1-norm; and the spatial convergence is forth order in the L^2-norm and third order in the H^1-norm. The results confirm our error estimates in Theorems 3.1 and 4.1 and show that they are sharp.

We then consider low regularity potential and nonlinearity. To show the validity of our results in general dimensions, we present a 2 dimensional example. In (1.1), we choose $\Omega = (-8,8) \times (-8,8)$, $\beta = 1$, $\sigma = 0.1$, and

$$V(\mathbf{x}) = \begin{cases} 10, & |x| \le 2, |y| \le 2, \\ 0, & \text{otherwise}, \end{cases} \quad \psi_0(\mathbf{x}) = x|x|^{0.51} e^{-\frac{|\mathbf{x}|^2}{2}}, \quad \mathbf{x} = (x,y)^T \in \Omega. \tag{5.2}$$

It follows immediately that $V \in L^\infty(\Omega)$ and $\psi_0 \in H^2(\Omega)$ in (5.2).

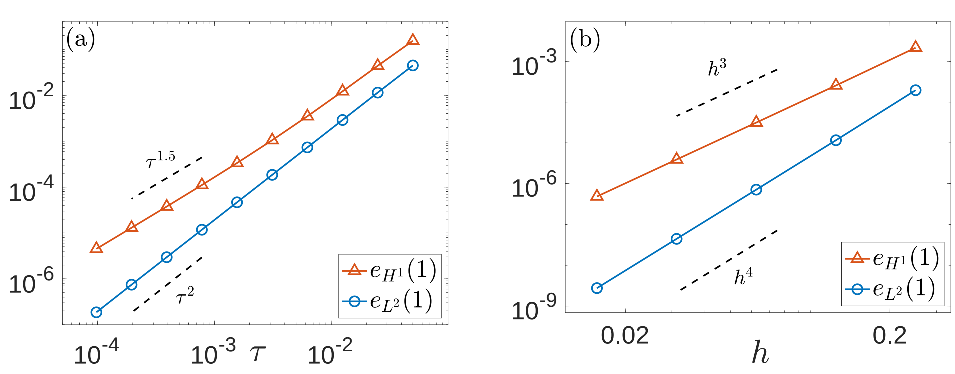

FIG. 5.1. *L^2- and H^1-errors of the sEWI for the NLSE with $\sigma = 1.1$ and $V \in H^2$ given in* (5.1)*:* (a) *temporal errors and* (b) *spatial errors. Note: color appears only in the online article.*

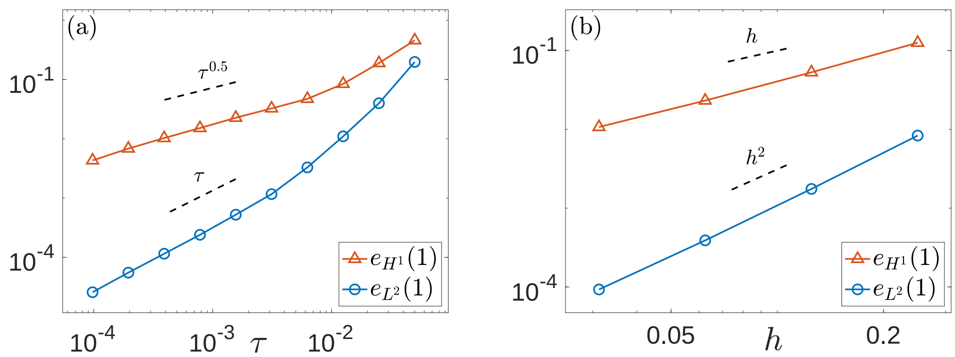

FIG. 5.2. *L^2- and H^1-errors of the sEWI for the NLSE with $\sigma = 0.1$ and $V \in L^\infty$ given in* (5.2)*:* (a) *temporal errors and* (b) *spatial errors. Note: color appears only in the online article.*

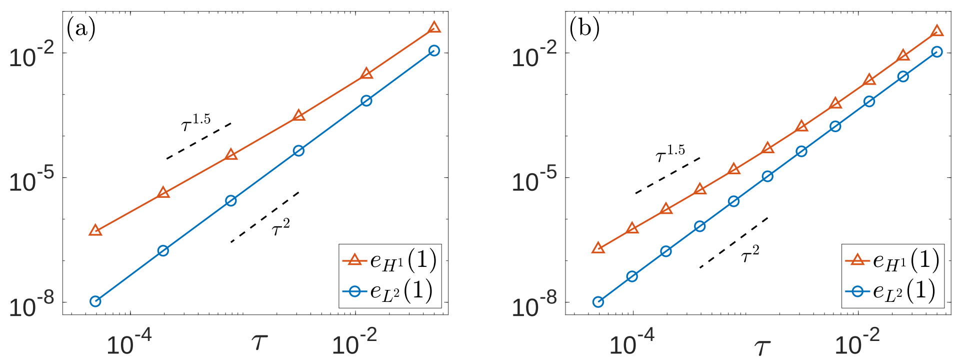

FIG. 5.3. *L^2- and H^1-errors of the sEWI for the NLSE with $\sigma = 0.5$:* (a) *errors computed with $h = \sqrt{10\tau}$ and* (b) *errors computed with $h = 2^{-9}$ fixed. Note: color appears only in the online article.*

In computation, we choose $T = 0.25$. The exact solution is computed by the sEWI-FS method with $\tau = 10^{-5}$ and $h_x = h_y = 2^{-7}$, where h_x and h_y are the mesh sizes in the x and y directions, respectively. We plot temporal and spatial errors in Figure 5.2, following the same manner as in the previous example.

From Figure 5.2, we observe that under L^∞-potential, $\sigma = 0.1$, and H^2-initial data, the temporal convergence of the sEWI is first order in the L^2-norm and half-order in the H^1-norm; and the spatial convergence is second order in the L^2-norm and first order in the H^1-norm. The observation validates our error estimates in Theorems 3.2 and 4.2 and indicates that they are sharp.

Then we consider another example in 1D under improved regularity assumptions. We set $T = 1$ and choose $\Omega = (-16, 16)$, $\beta = -1$, $\sigma = 0.5$, and $V(x) \equiv 0$ with the same H^4-initial datum ψ_0 given in (5.1). The exact solution is computed with $\tau = 10^{-5}$ and $h = 2^{-9}$. Differently from the two cases above, we compute the errors of the sEWI-FS with $h = \sqrt{10\tau}$ to satisfy the constraint $\tau \leq h^2/(2\pi)$. For comparison, we also plot the errors computed by varying τ with $h = 2^{-9}$ fixed (corresponding to the time semidiscrete case). The numerical results for the two cases are exhibited in Figure 5.3(a) and (b), respectively.

From Figure 5.3, we can observe that, the L^2-error of the sEWI-FS method is of $O(\tau^2)$ and the H^1-error is of $O(\tau^{\frac{3}{2}})$ with and without the time step size restriction $\tau \leq h^2/(2\pi)$. The numerical results validate our error estimates in Theorem 4.3, but also suggest that the time step size restriction might be relaxed. We will try to investigate this phenomenon in our future work.

It should be noted that while all the numerical results shown in Figures 5.1 to 5.3 indicate the sharpness of the convergence rates under given assumptions, they do not imply that all the assumptions are necessary. In particular, the same convergence rate observed in Figure 5.3 can also be seen when reducing σ from 0.5 to 0.1. This suggests that the assumption on nonlinearity in Theorem 4.3 might be further relaxed. However, the rigorous analysis is challenging and will be considered in our future work.

In the following, we test the long-time behavior of the sEWI. We consider two cases with potential and nonlinearity of different regularity and compute relative errors of mass and energy up to a very long time $T = 500$. In both cases, we fix $\Omega = (-16, 16)$, $\beta = 1$ and choose an odd initial datum $\psi_0(x) = xe^{-x^2/2}$ for $x \in \Omega$. In the case of good potential and nonlinearity, we choose $\sigma = 1.1$ and an H^2-potential V given in (5.1). In the case of low regularity potential and nonlinearity, we choose $\sigma = 0.1$ and an L^∞-potential V given by

$$V(x) = \begin{cases} 10, & x \geq 4 \text{ or } x \leq -4, \\ 0, & \text{otherwise}, \end{cases} \qquad x \in \Omega. \tag{5.3}$$

The numerical results are plotted in Figures 5.4 and 5.5 for the two cases, respectively. We can clearly observe that the mass and energy are nearly conserved for a very long time in both cases: The relative errors of mass and energy satisfy (based on numerical results)

$$\frac{|M(\psi_N^n) - M(\psi_0)|}{|M(\psi_0)|} \leq C_1\tau^2, \quad \frac{|E(\psi_N^n) - E(\psi_0)|}{|E(\psi_0)|} \leq C_2\tau^2, \quad 0 \leq n\tau \leq T = 500,$$

where C_1 and C_2 seem to be independent of T. It is rather surprising that even with extremely low regularity potential and nonlinearity, one can still obtain second-order temporal convergence of mass and energy. The rigorous analysis of these phenomena, including the long-time near conservation property and the high-order temporal convergence of mass and energy, will be taken as our future work.

Finally, we perform long-time simulation of a benchmark problem posed in [33] to showcase the superiority of the sEWI even in the smooth setting where the potential, nonlinearity, and initial datum are all smooth. In the NLSE (1.1), we take $V(x) \equiv 0$, $\beta = -2$, and $\sigma = 1$ with $\Omega = (-16, 16)$. The computation time is taken as $T = 200$ with the initial datum given by

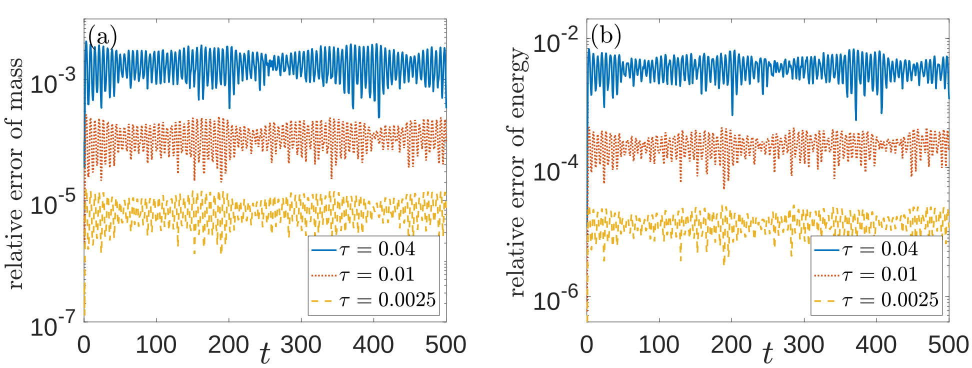

FIG. 5.4. *Relative errors of* (a) *mass and* (b) *energy of the sEWI for the NLSE with* $\sigma = 1.1$ *and* $V \in H^2$ *given in* (5.1). *Note: color appears only in the online article.*

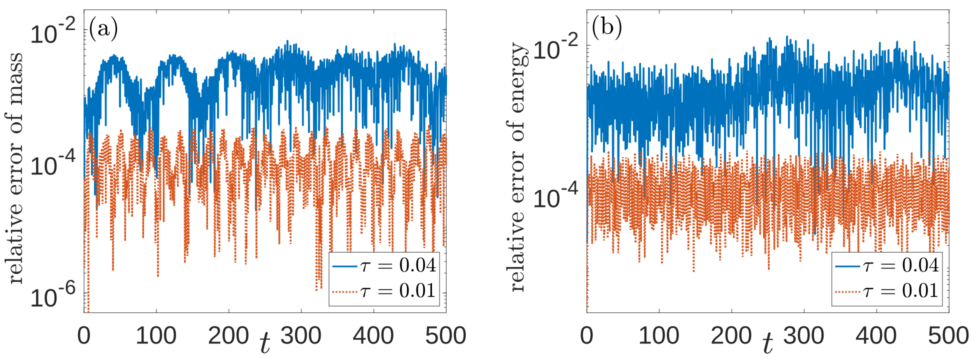

FIG. 5.5. *Relative errors of* (a) *mass and* (b) *energy of the sEWI for the NLSE with* $\sigma = 0.1$ *and* $V \in L^\infty$ *given in* (5.3)*. Note: color appears only in the online article.*

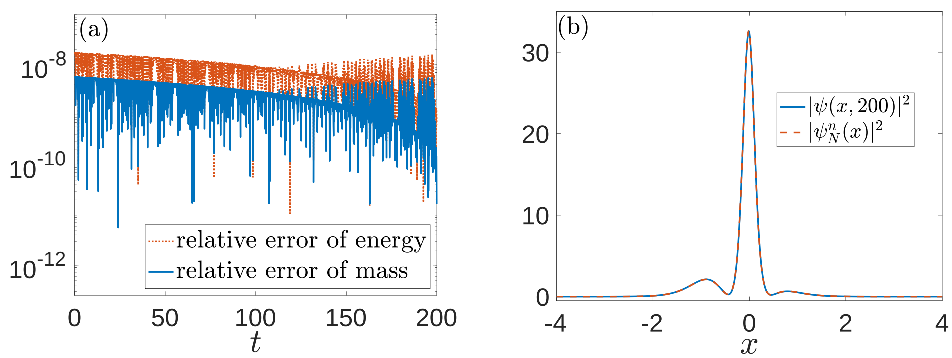

FIG. 5.6. *A benchmark problem:* (a) *relative errors of mass and energy and* (b) *plots of the density. Note: color appears only in the online article.*

$$\psi_0(x) = \frac{8(9e^{-4x} + 16e^{4x}) - 32(4e^{-2x} + 9e^{2x})}{-128 + 4e^{-6x} + 16e^{6x} + 81e^{-2x} + 64e^{2x}}, \quad x \in \Omega. \tag{5.4}$$

The exact solution can be given analytically by (24) of [33]. As discussed in [33], although it is a 1 dimensional experiment with known analytical solution, the problem is extremely hard to solve numerically. In computation, we take $\tau = 2.5 \times 10^{-6}$ and $h = 2^{-6}$, and the total computation time is about 4 hours on a personal computer. The relative errors of mass and energy as well as the density $|\psi|^2$ are plotted in Figure 5.6. We can observe not only near conservation of mass and energy up to a long time but also the density is correctly approximated without any evident difference. This example shows the sEWI is still advantageous in the smooth setting to simulate complicated interaction up to a long time.

6. Conclusion. We proposed and analyzed an sEWI for the NLSE with low regularity potential and nonlinearity. The sEWI is symmetric, explicit, and stable under a time step size restriction independent of the mesh size. Moreover, it exhibits excellent performance in solving the NLSE with low regularity potential and/or nonlinearity as well as in the long-time simulation of the NLSE. Rigorous error estimates of the sEWI were established under various regularity assumptions on potential and nonlinearity. Extended numerical results were reported to validate our error estimates and to demonstrate superb long-time behavior of the sEWI.

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