# ERROR ESTIMATES OF THE TIME-SPLITTING METHODS FOR THE NONLINEAR SCHRÖDINGER EQUATION WITH SEMI-SMOOTH NONLINEARITY 

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#### Abstract

We establish error bounds of the Lie-Trotter time-splitting sine pseudospectral method for the nonlinear Schrödinger equation (NLSE) with semi-smooth nonlinearity $f(\rho)=\rho^{\sigma}$, where $\rho=|\psi|^{2}$ is the density with $\psi$ the wave function and $\sigma>0$ is the exponent of the semi-smooth nonlinearity. Under the assumption of $H^{2}$-solution of the NLSE, we prove error bounds at $O\left(\tau^{\frac{1}{2}+\sigma}+h^{1+2 \sigma}\right)$ and $O\left(\tau+h^{2}\right)$ in $L^{2}$-norm for $0<\sigma \leq \frac{1}{2}$ and $\sigma \geq$ $\frac{1}{2}$, respectively, and an error bound at $O\left(\tau^{\frac{1}{2}}+h\right)$ in $H^{1}$-norm for $\sigma \geq \frac{1}{2}$, where $h$ and $\tau$ are the mesh size and time step size, respectively. In addition, when $\frac{1}{2}<\sigma<1$ and under the assumption of $H^{3}$-solution of the NLSE, we show an error bound at $O\left(\tau^{\sigma}+h^{2 \sigma}\right)$ in $H^{1}$-norm. Two key ingredients are adopted in our proof: one is to adopt an unconditional $L^{2}$-stability of the numerical flow in order to avoid an a priori estimate of the numerical solution for the case of $0<\sigma \leq \frac{1}{2}$, and to establish an $l^{\infty}$-conditional $H^{1}$-stability to obtain the $l^{\infty}$-bound of the numerical solution by using the mathematical induction and the error estimates for the case of $\sigma \geq \frac{1}{2}$; and the other one is to introduce a regularization technique to avoid the singularity of the semismooth nonlinearity in obtaining improved local truncation errors. Finally, numerical results are reported to demonstrate our error bounds.


## 1. Introduction

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

$$
\begin{equation*}
i \partial_{t} \psi(\mathbf{x}, t)=-\Delta \psi(\mathbf{x}, t)+V(\mathbf{x}) \psi(\mathbf{x}, t)+f\left(|\psi(\mathbf{x}, t)|^{2}\right) \psi(\mathbf{x}, t), \quad \mathbf{x} \in \Omega, \quad t>0 \tag{1.1}
\end{equation*}
$$

with the initial data

$$
\begin{equation*}
\psi(\mathbf{x}, 0)=\psi_{0}(\mathbf{x}), \quad \mathbf{x} \in \bar{\Omega} \tag{1.2}
\end{equation*}
$$

and the homogeneous Dirichlet boundary condition

$$
\begin{equation*}
\psi(\mathbf{x}, t)=0, \quad \mathbf{x} \in \partial \Omega, \quad t \geq 0 \tag{1.3}
\end{equation*}
$$

where $t$ is time, $\mathbf{x} \in \mathbb{R}^{d}(d=1,2,3)$ is the spatial coordinate, $\psi:=\psi(\mathbf{x}, t)$ is a complex-valued wave function, and $V:=V(\mathbf{x}): \Omega \rightarrow \mathbb{R}$ is a time-independent

[^0]real-valued potential. Here $\Omega=\Pi_{i=1}^{d}\left(a_{i}, b_{i}\right) \subset \mathbb{R}^{d}$ is a bounded domain, and the nonlinearity is given as
\[

$$
\begin{equation*}
f(\rho)=\beta \rho^{\sigma}, \quad \rho:=|\psi|^{2} \geq 0 \tag{1.4}
\end{equation*}
$$

\]

where $\beta \in \mathbb{R}$ is a given constant and $\sigma>0$ is the exponent of the nonlinearity. The NLSE (1.1) conserves the mass

$$
\begin{equation*}
M(\psi(\cdot, t))=\int_{\Omega}|\psi(\mathbf{x}, t)|^{2} \mathrm{~d} \mathbf{x} \equiv M\left(\psi_{0}\right), \quad t \geq 0 \tag{1.5}
\end{equation*}
$$

and the energy

$$
\begin{align*}
E(\psi(\cdot, t)) & =\int_{\Omega}\left[|\nabla \psi(\mathbf{x}, t)|^{2}+V(\mathbf{x})|\psi(\mathbf{x}, t)|^{2}+F\left(|\psi(\mathbf{x}, t)|^{2}\right)\right] \mathrm{d} \mathbf{x}  \tag{1.6}\\
& \equiv E\left(\psi_{0}\right), \quad t \geq 0
\end{align*}
$$

where the interaction energy density $F(\rho)$ is given as

$$
\begin{equation*}
F(\rho)=\int_{0}^{\rho} f(s) \mathrm{d} s=\frac{\beta}{\sigma+1} \rho^{\sigma+1}, \quad \rho \geq 0 \tag{1.7}
\end{equation*}
$$

When $\sigma=1$ in (1.4), i.e. $f(\rho)=\beta \rho$ and $F(\rho)=\frac{\beta}{2} \rho^{2}$, (1.1) collapses to the wellknown nonlinear Schrödinger equation with cubic nonlinearity (or smooth nonlinearity), also known as the Gross-Pitaevskii equation (GPE), which has been widely adopted for modeling and simulation in quantum mechanics, nonlinear optics, and Bose-Einstein condensation [6, 23, 44]. Arising from different physics applications, semi-smooth nonlinearity is introduced in the NLSE (1.1), i.e. $\sigma$ is taken as a noninteger in (1.4). Typical examples include, in the Schrödinger-Poisson- $\mathrm{X} \alpha$ model with $f(\rho)=-\alpha \rho^{1 / d}(\alpha>0)[14,16]$, i.e. $\sigma=\frac{1}{3}$ and $\sigma=\frac{1}{2}$ in three dimensions (3D) and two dimensions (2D), respectively; in the LHY correction (a next-order correction of the ground state energy proposed by Lee, Huang and Yang in 1957 [32]) for a beyond-mean-field term which is widely adopted in modeling and simulation for quantum droplets $[29,17,4,39,27]$ with $f(\rho)=\rho^{3 / 2}$ in 3 D , i.e. $\sigma=\frac{3}{2}$, $f(\rho)=\sqrt{\rho}$ in one dimension (1D), i.e. $\sigma=\frac{1}{2}$, and $f(\rho)=\rho \ln \rho$ in 2D; and in the mean field model for Bose-Fermi mixture [24, 18], with $f(\rho)=\rho^{2 / 3}$, i.e. $\sigma=\frac{2}{3}$. For all the aforementioned nonlinearities (actually for all $\sigma>0$ when $d=1,2,3$ ), the NLSE (1.1) is well-posed in $H^{2}$ under suitable assumptions on $V$, e.g. $V \in L^{p}$ with $p \geq 1$ and $p>d / 2[30,19]$. However, to our best knowledge, there is no guarantee of higher regularity to be propagated due to the low regularity of the semi-smooth nonlinearity, which is similar to the case of the logarithmic Schrödinger equation (LogSE) $[9,10,11]$. In fact, similar to the LogSE, the low regularity of the solution of the NLSE with semi-smooth nonlinearity is mainly due to the low regularity of the nonlinearity. We remark here that the potential $V$ could also be a source of low regularity of the solution, however, we will not consider the low regularity of $V$ in this paper but leave it as our future work.

For the cubic NLSE, i.e. $\sigma=1$, many accurate and efficient numerical methods have been proposed and analyzed in the last two decades, including the finite difference method $[1,7,6,3]$, the exponential wave integrator $[8,26,20]$, the timesplitting method $[13,15,33,22,6,34,3]$, the finite element method $[2,42,45,46,25]$, etc. Recently, new low regularity integrators or resonance based Fourier integrators are designed and analyzed for the cubic NLSE with low regularity initial data since the important work by Ostermann and Schratz [36], followed by [31, 35, 41, 38, 37]
and references therein for different dispersive partial differential equations. For all these numerical methods, optimal error bounds were rigorously established under different regularity assumptions of the cubic NLSE.

Most numerical methods for the cubic NLSE can be extended straightforwardly to solve the NLSE (1.1) with non-integer $\sigma>0$, e.g. semi-smooth nonlinearity with $0<\sigma<1$, which is different from the NLSE with singular nonlinearity, where regularization may be needed $[9,10,11,12]$. However, due to the low regularity of solution of the NLSE (1.1) with semi-smooth nonlinearity and the low regularity of the semi-smooth nonlinearity (1.4) in the NLSE (1.1) which causes order reduction in local truncation errors and results in difficulties in obtaining stability estimates, error analysis for different numerical methods applied to (1.1) with non-integer $\sigma>0$ is a very subtle and challenging question! For example, first order temporal convergence of the finite difference method requires boundedness of the secondorder time derivative, which roughly requires the exact solution to be in $H^{4}$, which is beyond the regularity property of the NLSE (1.1) with semi-smooth nonlinearity. In fact, based on our numerical experiments with a smooth initial datum $\psi_{0}(x)=$ $x e^{-x^{2} / 2}$, it indicates that $\psi(\cdot, t) \notin H^{4}$ for $t>0$ and $\sigma$ small! Since the time-splitting methods usually need lower regularity requirements on the exact solution than the finite difference methods, in this work, we consider the time-splitting method and in particular the first-order Lie-Trotter splitting method due to the low regularity of the semi-smooth nonlinearity and the low regularity of the exact solution of (1.1).

Error estimates of the time-splitting methods with different orders for the cubic NLSE (i.e. $\sigma=1$ ) have been well understood and we refer the readers to [33, $22,34,3]$ and references therein. However, for the NLSE with non-integer $\sigma$, only limited results are established for the filtered Lie-Trotter splitting scheme which requires a strong CFL-type time step size restriction $\tau=O\left(h^{2}\right)$. In [28], first order convergence in $L^{2}$-norm is established for $H^{2}$-solution and $\sigma \geq 1 / 2$. Then generalized in [21], half order convergence in $L^{2}$-norm is established for $H^{1}$-solution and $\sigma>0$. These convergence rates are optimal with respect to the regularity assumptions on the exact solution. However, there are still some questions related to error estimates to be addressed: (i) it is unclear whether higher convergence order can be obtained for $H^{2}$-solution when $0<\sigma<1 / 2$; (ii) their results are established for the filtered Lie-Trotter scheme, which is a semi-discretization scheme with a specific strong CFL-type time step size restriction, and it loses mass conservation and time symmetric property in the discretized level; and (iii) there is no optimal error estimate in $H^{1}$-norm, which is the natural norm of the NLSE.

The main aim of this paper is to establish error estimates of the time-splitting sine pseudospectral (TSSP) method (2.13) for the NLSE (1.1) with semi-smooth nonlinearity. We remark here that the TSSP is a fully discrete scheme and it preserves many good properties of the original NLSE in the discretized level, including mass conservation and time symmetry as well as dispersion relation. When $0<\sigma \leq \frac{1}{2}$, under the assumption of $H^{2}$-solution of the NLSE, we prove error bounds at $O\left(\tau^{\frac{1}{2}+\sigma}+h^{1+2 \sigma}\right)$ in $L^{2}$-norm without any CFL-type time step size restriction, which also fill the gap between the results in [28, 21]. When $\sigma \geq 1 / 2$, under the assumption of $H^{2}$-solution again, we prove error bounds at $O\left(\tau+h^{2}\right)$ and $O\left(\tau^{\frac{1}{2}}+h\right)$ in $L^{2}$-norm and $H^{1}$-norm, respectively, with a very mild CFL-type time step size restriction, which generalize the result in [28] to the mass-conservative
fully discrete scheme. In addition, when $\frac{1}{2}<\sigma<1$ and under the assumption of $H^{3}$-solution, we show a new error bound at $O\left(\tau^{\sigma}+h^{2 \sigma}\right)$ in $H^{1}$-norm.

The rest of the paper is organized as follows. In Section 2, we present the timesplitting sine pseudospectral (TSSP) method, introduce a local regularization for the semi-smooth nonlinearity to be used for obtaining improved local truncation errors and state our main results. Section 3 is devoted to error estimates of the TSSP method for $0<\sigma \leq 1 / 2$ and Section 4 is devoted to error estimates for $\sigma \geq 1 / 2$. 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 the corresponding norms, and denote by $C$ a generic positive constant independent of the mesh size $h$, time step $\tau$, and by $C(\alpha)$ a generic positive constant depending on $\alpha$. The notation $A \lesssim B$ is used to represent that there exists a generic constant $C>0$, such that $|A| \leq C B$.

## 2. Numerical methods and main results

2.1. The TSSP method. We shall use the Lie-Trotter splitting method for the temporal discretization and use the sine pseudospectral method for the spatial discretization. The operator splitting technique is based on the decomposition of the flow of (1.1)

$$
\begin{equation*}
\partial_{t} \psi=A(\psi)+B(\psi), \tag{2.1}
\end{equation*}
$$

where

$$
\begin{equation*}
A(\psi)=i \Delta \psi, \quad B(\psi)=B_{1}(\psi)+B_{2}(\psi):=-i V \psi-i f\left(|\psi|^{2}\right) \psi \tag{2.2}
\end{equation*}
$$

into two sub-problems. The first one is

$$
\left\{\begin{array}{l}
\partial_{t} \psi(\mathbf{x}, t)=A(\psi)=i \Delta \psi(\mathbf{x}, t), \quad \mathbf{x} \in \Omega, \quad t>0  \tag{2.3}\\
\psi(\mathbf{x}, 0)=\psi_{0}(\mathbf{x}), \quad \mathbf{x} \in \bar{\Omega}
\end{array}\right.
$$

which can be formally integrated exactly in time as

$$
\begin{equation*}
\psi(\cdot, t)=e^{i t \Delta} \psi_{0}(\cdot), \quad t \geq 0 \tag{2.4}
\end{equation*}
$$

The second one is to solve

$$
\left\{\begin{array}{l}
\partial_{t} \psi(\mathbf{x}, t)=B(\psi)=-i V(\mathbf{x}) \psi(\mathbf{x}, t)-i f\left(|\psi(\mathbf{x}, t)|^{2}\right) \psi(\mathbf{x}, t), \quad \mathbf{x} \in \Omega, t>0  \tag{2.5}\\
\psi(\mathbf{x}, 0)=\psi_{0}(\mathbf{x}), \quad \mathbf{x} \in \bar{\Omega}
\end{array}\right.
$$

which, by using the fact $|\psi(\mathbf{x}, t)|=\left|\psi_{0}(\mathbf{x})\right|$ for $t \geq 0$, can be integrated exactly in time as

$$
\begin{equation*}
\psi(\mathbf{x}, t)=\Phi_{B}^{t}\left(\psi_{0}\right):=e^{-i t V(\mathbf{x})} \Phi_{B_{2}}^{t}\left(\psi_{0}(\mathbf{x})\right), \quad \mathbf{x} \in \bar{\Omega}, \quad t \geq 0 \tag{2.6}
\end{equation*}
$$

where

$$
\begin{equation*}
\Phi_{B_{2}}^{t}(z)=z e^{-i t f\left(|z|^{2}\right)}, \quad z \in \mathbb{C}, \quad t \geq 0 \tag{2.7}
\end{equation*}
$$

In fact, in the second subproblem (2.5), the operator $B(\psi)=-i\left(V+f\left(\left|\psi_{0}\right|^{2}\right)\right) \psi$ becomes a bounded linear operator.

Choose a time step size $\tau>0$, denote time steps as $t_{k}=k \tau$ for $k=0,1, \ldots$, and let $\psi^{[k]}:=\psi^{[k]}(\mathbf{x})$ be the approximation of $\psi\left(\mathbf{x}, t_{k}\right)$ for $k \geq 0$. Then a first order semi-discretization of the NLSE (1.1) via the Lie-Trotter splitting is given as:

$$
\begin{equation*}
\psi^{[k+1]}=e^{i \tau \Delta} \Phi_{B}^{\tau}\left(\psi^{[k]}\right), \tag{2.8}
\end{equation*}
$$

with $\psi^{[0]}(\mathbf{x})=\psi_{0}(\mathbf{x})$ for $\mathbf{x} \in \bar{\Omega}$.

Then we discretize (2.8) in space by the sine pseudospectral method to obtain a full discretization for the NLSE (1.1). For simplicity of notations, here we only present the spatial discretization in 1D (taking $\Omega=(a, b)$ ), and the generalization to higher dimensions is straightforward. Choose a mesh size $h=(b-a) / N$ with $N$ being a positive integer and denote grid points as

$$
x_{j}=a+j h, \quad j=0,1, \cdots, N .
$$

Define the index sets

$$
\mathcal{T}_{N}=\{1,2, \cdots, N-1\}, \quad \mathcal{T}_{N}^{0}=\{0,1, \cdots, N\}
$$

and denote

$$
\begin{gather*}
X_{N}=\operatorname{span}\left\{\sin \left(\mu_{l}(x-a)\right): l \in \mathcal{T}_{N}\right\}, \quad \mu_{l}=\frac{\pi l}{b-a},  \tag{2.9}\\
Y_{N}=\left\{v=\left(v_{0}, v_{1}, \cdots, v_{N}\right)^{T} \in \mathbb{C}^{N+1}: v_{0}=v_{N}=0\right\}
\end{gather*}
$$

We define the $l^{p}(1 \leq p \leq \infty)$ norm on $Y_{N}$ as

$$
\|v\|_{l^{p}}=\left(h \sum_{j=0}^{N-1}\left|v_{j}\right|^{p}\right)^{\frac{1}{p}}, \quad 1 \leq p<\infty, \quad\|v\|_{l^{\infty}}=\max _{0 \leq j \leq N-1}\left|v_{j}\right|, \quad v \in Y_{N}
$$

We shall sometimes identify a function $\phi(\cdot) \in C_{0}(\bar{\Omega})$ with a vector $\phi=\left(\phi_{0}, \phi_{1}, \cdots\right.$, $\left.\phi_{N}\right)^{T} \in Y_{N}$ with $\phi_{j}=\phi\left(x_{j}\right)$ and then the discrete norm $\|\cdot\|_{l^{p}}$ can also be defined on $X_{N}$. For $v \in Y_{N}$, we define the forward finite difference operator as

$$
\begin{equation*}
\left(\delta_{x}^{+} v\right)_{j}=\delta_{x}^{+} v_{j}=\frac{v_{j+1}-v_{j}}{h}, \quad 0 \leq j \leq N-1 \tag{2.10}
\end{equation*}
$$

Let $P_{N}: L^{2}(\Omega) \rightarrow X_{N}$ be the standard $L^{2}$ projection onto $X_{N}$ and $I_{N}: Y_{N} \rightarrow X_{N}$ be the standard sine interpolation operator as

$$
\begin{align*}
& \left(P_{N} v\right)(x)=\sum_{l \in \mathcal{T}_{N}} \widehat{v}_{l} \sin \left(\mu_{l}(x-a)\right), \\
& \left(I_{N} w\right)(x)=\sum_{l \in \mathcal{T}_{N}} \widetilde{w}_{l} \sin \left(\mu_{l}(x-a)\right), \quad x \in \bar{\Omega}=[a, b]
\end{align*}
$$

where $v \in L^{2}(\Omega), w \in Y_{N}$, and

$$
\begin{align*}
& \widehat{v}_{l}=\frac{2}{b-a} \int_{a}^{b} v(x) \sin \left(\mu_{l}(x-a)\right) \mathrm{d} x \\
& \widetilde{w}_{l}=\frac{2}{N} \sum_{j \in \mathcal{T}_{N}} w_{j} \sin (j \pi l / N) \tag{2.12}
\end{align*}
$$

Let $\psi_{j}^{k}$ be the numerical approximations of $\psi\left(x_{j}, t_{k}\right)$ for $j \in \mathcal{T}_{N}^{0}$ and $k \geq 0$, and denote $\psi^{k}:=\left(\psi_{0}^{k}, \psi_{1}^{k}, \ldots, \psi_{N}^{k}\right)^{T} \in Y_{N}$. Then the time-splitting sine pseudospectral (TSSP) method for discretizing the NLSE (1.1) can be given for $k \geq 0$ as

$$
\begin{align*}
& \psi_{j}^{(1)}=e^{-i \tau\left(V\left(x_{j}\right)+f\left(\left|\psi_{j}^{k}\right|^{2}\right)\right)} \psi_{j}^{k} \\
& \psi_{j}^{k+1}=\sum_{l \in \mathcal{T}_{N}} e^{-i \tau \mu_{l}^{2}} \widetilde{\left(\psi^{(1)}\right)_{l}} \sin \left(\mu_{l}\left(x_{j}-a\right)\right), \quad j \in \mathcal{T}_{N}^{0} \tag{2.13}
\end{align*}
$$

where $\psi_{j}^{0}=\psi_{0}\left(x_{j}\right)$ for $j \in \mathcal{T}_{N}^{0}$.

Let $\Phi^{\tau}: X_{N} \rightarrow X_{N}$ be the numerical integrator defined as

$$
\begin{equation*}
\Phi^{\tau}(\phi)=e^{i \tau \Delta} I_{N} \Phi_{B}^{\tau}(\phi), \quad \phi \in X_{N} \tag{2.14}
\end{equation*}
$$

where $\Phi_{B}^{\tau}$ is defined in (2.6). Then one has

$$
\begin{align*}
& I_{N} \psi^{k+1}=\Phi^{\tau}\left(I_{N} \psi^{k}\right), \quad k \geq 0 \\
& I_{N} \psi^{0}=I_{N} \psi_{0} \tag{2.15}
\end{align*}
$$

Remark 2.1. In applications, the NLSE (1.1) can also be discretized by the LieTrotter splitting via a different order as:

$$
\begin{equation*}
\psi^{[k+1]}=\Phi_{B}^{\tau}\left(e^{i \tau \Delta} \psi^{[k]}\right), \quad k \geq 0 . \tag{2.16}
\end{equation*}
$$

Then a full discretization can be obtained straightforward by using the sine pseudospectral method in space.
2.2. A local regularization for $f(\rho)=\beta \rho^{\sigma}(\beta \in \mathbb{R})$. When $0<\sigma<1$ in (1.4), $f(\rho)$ is a semi-smooth function and it is not differentiable at $\rho=0$. Here, we want to regularize it to obtain higher order local error estimates later. Following the regularization methods used in [11] for the logarithmic Schrödinger equation, we regularize the semi-smooth nonlinearity $f(\rho)$ only locally in a small region near $\rho=0$. Taking $0<\varepsilon \ll 1$ as a regularization parameter, we approximate $f(\rho)$ locally in the region $\left\{\rho<\varepsilon^{2}\right\}$ by a polynomial and leave it unchanged in $\left\{\rho \geq \varepsilon^{2}\right\}$, i.e.

$$
f_{\varepsilon}(\rho)=\left\{\begin{array}{lr}
f(\rho), & \rho \geq \varepsilon^{2}  \tag{2.17}\\
\rho Q_{\varepsilon}(\rho), & 0 \leq \rho<\varepsilon^{2}
\end{array}\right.
$$

where $Q_{\varepsilon}(\rho)$ is a polynomial with degree at most 3 such that

$$
\begin{equation*}
f_{\varepsilon} \in C^{3}([0, \infty)) \tag{2.18}
\end{equation*}
$$

Note that $f_{\varepsilon}$ given by (2.17) is uniquely determined by the interpolation conditions (2.18) and it satisfies $f_{\varepsilon}(0)=f(0)=0$. Actually, the explicit formula of $Q_{\varepsilon}(\rho)$ can be given as

$$
\begin{equation*}
Q_{\varepsilon}(\rho)=\beta \varepsilon^{2 \sigma-2} \sum_{j=0}^{3}\binom{j-\sigma}{j}\left(1-\frac{\rho}{\varepsilon^{2}}\right)^{j}, \quad 0 \leq \rho<\varepsilon^{2} \tag{2.19}
\end{equation*}
$$

In fact, $f_{\varepsilon} \in C^{3}([0, \infty))$ can be regarded as a local regularization of the semismooth nonlinearity $f(\rho) \in C^{0}([0, \infty))$, which has much better regularity near $\rho=0$. For $f_{\varepsilon}$, we have the following estimates.

Lemma 2.2. When $0<\sigma<1$, we have

$$
\begin{align*}
&\left|f_{\varepsilon}(\rho)\right|+\left|\rho f_{\varepsilon}^{\prime}(\rho)\right| \leq C_{1} \rho^{\sigma}, \rho \geq 0  \tag{2.20}\\
&\left|\sqrt{\rho} f_{\varepsilon}^{\prime}(\rho)\right|+\left|\rho^{\frac{3}{2}} f_{\varepsilon}^{\prime \prime}(\rho)\right| \leq C_{2}\left\{\begin{array}{ll}
\frac{1}{\varepsilon^{1-2 \sigma}}, & 0<\sigma \leq \frac{1}{2} \\
\rho^{\sigma-\frac{1}{2}}, & \frac{1}{2}<\sigma<1
\end{array}, \quad \rho \geq 0\right. \tag{2.21}
\end{align*}
$$

and

$$
\begin{equation*}
\left|f_{\varepsilon}^{\prime}(\rho)\right|+\left|\rho f_{\varepsilon}^{\prime \prime}(\rho)\right|+\left|\rho^{2} f_{\varepsilon}^{\prime \prime \prime}(\rho)\right| \leq \frac{C_{3}}{\varepsilon^{2-2 \sigma}}, \quad \rho \geq 0 \tag{2.22}
\end{equation*}
$$

where $C_{1}, C_{2}$ and $C_{3}$ depend exclusively on $\sigma$ and $\beta$.

Proof. When $\rho \geq \varepsilon^{2}$, by (2.17), we have $f^{(k)}(\rho)=f_{\varepsilon}^{(k)}(\rho)$ for $0 \leq k \leq 3$, and (2.20)-(2.22) follows immediately from $f(\rho)=\beta \rho^{\sigma}$ and $0<\varepsilon<1$.

In the following, we assume that $0 \leq \rho<\varepsilon^{2}$. From (2.19), we easily obtain that

$$
\begin{equation*}
\left|Q_{\varepsilon}^{(k)}(\rho)\right| \lesssim \varepsilon^{2 \sigma-2-2 k}, \quad 0 \leq \rho<\varepsilon^{2}, \quad 0 \leq k \leq 3 \tag{2.23}
\end{equation*}
$$

From (2.17), using (2.23), one gets

$$
\begin{equation*}
\left|f_{\varepsilon}(\rho)\right| \leq \rho\left|Q_{\varepsilon}(\rho)\right| \lesssim \rho \varepsilon^{2 \sigma-2}=\rho^{\sigma}\left(\frac{\rho}{\varepsilon^{2}}\right)^{1-\sigma} \leq \rho^{\sigma} \tag{2.24}
\end{equation*}
$$

Similarly, one has

$$
\begin{equation*}
\left|\rho f_{\varepsilon}^{\prime}(\rho)\right| \leq\left|\rho^{2} Q_{\varepsilon}^{\prime}(\rho)\right|+\left|\rho Q_{\varepsilon}(\rho)\right| \lesssim\left(\frac{\rho}{\varepsilon^{2}}+1\right) \rho \varepsilon^{2 \sigma-2} \leq 2 \rho^{\sigma} \tag{2.25}
\end{equation*}
$$

which proves (2.20).
Recalling (2.17), using (2.23), one gets, when $0<\sigma<1$,

$$
\begin{align*}
\left|\sqrt{\rho} f_{\varepsilon}^{\prime}(\rho)\right| \leq \rho^{\frac{1}{2}}\left(\left|Q_{\varepsilon}(\rho)\right|+\rho\left|Q_{\varepsilon}{ }^{\prime}(\rho)\right|\right) & \lesssim \varepsilon\left(\varepsilon^{2 \sigma-2}+\varepsilon^{2} \varepsilon^{2 \sigma-4}\right) \lesssim \varepsilon^{2 \sigma-1}  \tag{2.26a}\\
\left|\sqrt{\rho} f_{\varepsilon}^{\prime}(\rho)\right| \leq \rho^{\frac{1}{2}}\left(\left|Q_{\varepsilon}(\rho)\right|+\rho\left|Q_{\varepsilon}{ }^{\prime}(\rho)\right|\right) & \lesssim \rho^{\frac{1}{2}} \varepsilon^{2 \sigma-2} \\
& =\rho^{\sigma-\frac{1}{2}}\left(\frac{\rho}{\varepsilon^{2}}\right)^{1-\sigma} \leq \rho^{\sigma-\frac{1}{2}} \tag{2.26~b}
\end{align*}
$$

Using (2.26a) when $0<\sigma \leq 1 / 2$ and using (2.26b) when $1 / 2<\sigma<1$, we obtain the desired estimate for $\left|\sqrt{\rho} f_{\varepsilon}^{\prime}(\rho)\right|$. The estimate of $\left|\rho^{\frac{3}{2}} f_{\varepsilon}^{\prime \prime}(\rho)\right|$ can be obtained similarly, which completes the proof of (2.21).

For (2.22), using (2.23) again, one has

$$
\begin{equation*}
\left|f_{\varepsilon}^{\prime}(\rho)\right| \leq\left|Q_{\varepsilon}(\rho)\right|+\rho\left|Q_{\varepsilon}^{\prime}(\rho)\right| \lesssim \varepsilon^{2 \sigma-2}+\varepsilon^{2} \varepsilon^{2 \sigma-4} \lesssim \varepsilon^{2 \sigma-2} \tag{2.27}
\end{equation*}
$$

The estimate of $\left|\rho f_{\varepsilon}^{\prime \prime}(\rho)\right|$ and $\left|\rho^{2} f_{\varepsilon}^{\prime \prime \prime}(\rho)\right|$ can be obtained similarly, which completes the proof of (2.22).

Corollary 2.3. When $0<\sigma \leq 1 / 2$, we have

$$
\begin{align*}
& \left\|f_{\varepsilon}\left(|v|^{2}\right) v\right\|_{L^{2}} \leq C_{1}\left(\|v\|_{L^{\infty}}\right)\|v\|_{L^{2}}, \quad v \in L^{\infty}(\Omega)  \tag{2.28}\\
& \left\|f_{\varepsilon}\left(|v|^{2}\right) v\right\|_{H^{1}} \leq C_{2}\left(\|v\|_{L^{\infty}}\right)\|v\|_{H^{1}}, \quad v \in H^{1}(\Omega) \cap L^{\infty}(\Omega)  \tag{2.29}\\
& \left\|f_{\varepsilon}\left(|v|^{2}\right) v\right\|_{H^{2}} \leq \frac{C_{3}\left(\|v\|_{H^{2}}\right)}{\varepsilon^{1-2 \sigma}}, \quad v \in H^{2}(\Omega) \tag{2.30}
\end{align*}
$$

When $0<\sigma<1$, we have

$$
\begin{equation*}
\left\|f_{\varepsilon}\left(|v|^{2}\right) v\right\|_{H^{3}} \leq \frac{C_{4}\left(\|v\|_{H^{3}}\right)}{\varepsilon^{2-2 \sigma}}, \quad v \in H^{3}(\Omega) \tag{2.31}
\end{equation*}
$$

Proof. By (2.20), one has

$$
\begin{equation*}
\left\|f_{\varepsilon}\left(|v|^{2}\right) v\right\|_{L^{2}} \leq\left\|f_{\varepsilon}\left(|v|^{2}\right)\right\|_{L^{\infty}}\|v\|_{L^{2}} \lesssim\|v\|_{L^{\infty}}^{2 \sigma}\|v\|_{L^{2}} \tag{2.32}
\end{equation*}
$$

which proves (2.28).
By direct calculation, using (2.20), one gets

$$
\begin{aligned}
\left\|\nabla\left(f_{\varepsilon}\left(|v|^{2}\right) v\right)\right\|_{L^{2}} & =\left\|f_{\varepsilon}\left(|v|^{2}\right) \nabla v+f_{\varepsilon}^{\prime}\left(|v|^{2}\right) v(v \nabla \bar{v}+\bar{v} \nabla v)\right\|_{L^{2}} \\
& \leq\left(\left\|f_{\varepsilon}\left(|v|^{2}\right)\right\|_{L^{\infty}}+\left\|f_{\varepsilon}^{\prime}\left(|v|^{2}\right) v^{2}\right\|_{L^{\infty}}+\left\|f_{\varepsilon}^{\prime}\left(|v|^{2}\right)|v|^{2}\right\|_{L^{\infty}}\right)\|\nabla v\|_{L^{2}} \\
& \lesssim\|v\|_{L^{\infty}}^{2 \sigma}\|v\|_{H^{1}}
\end{aligned}
$$

which shows (2.29).

To show (2.30), we note that

$$
\begin{align*}
\partial_{j k}\left(f_{\varepsilon}\left(|v|^{2}\right) v\right)= & \partial_{j}\left[\left(f_{\varepsilon}\left(|v|^{2}\right)+f_{\varepsilon}^{\prime}\left(|v|^{2}\right)|v|^{2}\right) \partial_{k} v+f_{\varepsilon}^{\prime}\left(|v|^{2}\right) v^{2} \partial_{k} \bar{v}\right] \\
= & \left(2 f_{\varepsilon}^{\prime}\left(|v|^{2}\right)+f_{\varepsilon}^{\prime \prime}\left(|v|^{2}\right)|v|^{2}\right) \partial_{j}|v|^{2} \partial_{k} v+\left(f_{\varepsilon}\left(|v|^{2}\right)+f_{\varepsilon}^{\prime}\left(|v|^{2}\right)|v|^{2}\right) \partial_{j k} v \\
& +f_{\varepsilon}^{\prime \prime}\left(|v|^{2}\right) v^{2} \partial_{j}|v|^{2} \partial_{k} \bar{v}+2 f_{\varepsilon}^{\prime}\left(|v|^{2}\right) v \partial_{j} v \partial_{k} \bar{v}+f_{\varepsilon}^{\prime}\left(|v|^{2}\right) v^{2} \partial_{j k} \bar{v}, \tag{2.34}
\end{align*}
$$

where $\partial_{j}=\partial_{x_{j}}$ and $\partial_{j k}=\partial_{x_{j}} \partial_{x_{k}}$ for $1 \leq j, k \leq d$. Here we adopt the notations $\mathbf{x}=$ $x_{1}($ or $x)$ when $d=1, \mathbf{x}=\left(x_{1}, x_{2}\right)^{T}\left(\right.$ or $\left.(x, y)^{T}\right)$ when $d=2$, and $\mathbf{x}=\left(x_{1}, x_{2}, x_{3}\right)^{T}$ (or $(x, y, z)^{T}$ ) when $d=3$. From Lemma 2.2, using (2.20) and (2.21) and noting that $\left.\left|\partial_{j}\right| v\right|^{2}|\leq 2| v| | \partial_{j} v \mid$, one gets

$$
\begin{align*}
\left|\partial_{j k}\left(f_{\varepsilon}\left(|v|^{2}\right) v\right)\right| \lesssim & \left(f_{\varepsilon}^{\prime}\left(|v|^{2}\right)|v|+f_{\varepsilon}^{\prime \prime}\left(|v|^{2}\right)|v|^{3}\right)\left|\partial_{j} v\right|\left|\partial_{k} v\right| \\
& +\left(f_{\varepsilon}\left(|v|^{2}\right)+f_{\varepsilon}^{\prime}\left(|v|^{2}\right)|v|^{2}\right)\left|\partial_{j k} v\right| \\
\lesssim & \frac{\left|\partial_{j} v\right|\left|\partial_{k} v\right|}{\varepsilon^{1-2 \sigma}}+|v|^{2 \sigma}\left|\partial_{j k} v\right|, \tag{2.35}
\end{align*}
$$

which, by using Hölder's inequality and Sobolev embedding $H^{2} \hookrightarrow W^{1,4}$ which holds for $d=1,2,3$, yields

$$
\begin{equation*}
\left\|\partial_{j k}\left(f_{\varepsilon}\left(|v|^{2}\right) v\right)\right\|_{L^{2}} \lesssim \frac{\left\|\partial_{j} v\right\|_{L^{4}}\left\|\partial_{k} v\right\|_{L^{4}}}{\varepsilon^{1-2 \sigma}}+\|v\|_{L^{\infty}}^{2 \sigma}\left\|\partial_{j k} v\right\|_{L^{2}} \leq \frac{C\left(\|v\|_{H^{2}}\right)}{\varepsilon^{1-2 \sigma}} \tag{2.36}
\end{equation*}
$$

which implies (2.30).
Following Lemma 2.2, noting (2.35) and (2.36) and using (2.22), we can similarly obtain (2.31) and the details are omitted here for brevity.

Lemma 2.4. When $0<\sigma<1$, we have

$$
\left|f(\rho)-f_{\varepsilon}(\rho)\right| \leq C \varepsilon^{2 \sigma} \mathbb{1}_{\rho<\varepsilon^{2}}, \quad \rho \geq 0
$$

Proof. Recalling (2.17), we have

$$
\begin{equation*}
\left|f(\rho)-f_{\varepsilon}(\rho)\right|=0, \quad \rho \geq \varepsilon^{2} \tag{2.37}
\end{equation*}
$$

and, by (1.4) and (2.20),

$$
\begin{equation*}
\left|f(\rho)-f_{\varepsilon}(\rho)\right| \leq|f(\rho)|+\left|f_{\varepsilon}(\rho)\right| \lesssim \rho^{\sigma} \leq \varepsilon^{2 \sigma}, \quad 0 \leq \rho<\varepsilon^{2} \tag{2.38}
\end{equation*}
$$

which completes the proof.
2.3. Main results. Let $T_{\max }$ be the maximal existing time for the solution of the NLSE (1.1) with (1.2) and (1.3) and take $0<T<T_{\max }$ be a fixed time. Based on the known existence and regularity results (see Remark 4.8.7 (iii) in [19] or Theorem II in [30]) for the solution of (1.1), we make the assumption that the solution $\psi$ satisfies $\psi \in C\left([0, T] ; H_{0}^{1}(\Omega) \cap H^{2}(\Omega)\right) \cap C^{1}\left([0, T] ; L^{2}(\Omega)\right)$ such that

$$
\begin{equation*}
\|\psi\|_{L^{\infty}\left([0, T] ; H^{2}\right)}+\left\|\partial_{t} \psi\right\|_{L^{\infty}\left([0, T] ; L^{2}\right)} \lesssim 1 \tag{A}
\end{equation*}
$$

Note that the solution to (1.1) that satisfies (A) must be unique [25].
Define

$$
\begin{equation*}
M_{2}:=\max \left\{\|\psi\|_{L^{\infty}\left([0, T] ; H^{2}\right)},\|\psi\|_{L^{\infty}\left([0, T] ; L^{\infty}\right)},\|V\|_{H^{2}}\right\} \tag{2.39}
\end{equation*}
$$

and assume the following time step size restriction $(h<1)$

$$
\tau \lesssim \begin{cases}1, & d=1  \tag{B}\\ \frac{1}{|\ln h|^{2}}, & d=2 \\ h, & d=3\end{cases}
$$

For the TSSP method (2.13), we can establish the following error estimates.
Theorem 2.5. When $0<\sigma \leq 1 / 2$, under the assumptions $V \in H^{2}(\Omega)$ and (A), for $0<\tau<1$ and $0<h<1$, we have

$$
\begin{equation*}
\left\|\psi\left(\cdot, t_{k}\right)-I_{N} \psi^{k}\right\|_{L^{2}} \lesssim \tau^{1 / 2+\sigma}+h^{1+2 \sigma}, \quad 0 \leq k \leq \frac{T}{\tau} \tag{2.40}
\end{equation*}
$$

Corollary 2.6. When $d=1$ and $0<\sigma \leq 1 / 2$, under the following much weaker assumptions

$$
V \in H^{1}(\Omega), \quad \psi \in C\left([0, T] ; H_{0}^{1}(\Omega)\right)
$$

we have for $0<\tau<1$ and $0<h<1$,

$$
\begin{equation*}
\left\|\psi\left(\cdot, t_{k}\right)-I_{N} \psi^{k}\right\|_{L^{2}} \lesssim \tau^{1 / 2}+h, \quad 0 \leq k \leq \frac{T}{\tau} \tag{2.41}
\end{equation*}
$$

Theorem 2.7. When $\sigma \geq 1 / 2$, under the assumptions $V \in H^{2}(\Omega) \cap W^{1, \infty}(\Omega)$ and (A), there exist $\tau_{0}>0$ and $h_{0}>0$ sufficiently small and depending on $M_{2}$, $\|V\|_{W^{1, \infty}}$ and $T$ such that for $\tau \leq \tau_{0}$ and $h \leq h_{0}$ satisfying (B), we have

$$
\begin{align*}
& \left\|\psi\left(\cdot, t_{k}\right)-I_{N} \psi^{k}\right\|_{L^{2}} \lesssim \tau+h^{2}, \quad\left\|\psi^{k}\right\|_{l^{\infty}} \leq 1+M_{2} \\
& \left\|\psi\left(\cdot, t_{k}\right)-I_{N} \psi^{k}\right\|_{H^{1}} \lesssim \tau^{\frac{1}{2}}+h, \quad 0 \leq k \leq \frac{T}{\tau} \tag{2.42}
\end{align*}
$$

Moreover, when $1 / 2<\sigma<1$, under the additional assumptions that $V \in H^{3}(\Omega)$, $\nabla V \in H_{0}^{1}(\Omega)$ and $\psi \in C\left([0, T] ; H_{*}^{3}(\Omega)\right) \cap C^{1}\left([0, T] ; H^{1}(\Omega)\right)$, we have

$$
\begin{equation*}
\left\|\psi\left(\cdot, t_{k}\right)-I_{N} \psi^{k}\right\|_{H^{1}} \lesssim \tau^{\sigma}+h^{2 \sigma}, \quad 0 \leq k \leq \frac{T}{\tau} \tag{2.43}
\end{equation*}
$$

where $H_{*}^{3}(\Omega):=\left\{\phi \in H^{3}(\Omega)|\phi(\mathbf{x})|_{\partial \Omega}=\left.\Delta \phi(\mathbf{x})\right|_{\partial \Omega}=0\right\}$.
Remark 2.8. When $\sigma \geq 1$, under the same assumptions as those for (2.43), one can obtain the following error bound for the TSSP method (2.13) as

$$
\left\|\psi\left(\cdot, t_{k}\right)-I_{N} \psi^{k}\right\|_{H^{1}} \lesssim \tau+h^{2}, \quad 0 \leq k \leq \frac{T}{\tau}
$$

3. Proof of Theorem 2.5 for the case $0<\sigma \leq 1 / 2$

Throughout this section, we assume that $V \in H^{2}(\Omega), 0<\sigma \leq 1 / 2$ and the assumption (A).
3.1. Some estimates for the operator $B$. For the operator $B$ defined in (2.2), we have

Lemma 3.1. Let $v \in H^{1}(\Omega)$ such that $\|v\|_{L^{\infty}} \leq M$. When $\sigma>0$, we have

$$
\begin{align*}
& \|B(v)\|_{L^{2}} \leq C_{1}\left(M,\|V\|_{L^{\infty}}\right)\|v\|_{L^{2}},  \tag{3.1}\\
& \|B(v)\|_{H^{1}} \leq\|v\|_{H^{1}} \begin{cases}C_{2}\left(M,\|V\|_{H^{1}}\right), & d=1 \\
C_{2}\left(M,\|V\|_{W^{1,4}}\right), & d=2,3\end{cases} \tag{3.2}
\end{align*}
$$

Proof. From the definition of $B$ in (2.2), we have

$$
\begin{equation*}
\|B(v)\|_{L^{2}} \leq\|V\|_{L^{\infty}}\|v\|_{L^{2}}+C\left(\|v\|_{L^{\infty}}\right)\|v\|_{L^{2}} \tag{3.3}
\end{equation*}
$$

which implies (3.1).

Introduce a continuous function $G: \mathbb{C} \rightarrow \mathbb{C}$ as

$$
G(z)=\left\{\begin{array}{ll}
f^{\prime}\left(|z|^{2}\right) z^{2}=\beta \sigma|z|^{2 \sigma-2} z^{2}, & z \neq 0  \tag{3.4}\\
0, & z=0,
\end{array} \quad z \in \mathbb{C}\right.
$$

and note that $f^{\prime}\left(|z|^{2}\right)|z|^{2}=\sigma f\left(|z|^{2}\right)$ for $z \in \mathbb{C}$. Further note that

$$
\begin{equation*}
f\left(|z|^{2}\right)+|G(z)| \lesssim|z|^{2 \sigma}, \quad z \in \mathbb{C}, \quad \sigma>0 \tag{3.5}
\end{equation*}
$$

Direct calculation yields

$$
\begin{align*}
\nabla B(v) & =-i\left[V \nabla v+v \nabla V+f\left(|v|^{2}\right) \nabla v+f^{\prime}\left(|v|^{2}\right) v(v \nabla \bar{v}+\bar{v} \nabla v)\right] \\
& =-i\left[V \nabla v+v \nabla V+(1+\sigma) f\left(|v|^{2}\right) \nabla v+G(v) \nabla \bar{v}\right] \tag{3.6}
\end{align*}
$$

where $G(v)(\mathbf{x}):=G(v(\mathbf{x}))$ for $\mathbf{x} \in \Omega$. From (3.6), using Hölder's inequality and noticing (3.5), we obtain

$$
\|\nabla B(v)\|_{L^{2}} \lesssim\|V\|_{L^{\infty}}\|\nabla v\|_{L^{2}}+\|v\|_{L^{\infty}}^{2 \sigma}\|\nabla v\|_{L^{2}}+\left\{\begin{array}{ll}
\|v\|_{L^{\infty}}\|\nabla V\|_{L^{2}}, & d=1  \tag{3.7}\\
\|v\|_{L^{4}}\|\nabla V\|_{L^{4}}, & d=2,3
\end{array},\right.
$$

where different estimates are used for $v \nabla V$ for $d=1$ and $d=2,3$. Thus we have, by Sobolev embedding $H^{1} \hookrightarrow L^{\infty}$ when $d=1$ and $H^{1} \hookrightarrow L^{4}$ when $d=2,3$,

$$
\|\nabla B(v)\|_{L^{2}} \leq C\left(\|v\|_{L^{\infty}}\right)\|v\|_{H^{1}}+\|v\|_{H^{1}} \begin{cases}C\left(\|V\|_{H^{1}}\right), & d=1 \\ C\left(\|V\|_{W^{1,4}}\right), & d=2,3\end{cases}
$$

which completes the proof.
Lemma 3.2. Let $v, w \in L^{\infty}(\Omega)$ such that $\|v\|_{L^{\infty}} \leq M$ and $\|w\|_{L^{\infty}} \leq M$. When $\sigma>0$, we have

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

Proof. Recalling (2.2), we have

$$
\begin{equation*}
\|B(v)-B(w)\|_{L^{2}} \leq\|V\|_{L^{\infty}}\|v-w\|_{L^{2}}+\left\|f\left(|v|^{2}\right) v-f\left(|w|^{2}\right) w\right\|_{L^{2}} \tag{3.8}
\end{equation*}
$$

For any $z_{1}, z_{2} \in \mathbb{C}$, let $z_{\theta}=(1-\theta) z_{1}+\theta z_{2}$ and let $\gamma(\theta)=f\left(\left|z_{\theta}\right|^{2}\right) z_{\theta}$ for $0 \leq \theta \leq 1$, we have

$$
\begin{equation*}
f\left(\left|z_{2}\right|^{2}\right) z_{2}-f\left(\left|z_{1}\right|^{2}\right) z_{1}=\gamma(1)-\gamma(0)=\int_{0}^{1} \gamma^{\prime}(\theta) \mathrm{d} \theta \tag{3.9}
\end{equation*}
$$

Recalling (1.4) and (3.4), we have

$$
\begin{equation*}
\gamma^{\prime}(\theta)=(1+\sigma) f\left(\left|z_{\theta}\right|^{2}\right)\left(z_{2}-z_{1}\right)+G\left(z_{\theta}\right) \overline{\left(z_{2}-z_{1}\right)} \tag{3.10}
\end{equation*}
$$

Plugging (3.10) into (3.9), noticing (3.5), we have

$$
\begin{equation*}
\left|f\left(\left|z_{1}\right|^{2}\right) z_{1}-f\left(\left|z_{2}\right|^{2}\right) z_{2}\right| \leq \sup _{0 \leq \theta \leq 1}\left|\gamma^{\prime}(\theta)\right| \lesssim \max \left\{\left|z_{1}\right|,\left|z_{2}\right|\right\}^{2 \sigma}\left|z_{1}-z_{2}\right| \tag{3.11}
\end{equation*}
$$

Thus we have

$$
\begin{equation*}
\left\|f\left(|v|^{2}\right) v-f\left(|w|^{2}\right) w\right\|_{L^{2}} \leq C\left(\max \left\{\|v\|_{L^{\infty}},\|w\|_{L^{\infty}}\right\}\right)\|v-w\|_{L^{2}} \tag{3.12}
\end{equation*}
$$

which plugged into (3.8) completes the proof.

Let $d B(\cdot)[\cdot]$ be the Gâteaux derivative defined as

$$
\begin{equation*}
d B(v)[w]:=\lim _{\varepsilon \rightarrow 0} \frac{B(v+\varepsilon w)-B(v)}{\varepsilon} \tag{3.13}
\end{equation*}
$$

where the limit is taken for real $\varepsilon$, and we identify $\mathbb{C}$ with $\mathbb{R}^{2}$ to be consistent with the complex valued setting (see also the appendix in [30]). Then we have

Lemma 3.3. Let $v \in L^{\infty}(\Omega)$ such that $\|v\|_{L^{\infty}} \leq M$ and $w \in L^{2}(\Omega)$. When $\sigma>0$, we have

$$
\|d B(v)[w]\|_{L^{2}} \leq C\left(M,\|V\|_{L^{\infty}}\right)\|w\|_{L^{2}} .
$$

Proof. Plugging (2.2) into (3.13), we obtain (see (4.26) in [11])

$$
\begin{align*}
d B(v)[w] & =-i V w+d B_{2}(v)[w] \\
& =-i\left[V w+(1+\sigma) f\left(|v|^{2}\right) w+G(v) \bar{w}\right] \tag{3.14}
\end{align*}
$$

where $G$ is defined in (3.4). From (3.14), noting (3.5), we have

$$
\|d B(v)[w]\|_{L^{2}} \leq\|V\|_{L^{\infty}}\|w\|_{L^{2}}+C\left(\|v\|_{L^{\infty}}\right)\|w\|_{L^{2}}
$$

which concludes the proof.
Lemma 3.4. When $0<\sigma \leq 1 / 2$, we have

$$
\left|\Phi_{B_{2}}^{\tau}\left(z_{1}\right)-\Phi_{B_{2}}^{\tau}\left(z_{2}\right)\right| \leq(1+C \tau)\left|z_{1}-z_{2}\right|, \quad z_{1}, z_{2} \in \mathbb{C}
$$

where $\Phi_{B_{2}}^{\tau}(z)=z e^{-i \tau f\left(|z|^{2}\right)}$ in (2.7) and $C=2 \sigma|\beta| \min \left\{\left|z_{1}\right|,\left|z_{2}\right|\right\}^{2 \sigma}$.
Proof. Without loss of generality, we assume that $\left|z_{2}\right| \leq\left|z_{1}\right|$. If $z_{2}=0$, the conclusion follows immediately. In the following, we assume that $z_{2} \neq 0$. Then, by noting that $\left|1-e^{i \theta}\right| \leq|\theta|$ for all $\theta \in \mathbb{R}$, we have

$$
\begin{align*}
\left|\Phi_{B_{2}}^{\tau}\left(z_{1}\right)-\Phi_{B_{2}}^{\tau}\left(z_{2}\right)\right| & =\left|z_{1} e^{-i \tau f\left(\left|z_{1}\right|^{2}\right)}-z_{2} e^{-i \tau f\left(\left|z_{2}\right|^{2}\right)}\right| \\
& \leq\left|z_{1}-z_{2}\right|+\left|z_{2}\right|\left|1-e^{-i \tau\left(f\left(\left|z_{1}\right|^{2}\right)-f\left(\left|z_{2}\right|^{2}\right)\right)}\right| \\
& \leq\left|z_{1}-z_{2}\right|+\tau\left|z_{2}\right|\left|f\left(\left|z_{1}\right|^{2}\right)-f\left(\left|z_{2}\right|^{2}\right)\right| \tag{3.15}
\end{align*}
$$

When $0<\sigma \leq 1 / 2$, since $0<\left|z_{2}\right| \leq\left|z_{1}\right|$, by the mean value theorem and the definition of $f$ in (1.4), we have

$$
\begin{align*}
\left|f\left(\left|z_{1}\right|^{2}\right)-f\left(\left|z_{2}\right|^{2}\right)\right| & =\left.|\beta|| | z_{1}\right|^{2 \sigma}-\left|z_{2}\right|^{2 \sigma} \mid \\
& \leq \frac{2 \sigma|\beta|\left|z_{1}-z_{2}\right|}{\min \left\{\left|z_{1}\right|,\left|z_{2}\right|\right\}^{1-2 \sigma}}=2 \sigma|\beta| \frac{\left|z_{1}-z_{2}\right|}{\left|z_{2}\right|^{1-2 \sigma}} . \tag{3.16}
\end{align*}
$$

Plugging (3.16) into (3.15), we get the desired result immediately.
3.2. Local truncation error. In this subsection, we shall prove the local truncation error estimates for the TSSP (2.13) in 1D, which can be directly generalized to 2 D and 3D. With the regularized function $f_{\varepsilon}$ introduced in Section 2.2, we can obtain $\sigma$ sensitive estimates as follows.

Lemma 3.5. Let $\phi \in X_{N}$ such that $\|\phi\|_{H^{2}} \leq M$ and let $0<\tau<1$ and $0<h<1$. Assume that $V \in H^{2}(\Omega)$. When $0<\sigma \leq 1 / 2$, we have

$$
\begin{align*}
& \left\|\left(I-e^{i \tau \Delta}\right) P_{N} B(\phi)\right\|_{L^{2}} \leq C_{1}\left(M,\|V\|_{H^{2}}\right) \tau^{1 / 2+\sigma}  \tag{3.17}\\
& \left\|I_{N} B(\phi)-P_{N} B(\phi)\right\|_{L^{2}} \leq C_{2}\left(M,\|V\|_{H^{2}}\right) h^{1+2 \sigma} \tag{3.18}
\end{align*}
$$

Proof. Recalling the standard estimates that (see, e.g., $[43,8,10]$ )

$$
\begin{align*}
& \left\|v-P_{N} v\right\|_{L^{2}} \lesssim h^{2}|v|_{H^{2}}, \quad\left\|I_{N} v-P_{N} v\right\|_{L^{2}} \lesssim h^{2}|v|_{H^{2}},  \tag{3.19}\\
& \left\|v-e^{i t \Delta} v\right\|_{L^{2}} \lesssim t\|v\|_{H^{2}}, \quad v \in H_{0}^{1}(\Omega) \cap H^{2}(\Omega) \tag{3.20}
\end{align*}
$$

noting that $H^{2}(\Omega)$ is an algebra when $1 \leq d \leq 3$, we have

$$
\begin{equation*}
\left\|\left(I-e^{i \tau \Delta}\right)(V \phi)\right\|_{L^{2}} \lesssim \tau\|V\|_{H^{2}}\|\phi\|_{H^{2}}, \quad\left\|\left(I_{N}-P_{N}\right)(V \phi)\right\|_{L^{2}} \lesssim h^{2}\|V\|_{H^{2}}\|\phi\|_{H^{2}} \tag{3.21}
\end{equation*}
$$

According to (2.2), it remains to show (3.17) and (3.18) with $f\left(|\phi|^{2}\right) \phi$ replacing $B(\phi)$. Using the regularized function $f_{\varepsilon}$ defined in (2.17) with $0<\varepsilon \ll 1$ and the triangle inequality, we have

$$
\begin{align*}
& \left\|\left(I-e^{i \tau \Delta}\right)\left(f\left(|\phi|^{2}\right) \phi\right)\right\|_{L^{2}} \\
& \leq\left\|\left(I-e^{i \tau \Delta}\right)\left(f\left(|\phi|^{2}\right) \phi-f_{\varepsilon}\left(|\phi|^{2}\right) \phi\right)\right\|_{L^{2}}+\left\|\left(I-e^{i \tau \Delta}\right)\left(f_{\varepsilon}\left(|\phi|^{2}\right) \phi\right)\right\|_{L^{2}} . \tag{3.22}
\end{align*}
$$

From (3.22), using $\left\|\left(I-e^{i \tau \Delta}\right) v\right\|_{L^{2}} \leq 2\|v\|_{L^{2}}$ for the first term and (3.20) for the second term, we have

$$
\begin{equation*}
\left\|\left(I-e^{i \tau \Delta}\right)\left(f\left(|\phi|^{2}\right) \phi\right)\right\|_{L^{2}} \lesssim\left\|f\left(|\phi|^{2}\right) \phi-f_{\varepsilon}\left(|\phi|^{2}\right) \phi\right\|_{L^{2}}+\tau\left\|f_{\varepsilon}\left(|\phi|^{2}\right) \phi\right\|_{H^{2}} \tag{3.23}
\end{equation*}
$$

By Lemma 2.4 and (2.30), we have

$$
\begin{align*}
& \left\|f\left(|\phi|^{2}\right) \phi-f_{\varepsilon}\left(|\phi|^{2}\right) \phi\right\|_{L^{2}} \lesssim \varepsilon^{2 \sigma}\left\|\phi \mathbb{1}_{|\phi|<\varepsilon}\right\|_{L^{2}} \leq|\Omega|^{\frac{1}{2}} \varepsilon^{1+2 \sigma}  \tag{3.24}\\
& \left\|f_{\varepsilon}\left(|\phi|^{2}\right) \phi\right\|_{H^{2}} \leq \frac{C(M)}{\varepsilon^{1-2 \sigma}} \tag{3.25}
\end{align*}
$$

Plugging (3.24) and (3.25) into (3.23), we have

$$
\left\|\left(I-e^{i \tau \Delta}\right)\left(f\left(|\phi|^{2}\right) \phi\right)\right\|_{L^{2}} \leq C(M) \inf _{0<\varepsilon<1}\left(\varepsilon^{1+2 \sigma}+\frac{\tau}{\varepsilon^{1-2 \sigma}}\right) \leq C(M) \tau^{1 / 2+\sigma}
$$

which combined with (3.21) yields (3.17).
Then we shall prove (3.18). Similar to (3.22) and (3.23), using the triangle inequality, the $L^{2}$-projection property of $P_{N},(3.24),(3.19)$ and (2.30), we have

$$
\begin{align*}
& \left\|\left(I_{N}-P_{N}\right)\left(f\left(|\phi|^{2}\right) \phi\right)\right\|_{L^{2}} \\
& \leq\left\|\left(I_{N}-P_{N}\right)\left(f\left(|\phi|^{2}\right) \phi-f_{\varepsilon}\left(|\phi|^{2}\right) \phi\right)\right\|_{L^{2}}+\left\|\left(I_{N}-P_{N}\right)\left(f_{\varepsilon}\left(|\phi|^{2}\right) \phi\right)\right\|_{L^{2}} \\
& \leq\left\|I_{N}\left(f\left(|\phi|^{2}\right) \phi-f_{\varepsilon}\left(|\phi|^{2}\right) \phi\right)\right\|_{L^{2}}+\left\|P_{N}\left(f\left(|\phi|^{2}\right) \phi-f_{\varepsilon}\left(|\phi|^{2}\right) \phi\right)\right\|_{L^{2}} \\
& \quad+h^{2}\left\|f_{\varepsilon}\left(|\phi|^{2}\right) \phi\right\|_{H^{2}} \\
& \leq\left\|I_{N}\left(f\left(|\phi|^{2}\right) \phi-f_{\varepsilon}\left(|\phi|^{2}\right) \phi\right)\right\|_{L^{2}}+|\Omega|^{\frac{1}{2}} \varepsilon^{1+2 \sigma}+h^{2} \frac{C(M)}{\varepsilon^{1-2 \sigma}} . \tag{3.26}
\end{align*}
$$

By Parseval's identity,

$$
\begin{equation*}
\left\|I_{N} v\right\|_{L^{2}}=\sqrt{h \sum_{j=1}^{N-1}\left|v\left(x_{j}\right)\right|^{2}} \leq \sqrt{h \sum_{j=1}^{N-1}\|v\|_{l^{\infty}}^{2}} \leq|\Omega|^{\frac{1}{2}}\|v\|_{l^{\infty}}, \quad v \in C_{0}(\bar{\Omega}) \tag{3.27}
\end{equation*}
$$

which implies, by using Lemma 2.4 again,

$$
\begin{align*}
\left\|I_{N}\left(f\left(|\phi|^{2}\right) \phi-f_{\varepsilon}\left(|\phi|^{2}\right) \phi\right)\right\|_{L^{2}} & \leq|\Omega|^{\frac{1}{2}}\left\|\left(f\left(|\phi|^{2}\right)-f_{\varepsilon}\left(|\phi|^{2}\right)\right) \phi\right\|_{l^{\infty}} \\
& \leq|\Omega|^{\frac{1}{2}} \varepsilon^{2 \sigma}\left\|\phi \mathbb{1}_{|\phi|<\varepsilon}\right\|_{l^{\infty}} \leq|\Omega|^{\frac{1}{2}} \varepsilon^{1+2 \sigma} . \tag{3.28}
\end{align*}
$$

Plugging (3.28) into (3.26), we have

$$
\left\|\left(I_{N}-P_{N}\right)\left(f\left(|\phi|^{2}\right) \phi\right)\right\|_{L^{2}} \leq C(M) \inf _{0<\varepsilon<1}\left(\varepsilon^{1+2 \sigma}+\frac{h^{2}}{\varepsilon^{1-2 \sigma}}\right) \leq C(M) h^{1+2 \sigma}
$$

which completes the proof.
Now we are able to show the local truncation error of the TSSP method.
Proposition 3.6 (local truncation error). Assume that $V \in H^{2}(\Omega)$. Under the assumption (A), for $0 \leq k \leq T / \tau-1$, we have

$$
\left\|P_{N} \psi\left(\cdot, t_{k+1}\right)-\Phi^{\tau}\left(P_{N} \psi\left(\cdot, t_{k}\right)\right)\right\|_{L^{2}(\Omega)} \leq C\left(M_{2}\right) \tau\left(\tau^{\frac{1}{2}+\sigma}+h^{1+2 \sigma}\right)
$$

Proof. For the simplicity of notations, we define $v(t)=\psi\left(t_{k}+t\right):=\psi\left(\cdot, t_{k}+t\right)$ for $0 \leq t \leq \tau$ and $v_{0}:=v(0)=\psi\left(t_{k}\right)$. By Sobolev embedding $H^{2} \hookrightarrow L^{\infty}$, noting the boundedness of $e^{i t \Delta}$ and $P_{N}$, we have

$$
\begin{align*}
& \left\|e^{i s \Delta} v(t)\right\|_{L^{\infty}} \lesssim\left\|e^{i s \Delta} v(t)\right\|_{H^{2}}=\|v(t)\|_{H^{2}} \leq M_{2}  \tag{3.29}\\
& \left\|P_{N} v(t)\right\|_{L^{\infty}} \lesssim\left\|P_{N} v(t)\right\|_{H^{2}} \leq\|v(t)\|_{H^{2}} \leq M_{2}, \quad 0 \leq s, t \leq \tau \tag{3.30}
\end{align*}
$$

By variation of constant formula (see (4.24)-(4.25) in [11])

$$
\begin{align*}
\psi\left(t_{k+1}\right)= & e^{i \tau \Delta} v_{0}+\int_{0}^{\tau} e^{i(\tau-s) \Delta} B\left(e^{i s \Delta} v_{0}\right) \mathrm{d} s \\
& +\int_{0}^{\tau} \int_{0}^{s} e^{i(\tau-s) \Delta} d B\left(e^{i(s-\sigma) \Delta} v(\sigma)\right)\left[e^{i(s-\sigma) \Delta} B(v(\sigma))\right] \mathrm{d} \sigma \mathrm{~d} s \tag{3.31}
\end{align*}
$$

where $d B(\cdot)[\cdot]$ is the Gâteaux derivative defined in (3.13). Applying $P_{N}$ on both sides of (3.31), noting that $e^{i \tau \Delta}$ and $P_{N}$ commute [6], one gets

$$
\begin{align*}
P_{N} \psi\left(t_{k+1}\right)= & e^{i \tau \Delta} P_{N} v_{0}+\int_{0}^{\tau} e^{i(\tau-s) \Delta} P_{N} B\left(e^{i s \Delta} v_{0}\right) \mathrm{d} s \\
& +\int_{0}^{\tau} \int_{0}^{s} e^{i(\tau-s) \Delta} P_{N}\left(d B\left(e^{i(s-\sigma) \Delta} v(\sigma)\right)\left[e^{i(s-\sigma) \Delta} B(v(\sigma))\right]\right) \mathrm{d} \sigma \mathrm{~d} s . \tag{3.32}
\end{align*}
$$

From (2.6), recalling that $v_{0}=\psi\left(t_{k}\right)$, we have

$$
\begin{equation*}
\Phi^{\tau}\left(P_{N} \psi\left(t_{k}\right)\right)=e^{i \tau \Delta} I_{N} \Phi_{B}^{\tau}\left(P_{N} v_{0}\right) \tag{3.33}
\end{equation*}
$$

Applying the first-order Taylor expansion (see proof of Theorem 4.2 in [11])

$$
\begin{equation*}
\Phi_{B}^{\tau}(w)=w+\tau B(w)+\tau^{2} \int_{0}^{1}(1-\theta) d B\left(\Phi_{B}^{\theta \tau}(w)\right)\left[B\left(\Phi_{B}^{\theta \tau}(w)\right)\right] \mathrm{d} \theta \tag{3.34}
\end{equation*}
$$

for $w=P_{N} v_{0}$ and plugging it into (3.33), we have

$$
\begin{align*}
\Phi^{\tau}\left(P_{N} \psi\left(t_{k}\right)\right)= & e^{i \tau \Delta} P_{N} v_{0}+\tau e^{i \tau \Delta} I_{N} B\left(P_{N} v_{0}\right) \\
& +\tau^{2} e^{i \tau \Delta} I_{N}\left(\int_{0}^{1}(1-\theta)\left(d B\left(\Phi_{B}^{\theta \tau}\left(P_{N} v_{0}\right)\right)\left[B\left(\Phi_{B}^{\theta \tau}\left(P_{N} v_{0}\right)\right)\right]\right) \mathrm{d} \theta\right) . \tag{3.35}
\end{align*}
$$

Subtracting (3.35) from (3.32), we have

$$
\begin{equation*}
P_{N} \psi\left(t_{k+1}\right)-\Phi^{\tau}\left(P_{N} \psi\left(t_{k}\right)\right)=e_{1}-e_{2}+e_{3} \tag{3.36}
\end{equation*}
$$

where

$$
\begin{align*}
& e_{1}=\int_{0}^{\tau} \int_{0}^{s} e^{i(\tau-s) \Delta} P_{N}\left(d B\left(e^{i(s-\sigma) \Delta} v(\sigma)\right)\left[e^{i(s-\sigma) \Delta} B(v(\sigma))\right]\right) \mathrm{d} \sigma \mathrm{~d} s,  \tag{3.37}\\
& e_{2}=\tau^{2} e^{i \tau \Delta} I_{N}\left(\int_{0}^{1}(1-\theta)\left(d B\left(\Phi_{B}^{\theta \tau}\left(P_{N} v_{0}\right)\right)\left[B\left(\Phi_{B}^{\theta \tau}\left(P_{N} v_{0}\right)\right)\right]\right) \mathrm{d} \theta\right),  \tag{3.38}\\
& e_{3}=\int_{0}^{\tau} e^{i(\tau-s) \Delta} P_{N} B\left(e^{i s \Delta} v_{0}\right) \mathrm{d} s-\tau e^{i \tau \Delta} I_{N} B\left(P_{N} v_{0}\right) . \tag{3.39}
\end{align*}
$$

Next, we shall first estimate $e_{1}$ and $e_{2}$. Noticing the property of $e^{i t \Delta}$ and $P_{N}$, using Lemma 3.3 and (3.29), we have

$$
\begin{align*}
& \left\|e^{i(\tau-s) \Delta} P_{N}\left(d B\left(e^{i(s-\sigma) \Delta} v(\sigma)\right)\left[e^{i(s-\sigma) \Delta} B(v(\sigma))\right]\right)\right\|_{L^{2}} \\
& \leq\left\|d B\left(e^{i(s-\sigma) \Delta} v(\sigma)\right)\left[e^{i(s-\sigma) \Delta} B(v(\sigma))\right]\right\|_{L^{2}} \\
& \leq C\left(\|V\|_{L^{\infty}},\left\|e^{i(s-\sigma) \Delta} v(\sigma)\right\|_{L^{\infty}}\right)\left\|e^{i(s-\sigma) \Delta} B(v(\sigma))\right\|_{L^{2}} \\
& \leq C\left(M_{2}\right)\|B(v(\sigma))\|_{L^{2} .} \tag{3.40}
\end{align*}
$$

From (3.37), using (3.40) and (3.1), we get

$$
\begin{aligned}
\left\|e_{1}\right\|_{L^{2}} & \leq \int_{0}^{\tau} \int_{0}^{s}\left\|e^{i(\tau-s) \Delta} P_{N}\left(d B\left(e^{i(s-\sigma) \Delta} v(\sigma)\right)\left[e^{i(s-\sigma) \Delta} B(v(\sigma))\right]\right)\right\|_{L^{2}} \mathrm{~d} \sigma \mathrm{~d} s \\
& \leq C\left(M_{2}\right) \int_{0}^{\tau} \int_{0}^{s}\|B(v(\sigma))\|_{L^{2}} \mathrm{~d} \sigma \mathrm{~d} s \leq C\left(M_{2}\right) \tau^{2} \max _{0 \leq \sigma \leq \tau}\|B(v(\sigma))\|_{L^{2}} \\
& \leq C\left(M_{2}\right) \tau^{2} C\left(M_{2}\right) \max _{0 \leq \sigma \leq \tau}\|v(\sigma)\|_{L^{2}} \leq C\left(M_{2}\right) \tau^{2} .
\end{aligned}
$$

From (2.6) and (2.2), using (3.30), one gets,

$$
\begin{align*}
& \left\|\Phi_{B}^{\theta \tau}\left(P_{N} v_{0}\right)\right\|_{L^{\infty}}=\left\|P_{N} v_{0}\right\|_{L^{\infty}} \leq C\left(M_{2}\right), \quad 0 \leq \theta \leq 1 \\
& \left\|B\left(\Phi_{B}^{\theta \tau}\left(P_{N} v_{0}\right)\right)\right\|_{L^{\infty}} \leq C\left(\|V\|_{L^{\infty}},\left\|P_{N} v_{0}\right\|_{L^{\infty}}\right)\left\|P_{N} v_{0}\right\|_{L^{\infty}} \leq C\left(M_{2}\right) \tag{3.42}
\end{align*}
$$

From (3.14), noticing (3.5), one easily gets

$$
\begin{equation*}
\left\|d B\left(w_{1}\right)\left[w_{2}\right]\right\|_{L^{\infty}} \leq C\left(\|V\|_{L^{\infty}},\left\|w_{1}\right\|_{L^{\infty}}\right)\left\|w_{2}\right\|_{L^{\infty}}, \quad w_{1}, w_{2} \in L^{\infty}(\Omega) \tag{3.43}
\end{equation*}
$$

which combined with (3.27) and (3.42), yields the estimate for $e_{2}$ in (3.38) as

$$
\begin{align*}
\left\|e_{2}\right\|_{L^{2}} & \leq \tau^{2}\left\|I_{N}\left(\int_{0}^{1}(1-\theta)\left(d B\left(\Phi_{B}^{\theta \tau}\left(P_{N} v_{0}\right)\right)\left[B\left(\Phi_{B}^{\theta \tau}\left(P_{N} v_{0}\right)\right)\right]\right) \mathrm{d} \theta\right)\right\|_{L^{2}} \\
& \leq \tau^{2}|\Omega|^{\frac{1}{2}} \max _{0 \leq \theta \leq 1}\left\|d B\left(\Phi_{B}^{\theta \tau}\left(P_{N} v_{0}\right)\right)\left[B\left(\Phi_{B}^{\theta \tau}\left(P_{N} v_{0}\right)\right)\right]\right\|_{l^{\infty}} \\
& \leq \tau^{2}|\Omega|^{\frac{1}{2}} C\left(\|V\|_{L^{\infty}},\left\|\Phi_{B}^{\theta \tau}\left(P_{N} v_{0}\right)\right\|_{L^{\infty}}\right)\left\|B\left(\Phi_{B}^{\theta \tau}\left(P_{N} v_{0}\right)\right)\right\|_{L^{\infty}} \\
& \leq C\left(M_{2}\right) \tau^{2} \tag{3.44}
\end{align*}
$$

Then we shall estimate $e_{3}$ in (3.39), which can be written as

$$
e_{3}=\int_{0}^{\tau}\left[e^{i(\tau-s) \Delta} P_{N} B\left(e^{i s \Delta} v_{0}\right)-e^{i \tau \Delta} I_{N} B\left(P_{N} v_{0}\right)\right] \mathrm{d} s
$$

which yields

$$
\begin{equation*}
\left\|e_{3}\right\|_{L^{2}} \leq \tau \max _{0 \leq s \leq \tau}\left\|e^{i(\tau-s) \Delta} P_{N} B\left(e^{i s \Delta} v_{0}\right)-e^{i \tau \Delta} I_{N} B\left(P_{N} v_{0}\right)\right\|_{L^{2}} \tag{3.45}
\end{equation*}
$$

Using standard properties of $e^{i t \Delta}$ and $P_{N}$, one gets

$$
\begin{align*}
& \left\|e^{i(\tau-s) \Delta} P_{N} B\left(e^{i s \Delta} v_{0}\right)-e^{i \tau \Delta} I_{N} B\left(P_{N} v_{0}\right)\right\|_{L^{2}} \\
& =\left\|P_{N} B\left(e^{i s \Delta} v_{0}\right)-e^{i s \Delta} I_{N} B\left(P_{N} v_{0}\right)\right\|_{L^{2}} \\
& \leq\left\|P_{N} B\left(e^{i s \Delta} v_{0}\right)-P_{N} B\left(v_{0}\right)\right\|_{L^{2}}+\left\|P_{N} B\left(v_{0}\right)-P_{N} B\left(P_{N} v_{0}\right)\right\|_{L^{2}} \\
& \quad+\left\|P_{N} B\left(P_{N} v_{0}\right)-e^{i s \Delta} P_{N} B\left(P_{N} v_{0}\right)\right\|_{L^{2}} \\
& \quad+\left\|e^{i s \Delta} P_{N} B\left(P_{N} v_{0}\right)-e^{i s \Delta} I_{N} B\left(P_{N} v_{0}\right)\right\|_{L^{2}} \\
& \leq\left\|B\left(e^{i s \Delta} v_{0}\right)-B\left(v_{0}\right)\right\|_{L^{2}}+\left\|B\left(v_{0}\right)-B\left(P_{N} v_{0}\right)\right\|_{L^{2}} \\
& \quad+\left\|\left(I-e^{i s \Delta}\right) P_{N} B\left(P_{N} v_{0}\right)\right\|_{L^{2}}+\left\|\left(P_{N}-I_{N}\right) B\left(P_{N} v_{0}\right)\right\|_{L^{2}} \\
& =:\left\|e_{3}^{1}\right\|_{L^{2}}+\left\|e_{3}^{2}\right\|_{L^{2}}+\left\|e_{3}^{3}\right\|_{L^{2}}+\left\|e_{3}^{4}\right\|_{L^{2}} . \tag{3.46}
\end{align*}
$$

For $e_{3}^{1}$ and $e_{3}^{2}$ in (3.46), using Lemma 3.2, recalling (3.19), (3.20), (3.29), and (3.30), we obtain

$$
\begin{align*}
\left\|e_{3}^{1}\right\|_{L^{2}} & =\left\|B\left(e^{i s \Delta} v_{0}\right)-B\left(v_{0}\right)\right\|_{L^{2}} \leq C\left(M_{2}\right)\left\|\left(I-e^{i s \Delta}\right) v_{0}\right\|_{L^{2}} \leq C\left(M_{2}\right) \tau  \tag{3.47}\\
\left\|e_{3}^{2}\right\|_{L^{2}} & =\left\|B\left(v_{0}\right)-B\left(P_{N} v_{0}\right)\right\|_{L^{2}} \leq C\left(M_{2}\right)\left\|v_{0}-P_{N} v_{0}\right\|_{L^{2}} \leq C\left(M_{2}\right) h^{2}
\end{align*}
$$

For $e_{3}^{3}$ and $e_{3}^{4}$ in (3.46), using Lemma 3.5, we get

$$
\begin{align*}
& \left\|e_{3}^{3}\right\|_{L^{2}}=\left\|\left(I-e^{i s \Delta}\right) P_{N} B\left(P_{N} v_{0}\right)\right\|_{L^{2}} \leq C\left(M_{2}\right) \tau^{\frac{1+2 \sigma}{2}}  \tag{3.48}\\
& \left\|e_{3}^{4}\right\|_{L^{2}}=\left\|\left(I_{N}-P_{N}\right) B\left(P_{N} v_{0}\right)\right\|_{L^{2}} \leq C\left(M_{2}\right) h^{1+2 \sigma}
\end{align*}
$$

Plugging (3.47) and (3.48) into (3.46), and noticing (3.45), we get

$$
\begin{equation*}
\left\|e_{3}\right\|_{L^{2}} \leq C\left(M_{2}\right) \tau\left(\tau^{\frac{1+2 \sigma}{2}}+h^{1+2 \sigma}\right) \tag{3.49}
\end{equation*}
$$

Combing (3.41), (3.44), and (3.49), and noting (3.36), we get the desired result.
Remark 3.7. The proof of Proposition 3.6 can be generalized to 2 D and 3 D directly. Moreover, in 1D, under much weaker assumption that $V \in H^{1}(\Omega)$ and $\psi \in C\left([0, T] ; H_{0}^{1}(\Omega)\right)$, by using Sobolev embedding $H^{1} \hookrightarrow L^{\infty}$ and the estimates (see, e.g., $[10,11]$ )

$$
\begin{equation*}
\left\|v-e^{i t \Delta} v\right\|_{L^{2}} \lesssim \sqrt{\tau}\|v\|_{H^{1}}, \quad\left\|v-P_{N} v\right\|_{L^{2}} \lesssim h|v|_{H^{1}}, \quad v \in H_{0}^{1}(\Omega) \tag{3.50}
\end{equation*}
$$

and following the proof of Proposition 3.6, we can obtain

$$
\begin{equation*}
\left\|P_{N} \psi\left(t_{k+1}\right)-\Phi^{\tau}\left(P_{N} \psi\left(t_{k}\right)\right)\right\|_{L^{2}(\Omega)} \leq C \tau(\sqrt{\tau}+h) \tag{3.51}
\end{equation*}
$$

where $C$ depends on $\|V\|_{H^{1}}$ and $\|\psi\|_{L^{\infty}\left([0, T] ; H^{1}\right)}$.
3.3. Unconditional $L^{2}$-stability and proof of Theorem 2.5. We shall show the unconditional $L^{2}$-stability of the numerical flow by using Lemma 3.4. With the estimate of the local truncation error and the unconditional $L^{2}$-stability of the numerical flow, we are able to obtain the error estimates.
Proposition 3.8 (unconditional $L^{2}$-stability). Let $v \in X_{N}$ and $w \in X_{N}$ such that $\min \left\{\|v\|_{L^{\infty}},\|w\|_{L^{\infty}}\right\} \leq M$. When $0<\sigma \leq 1 / 2$, we have

$$
\left\|\Phi^{\tau}(v)-\Phi^{\tau}(w)\right\|_{L^{2}} \leq(1+C(M) \tau)\|v-w\|_{L^{2}}
$$

where $\Phi^{\tau}$ is defined in (2.14) and $C(M) \sim M^{2 \sigma}$.

Proof. Recalling (2.14), noting that $e^{i \tau \Delta}$ preserves the $L^{2}$ norm, one gets

$$
\begin{align*}
\left\|\Phi^{\tau}(v)-\Phi^{\tau}(w)\right\|_{L^{2}} & =\left\|e^{i \tau \Delta} I_{N} \Phi_{B}^{\tau}(v)-e^{i \tau \Delta} I_{N} \Phi_{B}^{\tau}(w)\right\|_{L^{2}} \\
& =\left\|I_{N} \Phi_{B}^{\tau}(v)-I_{N} \Phi_{B}^{\tau}(w)\right\|_{L^{2}} \tag{3.52}
\end{align*}
$$

From (3.52), by (3.27) and Lemma 3.4, noting that $I_{N}$ is an identity on $X_{N}$, and recalling (2.6), we have

$$
\begin{aligned}
& \left\|I_{N} \Phi_{B}^{\tau}(v)-I_{N} \Phi_{B}^{\tau}(w)\right\|_{L^{2}}^{2} \\
& =h \sum_{j=1}^{N-1}\left|\Phi_{B}^{\tau}(v)\left(x_{j}\right)-\Phi_{B}^{\tau}(w)\left(x_{j}\right)\right|^{2} \\
& =h \sum_{j=1}^{N-1}\left|e^{-i \tau V\left(x_{j}\right)} \Phi_{B_{2}}^{\tau}(v)\left(x_{j}\right)-e^{-i \tau V\left(x_{j}\right)} \Phi_{B_{2}}^{\tau}(w)\left(x_{j}\right)\right|^{2} \\
& =h \sum_{j=1}^{N-1}\left|\Phi_{B_{2}}^{\tau}(v)\left(x_{j}\right)-\Phi_{B_{2}}^{\tau}(w)\left(x_{j}\right)\right|^{2} \\
& \leq(1+C(M) \tau)^{2} h \sum_{j=1}^{N-1}\left|v\left(x_{j}\right)-w\left(x_{j}\right)\right|^{2} \\
& =(1+C(M) \tau)^{2}\left\|I_{N} v-I_{N} w\right\|_{L^{2}}^{2} \\
& =(1+C(M) \tau)^{2}\|v-w\|_{L^{2}}^{2} .
\end{aligned}
$$

The proof is completed.
Remark 3.9. In the error estimates, $v$ and $w$ in Proposition 3.8 are related to the exact solution and the numerical solution, respectively. Hence, to control the constant $C(M)$ in Proposition 3.8, we can assume bound of the exact solution and thus get rid of the a priori estimate of the numerical solution, which explains why Proposition 3.8 is called the unconditional $L^{2}$-stability.

Proof of Theorem 2.5. Under the assumption (A), using (3.19), one gets

$$
\begin{equation*}
\left\|\psi\left(\cdot, t_{k}\right)-P_{N} \psi\left(\cdot, t_{k}\right)\right\|_{L^{2}} \leq C\left(M_{2}\right) h^{2} \tag{3.54}
\end{equation*}
$$

Hence, it suffices to estimate $e^{k}:=I_{N} \psi^{k}-P_{N} \psi\left(\cdot, t_{k}\right) \in X_{N}$ for $0 \leq k \leq T / \tau$. By (2.15), for $0 \leq k \leq T / \tau-1$, one has

$$
\begin{align*}
&\left\|e^{k+1}\right\|_{L^{2}}=\left\|I_{N} \psi^{k+1}-P_{N} \psi\left(\cdot, t_{k+1}\right)\right\|_{L^{2}}=\left\|\Phi^{\tau}\left(I_{N} \psi^{k}\right)-P_{N} \psi\left(\cdot, t_{k+1}\right)\right\|_{L^{2}} \\
&(3.55) \quad \leq\left\|\Phi^{\tau}\left(I_{N} \psi^{k}\right)-\Phi^{\tau}\left(P_{N} \psi\left(\cdot, t_{k}\right)\right)\right\|_{L^{2}}+\left\|\Phi^{\tau}\left(P_{N} \psi\left(\cdot, t_{k}\right)\right)-P_{N} \psi\left(\cdot, t_{k+1}\right)\right\|_{L^{2}} . \tag{3.55}
\end{align*}
$$

By Propositions 3.6 and 3.8, noting that $\left\|P_{N} \psi\left(\cdot, t_{k}\right)\right\|_{L^{\infty}} \lesssim\left\|P_{N} \psi\left(\cdot, t_{k}\right)\right\|_{H^{2}} \leq$ $\left\|\psi\left(\cdot, t_{k}\right)\right\|_{H^{2}} \leq M_{2}$, one has
$\left\|e^{k}\right\|_{L^{2}(\Omega)} \leq\left(1+C\left(M_{2}\right) \tau\right)\left\|e^{k-1}\right\|_{L^{2}(\Omega)}+C\left(M_{2}\right) \tau\left(\tau^{1 / 2+\sigma}+h^{1+2 \sigma}\right), \quad 1 \leq k \leq T / \tau$.
It follows from the discrete Gronwall's inequality and $\left\|e^{0}\right\|_{L^{2}}=\left\|I_{N} \psi_{0}-P_{N} \psi_{0}\right\| \leq$ $C\left(M_{2}\right) h^{2}$ that

$$
\left\|e^{k}\right\|_{L^{2}(\Omega)} \leq C\left(T, M_{2}\right)\left(\tau^{\frac{1+2 \sigma}{2}}+h^{1+2 \sigma}\right), \quad 0 \leq k \leq T / \tau
$$

which completes the proof.

The proof of Corollary 2.6 follows the proof of Theorem 2.5 by replacing Proposition 3.6 with (3.51) and we shall omit it for brevity.

## 4. Proof of Theorem 2.7 for the case $\sigma \geq 1 / 2$

In this section, we assume that $V \in H^{2}(\Omega) \cap W^{1, \infty}(\Omega), \sigma \geq 1 / 2$ and the assumption (A). The assumption $V \in W^{1, \infty}(\Omega)$ is only used in Proposition 4.8 and can be obtained from $V \in H^{2}(\Omega)$ in 1D or $V \in H^{3}(\Omega)$ in 2D and 3D. Also, we shall use the equivalent norm $\|\nabla \cdot\|_{L^{2}}$ on $H_{0}^{1}(\Omega)$ to avoid frequent use of Poincaré inequality.

### 4.1. Some estimates for the operator $B$.

Lemma 4.1. Let $v \in H^{2}(\Omega)$ such that $\|v\|_{H^{2}} \leq M$. When $\sigma \geq 1 / 2$, we have

$$
\|B(v)\|_{H^{2}(\Omega)} \leq C\left(M,\|V\|_{H^{2}}\right)
$$

Proof. Recalling (2.2), noting that $H^{2}(\Omega)$ is an algebra when $1 \leq d \leq 3$, we have

$$
\begin{equation*}
\|B(v)\|_{H^{2}} \leq\|V v\|_{H^{2}}+\left\|f\left(|v|^{2}\right) v\right\|_{H^{2}} \leq\|V\|_{H^{2}}\|v\|_{H^{2}}+\left\|f\left(|v|^{2}\right) v\right\|_{H^{2}} . \tag{4.1}
\end{equation*}
$$

When $\sigma \geq 1 / 2$, recalling (1.4) and (3.4), by similar calculation as (2.34) and (2.35) and noting (3.5) as well as

$$
\begin{equation*}
\left|f^{\prime}\left(|z|^{2}\right) z\right|+\left|f^{\prime}\left(|z|^{2}\right) \bar{z}\right|+\left|f^{\prime \prime}\left(|z|^{2}\right) z^{3}\right|+\left|f^{\prime \prime}\left(|z|^{2}\right) z^{2} \bar{z}\right| \lesssim|z|^{2 \sigma-1}, z \in \mathbb{C}, \sigma \geq \frac{1}{2} \tag{4.2}
\end{equation*}
$$

we have

$$
\begin{equation*}
\left|\partial_{j k}\left(f\left(|v|^{2}\right) v\right)\right| \lesssim|v|^{2 \sigma}\left|\partial_{j k} v\right|+|v|^{2 \sigma-1}\left|\partial_{j} v\right|\left|\partial_{k} v\right| \tag{4.3}
\end{equation*}
$$

which yields, by Sobolev embedding $H^{2} \hookrightarrow W^{1,4}$ for $d=1,2,3$, that

$$
\begin{equation*}
\left\|\partial_{j k}\left(f\left(|v|^{2}\right) v\right)\right\|_{L^{2}} \lesssim\|v\|_{L^{\infty}}^{2 \sigma}\left\|\partial_{j k} v\right\|_{L^{2}}+\|v\|_{L^{\infty}}^{2 \sigma-1}\|\nabla v\|_{L^{4}}^{2} \leq C(M) \tag{4.4}
\end{equation*}
$$

Combing (4.4) and Lemma 3.1, noting (4.1), we obtain the desired result.
Lemma 4.2. Let $v, w \in H^{2}(\Omega)$ such that $\|v\|_{H^{2}} \leq M$ and $\|w\|_{H^{2}} \leq M$. When $\sigma \geq 1 / 2$, we have

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

Proof. From (3.6), one gets

$$
\begin{align*}
\nabla(B(v)-B(w))= & -i\left[\nabla(V(v-w))+i(1+\sigma)\left(f\left(|v|^{2}\right) \nabla v-f\left(|w|^{2}\right) \nabla w\right)\right. \\
& +G(v) \nabla \bar{v}-G(w) \nabla \bar{w}] \tag{4.5}
\end{align*}
$$

Using Hölder's inequality and Sobolev embedding $H^{1} \hookrightarrow L^{4}$ and $W^{1,4} \hookrightarrow L^{\infty}$ (both hold for $d=1,2,3$ ), we have

$$
\begin{align*}
\|\nabla(V(v-w))\|_{L^{2}} & \leq\|\nabla V\|_{L^{4}}\|v-w\|_{L^{4}}+\|V\|_{L^{\infty}}\|\nabla(v-w)\|_{L^{2}} \\
& \lesssim\|V\|_{W^{1,4}}\|v-w\|_{H^{1}} \tag{4.6}
\end{align*}
$$

By (4.5), it remains to show that

$$
\begin{align*}
& \left\|f\left(|v|^{2}\right) \nabla v-f\left(|w|^{2}\right) \nabla w\right\|_{L^{2}} \leq C(M)\|v-w\|_{H^{1}}  \tag{4.7}\\
& \|G(v) \nabla \bar{v}-G(w) \nabla \bar{w}\|_{L^{2}} \leq C(M)\|v-w\|_{H^{1}} \tag{4.8}
\end{align*}
$$

When $\sigma \geq 1 / 2$, following the proof of (3.11), we have, for $z_{1}, z_{2} \in \mathbb{C}$,

$$
\begin{align*}
& \left|f\left(\left|z_{1}\right|^{2}\right)-f\left(\left|z_{2}\right|^{2}\right)\right| \lesssim \max \left\{\left|z_{1}\right|,\left|z_{2}\right|\right\}^{2 \sigma-1}\left|z_{1}-z_{2}\right|,  \tag{4.9}\\
& \left|G\left(z_{1}\right)-G\left(z_{2}\right)\right| \lesssim \max \left\{\left|z_{1}\right|,\left|z_{2}\right|\right\}^{2 \sigma-1}\left|z_{1}-z_{2}\right| . \tag{4.10}
\end{align*}
$$

Using (4.9) and Sobolev embedding $H^{1} \hookrightarrow L^{4}$ and $H^{2} \hookrightarrow L^{\infty}$, we have

$$
\begin{aligned}
& \left\|f\left(|v|^{2}\right) \nabla v-f\left(|w|^{2}\right) \nabla w\right\|_{L^{2}} \\
& \leq\left\|f\left(|v|^{2}\right) \nabla(v-w)\right\|_{L^{2}}+\left\|\left(f\left(|v|^{2}\right)-f\left(|w|^{2}\right)\right) \nabla w\right\|_{L^{2}} \\
& \leq C\left(\|v\|_{L^{\infty}}\right)\|v-w\|_{H^{1}}+C\left(\max \left\{\|v\|_{L^{\infty}},\|w\|_{L^{\infty}}\right\}\right)\|(v-w) \nabla w\|_{L^{2}} \\
& \leq C(M)\|v-w\|_{H^{1}}+C(M)\|v-w\|_{L^{4}}\|\nabla w\|_{L^{4}} \\
& \leq C(M)\|v-w\|_{H^{1}},
\end{aligned}
$$

which proves (4.7). Similarly, we can prove (4.8), which completes the proof.
Lemma 4.3. Let $v, w \in H^{1}(\Omega) \cap L^{\infty}(\Omega)$ such that $\|v\|_{L^{\infty}}+\|v\|_{H^{1}} \leq M$ and $\|w\|_{L^{\infty}}+\|w\|_{H^{1}} \leq M$. When $\sigma \geq 1 / 2$, we have

$$
\|d B(v)[w]\|_{H^{1}} \leq C\left(M,\|V\|_{W^{1,4}}\right)
$$

Proof. From (3.14), using (4.6), we have

$$
\begin{align*}
\|d B(v)[w]\|_{H^{1}} & \leq\|V w\|_{H^{1}}+(1+\sigma)\left\|f\left(|v|^{2}\right) w\right\|_{H^{1}}+\|G(v) \bar{w}\|_{H^{1}} \\
& \lesssim\|V\|_{W^{1,4}}\|w\|_{H^{1}}+\left\|f\left(|v|^{2}\right) w\right\|_{H^{1}}+\|G(v) \bar{w}\|_{H^{1}} . \tag{4.11}
\end{align*}
$$

When $\sigma \geq 1 / 2$, recalling (4.2), we have

$$
\begin{aligned}
\left\|f\left(|v|^{2}\right)\right\|_{H^{1}} & =\left\|f\left(|v|^{2}\right)\right\|_{L^{2}}+\left\|\nabla f\left(|v|^{2}\right)\right\|_{L^{2}} \lesssim\|v\|_{L^{\infty}}^{2 \sigma}+\left\|f^{\prime}\left(|v|^{2}\right) v \nabla v\right\|_{L^{2}} \\
& \leq\|v\|_{L^{\infty}}^{2 \sigma}+\|v\|_{L^{\infty}}^{2 \sigma-1}\|\nabla v\|_{L^{2}} \leq C(M) .
\end{aligned}
$$

Similarly, one gets $\|G(v)\|_{H^{1}} \leq C(M)$. Then using

$$
\begin{equation*}
\left\|u_{1} u_{2}\right\|_{H^{1}} \leq\left\|u_{1}\right\|_{L^{\infty}}\left\|u_{2}\right\|_{H^{1}}+\left\|u_{2}\right\|_{L^{\infty}}\left\|u_{1}\right\|_{H^{1}}, \quad u_{1}, u_{2} \in H^{1}(\Omega) \cap L^{\infty}(\Omega), \tag{4.13}
\end{equation*}
$$

and recalling (3.5), we have

$$
\begin{align*}
& \left\|f\left(|v|^{2}\right) w\right\|_{H^{1}} \leq\left\|f\left(|v|^{2}\right)\right\|_{L^{\infty}}\|w\|_{H^{1}}+\|w\|_{L^{\infty}}\left\|f\left(|v|^{2}\right)\right\|_{H^{1}} \leq C(M),  \tag{4.14}\\
& \|G(v) \bar{w}\|_{H^{1}} \leq\|G(v)\|_{L^{\infty}}\|\bar{w}\|_{H^{1}}+\|\bar{w}\|_{L^{\infty}}\|G(v)\|_{H^{1}} \leq C(M) . \tag{4.15}
\end{align*}
$$

Plugging (4.14) and (4.15) into (4.11) yields the desired result.
Lemma 4.4. Let $v, w \in H^{2}(\Omega)$ such that $\|v\|_{H^{2}} \leq M$ and $\|w\|_{H^{2}} \leq M$. If $|w(\mathbf{x})| \leq C|v(\mathbf{x})|$ for all $\mathbf{x} \in \Omega$, when $\sigma \geq 1 / 2$, we have

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

Proof. The proof can be obtained similarly as the proof of Lemma 4.1 and we shall omit it here for brevity.

Lemma 4.5. Let $0<\tau<1$ and $v \in X_{N}$ such that $\|v\|_{L^{\infty}} \leq M$ and $\|v\|_{H^{2}} \leq M_{1}$. When $\sigma>0$, we have

$$
\begin{equation*}
\left\|\Phi_{B}^{\tau}(v)\right\|_{H^{1}} \leq\left(1+C_{1}\left(M,\|V\|_{W^{1,4}}\right) \tau\right)\|v\|_{H^{1}(\Omega)}, \tag{4.16}
\end{equation*}
$$

and when $\sigma \geq 1 / 2$, we have

$$
\begin{equation*}
\left\|\Phi_{B}^{\tau}(v)\right\|_{H^{2}} \leq C_{2}\left(M_{1},\|V\|_{H^{2}}\right) . \tag{4.17}
\end{equation*}
$$

Proof. Recalling that $\Phi_{B}^{\tau}(v)=v e^{-i \tau\left(V+f\left(|v|^{2}\right)\right)}$ in (2.6), the proof of (4.16) and (4.17) follows similarly from the proof of Lemma 3.1 and Lemma 4.1, respectively.

Lemma 4.6. Let $z_{1}, z_{2} \in \mathbb{C}$. When $\sigma \geq 1 / 2$, one has

$$
\left|\Phi_{B_{2}}^{\tau}\left(z_{1}\right)-\Phi_{B_{2}}^{\tau}\left(z_{2}\right)\right| \leq(1+C \tau)\left|z_{1}-z_{2}\right|,
$$

where $\Phi_{B_{2}}^{\tau}(z)=z e^{-i \tau f\left(|z|^{2}\right)}$ in (2.7) and $C \sim \max \left\{\left|z_{1}\right|,\left|z_{2}\right|\right\}^{2 \sigma}$.
Proof. The proof follows from the proof of Lemma 3.4 by replacing (3.16) with (4.9).

### 4.2. Local truncation error.

Proposition 4.7 (local truncation error). Assume that $0<\tau<1,0<h<1$, $V \in H^{2}$ and $\sigma \geq 1 / 2$. Under the assumption (A), for $0 \leq k \leq T / \tau-1$, we have

$$
\begin{align*}
& \left\|P_{N} \psi\left(\cdot, t_{k+1}\right)-\Phi^{\tau}\left(P_{N} \psi\left(\cdot, t_{k}\right)\right)\right\|_{L^{2}(\Omega)} \leq C_{1}\left(M_{2}\right) \tau\left(\tau+h^{2}\right)  \tag{4.18}\\
& \left\|P_{N} \psi\left(\cdot, t_{k+1}\right)-\Phi^{\tau}\left(P_{N} \psi\left(\cdot, t_{k}\right)\right)\right\|_{H^{1}(\Omega)} \leq C_{2}\left(M_{2}\right) \tau\left(\tau^{\frac{1}{2}}+h\right) . \tag{4.19}
\end{align*}
$$

Proof. Following the notations in the proof of Proposition 3.6, we let $v(t)=\psi\left(\cdot, t_{k}+\right.$ $t$ ) for $0 \leq t \leq \tau$ and $v_{0}:=v(0)=\psi\left(\cdot, t_{k}\right)$. When $\sigma \geq 1 / 2$, (3.29) and (3.30) are also valid and we have the same error decomposition (3.36). When $\sigma \geq 1 / 2$, the $L^{2}$ estimate (4.18) follows from the proof of Proposition 3.6 by replacing (3.48) with

$$
\begin{align*}
& \left\|e_{3}^{3}\right\|_{L^{2}} \lesssim \tau\left\|P_{N} B\left(P_{N} v_{0}\right)\right\|_{H^{2}} \leq \tau\left\|B\left(P_{N} v_{0}\right)\right\|_{H^{2}} \leq C\left(M_{2}\right) \tau, \\
& \left\|e_{3}^{4}\right\|_{L^{2}} \lesssim h^{2}\left\|B\left(P_{N} v_{0}\right)\right\|_{H^{2}} \leq C\left(M_{2}\right) h^{2}, \tag{4.20}
\end{align*}
$$

where (3.20), (3.19) and Lemma 4.1 are used.
In the following, we shall show (4.19). Using Sobolev embedding $H^{2} \hookrightarrow L^{\infty}$, the isometry property of $e^{i t \Delta}$ and Lemmas 3.1 and 4.1, one gets

$$
\begin{align*}
& \left\|e^{i(s-\sigma) \Delta} B(v(\sigma))\right\|_{H^{1}}=\|B(v(\sigma))\|_{H^{1}} \leq C\left(M_{2}\right)  \tag{4.21}\\
& \left\|e^{i(s-\sigma) \Delta} B(v(\sigma))\right\|_{L^{\infty}} \lesssim\left\|e^{i(s-\sigma) \Delta} B(v(\sigma))\right\|_{H^{2}}=\|B(v(\sigma))\|_{H^{2}} \leq C\left(M_{2}\right)
\end{align*}
$$

Recalling the boundedness of $e^{i t \Delta}$ and $P_{N}$, using Lemma 4.3, noticing (3.29) and (4.21), we have

$$
\begin{align*}
& \left\|e^{i(\tau-s) \Delta} P_{N}\left(d B\left(e^{i(s-\sigma) \Delta} v(\sigma)\right)\left[e^{i(s-\sigma) \Delta} B(v(\sigma))\right]\right)\right\|_{H^{1}} \\
& \leq\left\|d B\left(e^{i(s-\sigma) \Delta} v(\sigma)\right)\left[e^{i(s-\sigma) \Delta} B(v(\sigma))\right]\right\|_{H^{1}} \\
& \leq C\left(\|V\|_{W^{1,4}},\left\|e^{i(s-\sigma) \Delta} v(\sigma)\right\|_{L^{\infty} \cap H^{1}},\left\|e^{i(s-\sigma) \Delta} B(v(\sigma))\right\|_{L^{\infty} \cap H^{1}}\right) \\
& \leq C\left(M_{2}\right), \tag{4.22}
\end{align*}
$$

which yields, for $e_{1}$ in (3.37),

$$
\begin{align*}
\left\|e_{1}\right\|_{H^{1}} & \leq \int_{0}^{\tau} \int_{0}^{s}\left\|e^{i(\tau-s) \Delta} P_{N}\left(d B\left(e^{i(s-\sigma) \Delta} v(\sigma)\right)\left[e^{i(s-\sigma) \Delta} B(v(\sigma))\right]\right)\right\|_{H^{1}} \mathrm{~d} \sigma \mathrm{~d} s \\
& \leq C\left(M_{2}\right) \tau^{2} . \tag{4.23}
\end{align*}
$$

For $e_{2}$ in (3.38), using the estimate for $\phi \in H_{0}^{1}(\Omega) \cap H^{2}(\Omega)$,

$$
\begin{equation*}
\left\|I_{N} \phi\right\|_{H^{1}} \leq\|\phi\|_{H^{1}}+\left\|\phi-I_{N} \phi\right\|_{H^{1}} \lesssim\|\phi\|_{H^{1}}+h|\phi|_{H^{2}} \lesssim\|\phi\|_{H^{2}} \tag{4.24}
\end{equation*}
$$

one gets

$$
\begin{align*}
\left\|e_{2}\right\|_{H^{1}} & =\tau^{2}\left\|I_{N}\left(\int_{0}^{1}(1-\theta)\left(d B\left(\Phi_{B}^{\theta \tau}\left(P_{N} v_{0}\right)\right)\left[B\left(\Phi_{B}^{\theta \tau}\left(P_{N} v_{0}\right)\right)\right]\right) \mathrm{d} \theta\right)\right\|_{H^{1}} \\
& \lesssim \tau^{2}\left\|d B\left(\Phi_{B}^{\theta \tau}\left(P_{N} v_{0}\right)\right)\left[B\left(\Phi_{B}^{\theta \tau}\left(P_{N} v_{0}\right)\right)\right]\right\|_{H^{2}} \tag{4.25}
\end{align*}
$$

From (4.25), noting that

$$
\begin{equation*}
\left|\left[B\left(\Phi_{B}^{\theta \tau}\left(P_{N} v_{0}\right)\right)\right](\mathbf{x})\right| \lesssim\left|\Phi_{B}^{\theta \tau}\left(P_{N} v_{0}\right)(\mathbf{x})\right|=\left(P_{N} v_{0}\right)(\mathbf{x}), \quad \mathbf{x} \in \Omega \tag{4.26}
\end{equation*}
$$

and using Lemma 4.4, we have

$$
\begin{equation*}
\left\|e_{2}\right\|_{H^{1}} \leq C\left(M_{2}\right) \tau^{2} \tag{4.27}
\end{equation*}
$$

Then we shall estimate $e_{3}$ in (3.39). Similar to (3.45) and (3.46), it suffices to bound the $H^{1}$-norm of the four terms $e_{3}^{j}(1 \leq j \leq 4)$ defined in (3.46). Using the standard estimates (see, e.g., $[43,10]$ ),

$$
\begin{align*}
& \left\|\phi-P_{N} \phi\right\|_{H^{1}} \lesssim h|\phi|_{H^{2}}, \quad\left\|I_{N} \phi-P_{N} \phi\right\|_{H^{1}} \lesssim h|\phi|_{H^{2}},  \tag{4.28}\\
& \left\|\phi-e^{i t \Delta} \phi\right\|_{H^{1}} \lesssim \sqrt{t}\|\phi\|_{H^{2}}, \quad \phi \in H_{0}^{1}(\Omega) \cap H^{2}(\Omega), \tag{4.29}
\end{align*}
$$

and Lemmas 4.1 and 4.2, we have

$$
\begin{align*}
\left\|e_{3}^{1}\right\|_{H^{1}} & \leq C\left(M_{2}\right)\left\|e^{i s \Delta} v_{0}-v_{0}\right\|_{H^{1}} \leq C\left(M_{2}\right) \sqrt{\tau}\left\|v_{0}\right\|_{H^{2}} \leq C\left(M_{2}\right) \sqrt{\tau}  \tag{4.30}\\
\left\|e_{3}^{2}\right\|_{H^{1}} & \leq C\left(M_{2}\right)\left\|v_{0}-P_{N} v_{0}\right\|_{H^{1}} \leq C\left(M_{2}\right) h\left\|v_{0}\right\|_{H^{2}} \leq C\left(M_{2}\right) h \\
\left\|e_{3}^{3}\right\|_{H^{1}} & \lesssim \sqrt{\tau}\left\|P_{N} B\left(P_{N} v_{0}\right)\right\|_{H^{2}} \leq \sqrt{\tau}\left\|B\left(P_{N} v_{0}\right)\right\|_{H^{2}} \leq C\left(M_{2}\right) \sqrt{\tau} \\
\left\|e_{3}^{4}\right\|_{H^{1}} & \lesssim h\left\|B\left(P_{N} v_{0}\right)\right\|_{H^{2}} \leq C\left(M_{2}\right) h \tag{4.31}
\end{align*}
$$

which yields immediately

$$
\begin{equation*}
\left\|e_{3}\right\|_{H^{1}} \leq C\left(M_{2}\right) \tau(\sqrt{\tau}+h) \tag{4.32}
\end{equation*}
$$

Combining (4.23), (4.27), and (4.32), we obtain (4.19), which completes the proof.

## 4.3. $l^{\infty}$-conditional $L^{2}$ - and $H^{1}$-stability .

Proposition 4.8 ( $l^{\infty}$-conditional stability). Let $0<\tau<1$ and $v, w \in X_{N}$ such that $\|v\|_{l^{\infty}} \leq M,\|w\|_{l^{\infty}} \leq M$ and $\|v\|_{H^{2}} \leq M_{1}$. When $\sigma \geq 1 / 2$, we have

$$
\begin{align*}
& \left\|\Phi^{\tau}(v)-\Phi^{\tau}(w)\right\|_{L^{2}} \leq\left(1+C_{1}(M) \tau\right)\|v-w\|_{L^{2}}  \tag{4.33}\\
& \left\|\Phi^{\tau}(v)-\Phi^{\tau}(w)\right\|_{H^{1}} \leq\left(1+C_{2}\left(M, M_{1},\|V\|_{W^{1, \infty}}\right) \tau\right)\|v-w\|_{H^{1}} \tag{4.34}
\end{align*}
$$

Proof. The $L^{2}$-stability (4.33) can be obtained from (3.53) by using Lemma 4.6 instead of Lemma 3.4. In the following, we show the $H^{1}$-stability (4.34). By (2.6) and the isometry property of $e^{i \tau \Delta}$, (4.34) reduces to

$$
\begin{equation*}
\left\|I_{N} \Phi_{B}^{\tau}(v)-I_{N} \Phi_{B}^{\tau}(w)\right\|_{H^{1}} \leq\left(1+C\left(M, M_{1},\|V\|_{W^{1, \infty}}\right) \tau\right)\|v-w\|_{H^{1}} \tag{4.35}
\end{equation*}
$$

The proof is based on the following well-known equivalence relation (see, e.g., Lemma 3.2 in [8]): with $\delta_{x}^{+}$defined in (2.10),

$$
\begin{equation*}
\left\|\delta_{x}^{+} \phi\right\|_{l^{2}} \leq\left\|\nabla I_{N} \phi\right\|_{L^{2}} \leq \frac{\pi}{2}\left\|\delta_{x}^{+} \phi\right\|_{l^{2}}, \quad \phi \in X_{N}, \tag{4.36}
\end{equation*}
$$

which implies,
$\left\|I_{N} \Phi_{B}^{\tau}(v)-I_{N} \Phi_{B}^{\tau}(w)\right\|_{H^{1}} \leq\|v-w\|_{H^{1}}+\left\|I_{N}\left(\Phi_{B}^{\tau}(v)-v\right)-I_{N}\left(\Phi_{B}^{\tau}(w)-w\right)\right\|_{H^{1}}$

$$
\begin{equation*}
\leq\|v-w\|_{H^{1}}+C\left\|\delta_{x}^{+}\left(\Phi_{B}^{\tau}(v)-v\right)-\delta_{x}^{+}\left(\Phi_{B}^{\tau}(w)-w\right)\right\|_{l^{2}} \tag{4.37}
\end{equation*}
$$

We define

$$
\begin{aligned}
& v_{j}^{\theta}=(1-\theta) v_{j}+\theta v_{j+1}, \quad w_{j}^{\theta}=(1-\theta) w_{j}+\theta w_{j+1} \\
& V_{j}^{\theta}=(1-\theta) V\left(x_{j}\right)+\theta V\left(x_{j+1}\right), \quad 0 \leq \theta \leq 1, \quad j=0, \cdots, N-1
\end{aligned}
$$

By some elementary calculations, recalling (3.4) and $f^{\prime}\left(|z|^{2}\right)|z|^{2}=\sigma f\left(|z|^{2}\right)$, one gets, for $0 \leq j \leq N-1$,

$$
\begin{align*}
& \delta_{x}^{+}\left(\Phi_{B}^{\tau}(v)-v\right)_{j}=\delta_{x}^{+}\left(v\left(e^{-i \tau\left(V+f\left(|v|^{2}\right)\right)}-1\right)\right)_{j} \\
& =\frac{1}{h} \int_{0}^{1} \frac{\mathrm{~d}}{\mathrm{~d} \theta}\left(v_{j}^{\theta}\left(e^{-i \tau\left(V_{j}^{\theta}+f\left(\left|v_{j}^{\theta}\right|^{2}\right)\right)}-1\right)\right) \mathrm{d} \theta \\
& =\int_{0}^{1}\left[\delta_{x}^{+} v_{j}\left(e^{-i \tau\left(V_{j}^{\theta}+f\left(\left|v_{j}^{\theta}\right|^{2}\right)\right)}-1\right)-i \tau e^{-i \tau V_{j}^{\theta}} v_{j}^{\theta} \delta_{x}^{+} V\left(x_{j}\right) e^{-i \tau f\left(\left|v_{j}^{\theta}\right|^{2}\right)}\right. \\
& \left.\quad-i \tau e^{-i \tau V_{j}^{\theta}}\left(\sigma f\left(\left|v_{j}^{\theta}\right|^{2}\right) \delta_{x}^{+} v_{j}+G\left(v_{j}^{\theta}\right) \delta_{x}^{+} \overline{v_{j}}\right) e^{-i \tau f\left(\left|v_{j}^{\theta}\right|^{2}\right)}\right] \mathrm{d} \theta \tag{4.38}
\end{align*}
$$

Similarly, for $0 \leq j \leq N-1$,

$$
\begin{align*}
& \delta_{x}^{+}\left(\Phi_{B}^{\tau}(w)-w\right)_{j} \\
& =\int_{0}^{1}\left[\delta_{x}^{+} w_{j}\left(e^{-i \tau\left(V_{j}^{\theta}+f\left(\left|w_{j}^{\theta}\right|^{2}\right)\right)}-1\right)-i \tau e^{-i \tau V_{j}^{\theta}} w_{j}^{\theta} \delta_{x}^{+} V\left(x_{j}\right) e^{-i \tau f\left(\left|w_{j}^{\theta}\right|^{2}\right)}\right. \\
& \left.\quad-i \tau e^{-i \tau V_{j}^{\theta}}\left(\sigma f\left(\left|w_{j}^{\theta}\right|^{2}\right) \delta_{x}^{+} w_{j}+G\left(w_{j}^{\theta}\right) \delta_{x}^{+} \overline{w_{j}}\right) e^{-i \tau f\left(\left|w_{j}^{\theta}\right|^{2}\right)}\right] \mathrm{d} \theta \tag{4.39}
\end{align*}
$$

We define the function $e \in Y_{N}$ with

$$
e_{j}=v_{j}-w_{j}, \quad j=0, \cdots, N
$$

Subtracting (4.39) from (4.38), for $0 \leq j \leq N-1$, we have

$$
\begin{align*}
&\left|\delta_{x}^{+}\left(\Phi_{B}^{\tau}(v)-v\right)_{j}-\delta_{x}^{+}\left(\Phi_{B}^{\tau}(w)-w\right)_{j}\right| \\
& \leq \int_{0}^{1}\left[\left|\delta_{x}^{+} v_{j}\left(e^{-i \tau\left(V_{j}^{\theta}+f\left(\left|v_{j}^{\theta}\right|^{2}\right)\right)}-1\right)-\delta_{x}^{+} w_{j}\left(e^{-i \tau\left(V_{j}^{\theta}+f\left(\left|w_{j}^{\theta}\right|^{2}\right)\right)}-1\right)\right|\right. \\
&+\tau\left|\delta_{x}^{+} V\left(x_{j}\right)\right|\left|v_{j}^{\theta} e^{-i \tau f\left(\left|v_{j}^{\theta}\right|^{2}\right)}-w_{j}^{\theta} e^{-i \tau f\left(\left|w_{j}^{\theta}\right|^{2}\right)}\right| \\
&+\sigma \tau\left|\delta_{x}^{+} v_{j} f\left(\left|v_{j}^{\theta}\right|^{2}\right) e^{-i \tau f\left(\left|v_{j}^{\theta}\right|^{2}\right)}-\delta_{x}^{+} w_{j} f\left(\left|w_{j}^{\theta}\right|^{2}\right) e^{-i \tau f\left(\left|w_{j}^{\theta}\right|^{2}\right)}\right| \\
&\left.+\tau\left|\delta_{x}^{+} \overline{v_{j}} G\left(v_{j}^{\theta}\right) e^{-i \tau f\left(\left|v_{j}^{\theta}\right|^{2}\right)}-\delta_{x}^{+} \overline{w_{j}} G\left(w_{j}^{\theta}\right) e^{-i \tau f\left(\left|w_{j}^{\theta}\right|^{2}\right)}\right|\right] \mathrm{d} \theta \\
&= \int_{0}^{1}\left(J_{j}^{1}+J_{j}^{2}+J_{j}^{3}+J_{j}^{4}\right) \mathrm{d} \theta . \tag{4.40}
\end{align*}
$$

For $J_{j}^{1}$, by (4.9), one gets

$$
\begin{align*}
J_{j}^{1} \leq & \left|\delta_{x}^{+} v_{j}\right|\left|e^{-i \tau\left(V_{j}^{\theta}+f\left(\left|v_{j}^{\theta}\right|^{2}\right)\right)}-e^{-i \tau\left(V_{j}^{\theta}+f\left(\left|w_{j}^{\theta}\right|^{2}\right)\right)}\right| \\
& +\left|\delta_{x}^{+} v_{j}-\delta_{x}^{+} w_{j}\right|\left|e^{-i \tau\left(V_{j}^{\theta}+f\left(\left|w_{j}^{\theta}\right|^{2}\right)\right)}-1\right| \\
\leq & \tau\left|\delta_{x}^{+} v_{j}\right|\left|f\left(\left|v_{j}^{\theta}\right|^{2}\right)-f\left(\left|w_{j}^{\theta}\right|^{2}\right)\right|+\tau\left|V_{j}^{\theta}+f\left(\left|w_{j}^{\theta}\right|^{2}\right)\right|\left|\delta_{x}^{+} v_{j}-\delta_{x}^{+} w_{j}\right| \\
\leq & C(M) \tau\left|\delta_{x}^{+} v_{j}\right|\left(\left|e_{j}\right|+\left|e_{j+1}\right|\right)+C\left(M,\|V\|_{L^{\infty}}\right) \tau\left|\delta_{x}^{+} e_{j}\right| . \tag{4.41}
\end{align*}
$$

For $J_{j}^{2}$, recalling (2.7), by Lemma 4.6 and $0<\tau<1$, one gets

$$
\begin{align*}
J_{j}^{2} & =\tau\left|\delta_{x}^{+} V\left(x_{j}\right)\right|\left|\Phi_{B_{2}}^{\tau}\left(v_{j}^{\theta}\right)-\Phi_{B_{2}}^{\tau}\left(w_{j}^{\theta}\right)\right| \\
& \leq \tau\left|\delta_{x}^{+} V\left(x_{j}\right)\right|(1+C(M) \tau)\left(\left|e_{j}\right|+\left|e_{j+1}\right|\right) \\
& \leq C(M) \tau\left|\delta_{x}^{+} V\left(x_{j}\right)\right|\left(\left|e_{j}\right|+\left|e_{j+1}\right|\right) \tag{4.42}
\end{align*}
$$

For $J_{j}^{3}$, by (4.9) and $0<\tau<1$, one gets

$$
\begin{aligned}
J_{j}^{3} \lesssim & \tau\left|\delta_{x}^{+} v_{j}\right|\left|f\left(\left|v_{j}^{\theta}\right|^{2}\right) e^{-i \tau f\left(\left|v_{j}^{\theta}\right|^{2}\right)}-f\left(\left|w_{j}^{\theta}\right|^{2}\right) e^{-i \tau f\left(\left|w_{j}^{\theta}\right|^{2}\right)}\right| \\
& +\tau\left|\delta_{x}^{+} v_{j}-\delta_{x}^{+} w_{j}\right|\left|f\left(\left|w_{j}^{\theta}\right|^{2}\right) e^{-i \tau f\left(\left|w_{j}^{\theta}\right|^{2}\right)}\right| \\
\leq & \tau\left|\delta_{x}^{+} v_{j}\right|\left(\left|f\left(\left|v_{j}^{\theta}\right|^{2}\right)-f\left(\left|w_{j}^{\theta}\right|^{2}\right)\right|+\left|f\left(\left|w_{j}^{\theta}\right|^{2}\right)\right|\left|e^{-i \tau f\left(\left|v_{j}^{\theta}\right|^{2}\right)}-e^{-i \tau f\left(\left|w_{j}^{\theta}\right|^{2}\right)}\right|\right) \\
& +\tau C(M)\left|\delta_{x}^{+} v_{j}-\delta_{x}^{+} w_{j}\right| \\
\leq & \tau\left|\delta_{x}^{+} v_{j}\right| C(M)(1+\tau)\left|v_{j}^{\theta}-w_{j}^{\theta}\right|+\tau C(M)\left|\delta_{x}^{+} v_{j}-\delta_{x}^{+} w_{j}\right| \\
(4.43) \leq & C(M) \tau\left|\delta_{x}^{+} v_{j}\right|\left(\left|e_{j}\right|+\left|e_{j+1}\right|\right)+C(M) \tau\left|\delta_{x}^{+} e_{j}\right| .
\end{aligned}
$$

Similar to (4.43), using (4.10) instead of (4.9), one gets, for $J_{j}^{4}$,

$$
\begin{equation*}
J_{j}^{4} \leq C(M) \tau\left|\delta_{x}^{+} v_{j}\right|\left(\left|e_{j}\right|+\left|e_{j+1}\right|\right)+C(M) \tau\left|\delta_{x}^{+} e_{j}\right| \tag{4.44}
\end{equation*}
$$

Plugging (4.41)-(4.44) into (4.40), we have

$$
\begin{aligned}
& \left|\delta_{x}^{+}\left(\Phi_{B}^{\tau}(v)-v\right)_{j}-\delta_{x}^{+}\left(\Phi_{B}^{\tau}(w)-w\right)_{j}\right| \\
& \leq C(M) \tau\left(\left|\delta_{x}^{+} V\left(x_{j}\right)\right|+\left|\delta_{x}^{+} v_{j}\right|\right)\left(\left|e_{j}\right|+\left|e_{j+1}\right|\right)+C\left(M,\|V\|_{L^{\infty}}\right) \tau\left|\delta_{x}^{+} e_{j}\right|
\end{aligned}
$$

which yields

$$
\begin{align*}
&\left\|\delta_{x}^{+}\left(\Phi_{B}^{\tau}(v)-v\right)-\delta_{x}^{+}\left(\Phi_{B}^{\tau}(w)-w\right)\right\|_{l^{2}}^{2} \\
&= h \sum_{j=0}^{N-1}\left|\delta_{x}^{+}\left(\Phi_{B}^{\tau}(v)-v\right)_{j}-\delta_{x}^{+}\left(\Phi_{B}^{\tau}(w)-w\right)_{j}\right|^{2} \\
& \leq C(M) \tau^{2} h \sum_{j=0}^{N-1}\left(\left|\delta_{x}^{+} V\left(x_{j}\right)\right|^{2}+\left|\delta_{x}^{+} v_{j}\right|^{2}\right)\left(\left|e_{j}\right|^{2}+\left|e_{j+1}\right|^{2}\right) \\
&+C\left(M,\|V\|_{L^{\infty}}\right) \tau^{2} h \sum_{j=0}^{N-1}\left|\delta_{x}^{+} e_{j}\right|^{2} \\
& \leq C(M) \tau^{2}\left(\|\nabla V\|_{L^{\infty}}^{2}\|e\|_{l^{2}}^{2}+h \sum_{j=0}^{N-1}\left|\delta_{x}^{+} v_{j}\right|^{2}\left(\left|e_{j}\right|^{2}+\left|e_{j+1}\right|^{2}\right)\right) \\
&+C\left(M,\|V\|_{L^{\infty}}\right) \tau^{2}\left\|\delta_{x}^{+} e\right\|_{l^{2}}^{2} . \tag{4.45}
\end{align*}
$$

When $d=1$, one has $\left|\delta_{x}^{+} v_{j}\right| \leq\|\nabla v\|_{L^{\infty}} \leq C\left(M_{1}\right)$, which yields directly that

$$
\begin{equation*}
h \sum_{j=0}^{N-1}\left|\delta_{x}^{+} v_{j}\right|^{2}\left(\left|e_{j}\right|^{2}+\left|e_{j+1}\right|^{2}\right) \leq C\left(M_{1}\right)\|e\|_{l^{2}}^{2} \tag{4.46}
\end{equation*}
$$

However, (4.46) cannot be directly generalized to 2 D and 3 D without assuming higher regularity on $v$. Here, we present an alternative approach that can be generalized to 2D and 3D (see also Remark 4.9). Using the discrete Gagliardo-Nirenberg
inequality $((2.4)$ in [1] or (3.3) in [7]) and the discrete Poincaré inequality ((3.3) in [7]), we have

$$
\begin{equation*}
\|\phi\|_{l^{4}} \lesssim\|\phi\|_{l^{2}}^{\frac{3}{4}}\left\|\delta_{x}^{+} \phi\right\|_{l^{2}}^{\frac{1}{4}} \lesssim\left\|\delta_{x}^{+} \phi\right\|_{l^{2}}, \quad \phi \in Y_{N} \tag{4.47}
\end{equation*}
$$

which implies, by first applying Hölder's inequality in (4.46),

$$
\begin{equation*}
h \sum_{j=0}^{N-1}\left|\delta_{x}^{+} v_{j}\right|^{2}\left(\left|e_{j}\right|^{2}+\left|e_{j+1}\right|^{2}\right) \lesssim\left\|\delta_{x}^{+} v\right\|_{l^{4}}^{2}\|e\|_{l^{4}}^{2} \lesssim\left\|\delta_{x}^{+} v\right\|_{l^{4}}^{2}\left\|\delta_{x}^{+} e\right\|_{l^{2}}^{2} \tag{4.48}
\end{equation*}
$$

Using the following discrete version of the Sobolev embedding $H^{2} \hookrightarrow W^{1,4}$ (see (3.3) in [7] and also the appendix)

$$
\begin{equation*}
\left\|\delta_{x}^{+} \phi\right\|_{l^{4}} \lesssim\|\phi\|_{H^{2}}, \quad \phi \in X_{N} \tag{4.49}
\end{equation*}
$$

we get $\left\|\delta_{x}^{+} v\right\|_{l^{4}} \lesssim\|v\|_{H^{2}} \leq M_{1}$, which plugged into (4.48) yields from (4.45)

$$
\begin{align*}
& \left\|\delta_{x}^{+}\left(\Phi_{B}^{\tau}(v)-v\right)-\delta_{x}^{+}\left(\Phi_{B}^{\tau}(w)-w\right)\right\|_{l^{2}}^{2} \\
& \leq C\left(M, M_{1},\|V\|_{W^{1, \infty}}\right)\left(\|e\|_{l^{2}}^{2}+\left\|\delta_{x}^{+} e\right\|_{l^{2}}^{2}\right) \tag{4.50}
\end{align*}
$$

From (4.50), using the discrete Poincaré inequality and (3.27) and (4.36), we have

$$
\begin{align*}
\left\|\delta_{x}^{+}\left(\Phi_{B}^{\tau}(v)-v\right)-\delta_{x}^{+}\left(\Phi_{B}^{\tau}(w)-w\right)\right\|_{l^{2}}^{2} & \leq C\left(M, M_{1},\|V\|_{W^{1, \infty}}\right)\left\|\delta_{x}^{+} e\right\|_{l^{2}}^{2} \\
& \leq C\left(M, M_{1},\|V\|_{W^{1, \infty}}\right)\left\|\nabla I_{N} e\right\|_{L^{2}}^{2} \tag{4.51}
\end{align*}
$$

which plugged into (4.37) yields (4.35), and completes the proof.
Remark 4.9. The 2D case follows exactly (4.47)-(4.49). The proof of (4.49) in 2D proceeds similarly to our proof in 1D in the appendix by following the proof of (3.3) in [7] with additional attention paid to the boundary terms. The 3D case follows (4.47)-(4.49) with slight modification: using Hölder's inequality with index $(3 / 2,3)$ in (4.48). Then the discrete version of $H^{1} \hookrightarrow L^{6}$ and $H^{2} \hookrightarrow W^{1,3}$ in 3D are needed. The proof of the first one can be found in [40] while the proof of the second one will follow the proof of (4.49) in 2D, which is the reason why we modify the estimates in 3D.
4.4. Proof of (2.42) in Theorem 2.7. With Propositions 4.7 and 4.8, we are able to obtain (2.42).

Proof of (2.42) in Theorem 2.7. Following the proof of Theorem 2.7, we only need to estimate $e^{k}=I_{N} \psi^{k}-P_{N} \psi\left(\cdot, t_{k}\right)$ for $0 \leq k \leq T / \tau$. We shall first prove the error estimate in $H^{1}$ norm by the standard argument of the mathematical induction. Replacing $\|\cdot\|_{L^{2}}$ with $\|\cdot\|_{H^{1}}$ in (3.55), one has for $0 \leq k \leq T / \tau-1$,

$$
\begin{align*}
\left\|e^{k+1}\right\|_{H^{1}} \leq & \left\|\Phi^{\tau}\left(I_{N} \psi^{k}\right)-\Phi^{\tau}\left(P_{N} \psi\left(\cdot, t_{k}\right)\right)\right\|_{H^{1}} \\
& +\left\|\Phi^{\tau}\left(P_{N} \psi\left(\cdot, t_{k}\right)\right)-P_{N} \psi\left(\cdot, t_{k+1}\right)\right\|_{H^{1}} . \tag{4.52}
\end{align*}
$$

When $k=0$, by (4.28), one gets

$$
\left\|e^{0}\right\|_{H^{1}}=\left\|I_{N} \psi_{0}-P_{N} \psi_{0}\right\|_{H^{1}} \lesssim h\left\|\psi_{0}\right\|_{H^{2}} \leq C\left(M_{2}\right) h,\left\|\psi^{0}\right\|_{l^{\infty}} \leq\left\|\psi_{0}\right\|_{L^{\infty}} \leq 1+M_{2}
$$

We assume that for $0 \leq k \leq m \leq T / \tau-1$,

$$
\begin{equation*}
\left\|e^{k}\right\|_{H^{1}} \lesssim \tau^{\frac{1}{2}}+h, \quad\left\|\psi^{k}\right\|_{l \infty} \leq 1+M_{2} \tag{4.53}
\end{equation*}
$$

We shall prove (4.53) for $m+1$. From (4.52), using (4.19) and (4.34), and noting the assumption (4.53), we have

$$
\begin{equation*}
\left\|e^{m+1}\right\|_{H^{1}} \leq\left(1+C_{1} \tau\right)\left\|e^{m}\right\|_{H^{1}}+C_{2} \tau\left(\tau^{\frac{1}{2}}+h\right) \tag{4.54}
\end{equation*}
$$

where $C_{1}$ and $C_{2}$ are the constants in (4.19) and (4.34) respectively, which depend exclusively on $M_{2}$ and $\|V\|_{W^{1, \infty}}$. From (4.54), standard discrete Gronwall's inequality yields

$$
\begin{equation*}
\left\|e^{m+1}\right\|_{H^{1}} \leq 2 e^{C_{0} T} C_{1}\left(\tau^{\frac{1}{2}}+h\right) \tag{4.55}
\end{equation*}
$$

Recalling that $e^{k}=I_{N} \psi^{k}-P_{N} \psi\left(t_{k}\right)$ and $\left\|\psi\left(\cdot, t_{k}\right)\right\|_{L^{\infty}} \leq M_{2}$, using the inverse inequality $\|\phi\|_{L^{\infty}} \lesssim h^{-1 / 2}\|\phi\|_{L^{2}}, \phi \in X_{N}$ [43], we have

$$
\begin{aligned}
\left\|\psi^{m+1}\right\|_{l^{\infty}} & =\left\|I_{N} \psi^{m+1}\right\|_{l^{\infty}} \leq\left\|e^{m+1}\right\|_{l^{\infty}}+\left\|P_{N} \psi\left(\cdot, t_{m+1}\right)\right\|_{l^{\infty}} \\
& \leq\left\|e^{m+1}\right\|_{l^{\infty}}+\left\|\psi\left(\cdot, t_{m+1}\right)-P_{N} \psi\left(\cdot, t_{m+1}\right)\right\|_{l^{\infty}}+\left\|\psi\left(\cdot, t_{m+1}\right)\right\|_{l^{\infty}} \\
& \leq\left\|e^{m+1}\right\|_{l^{\infty}}+h^{-\frac{1}{2}}\left\|\psi\left(\cdot, t_{m+1}\right)-P_{N} \psi\left(\cdot, t_{m+1}\right)\right\|_{L^{2}}+M_{2}
\end{aligned}
$$

Hence, for $\tau \leq \tau_{0}$ and $h \leq h_{0}$ with $\tau_{0}>0$ and $h_{0}>0$ depending on $M_{2}$ and $T$, by Sobolev embedding $H^{1} \hookrightarrow L^{\infty}$ in 1 D , and (3.19) and (4.55), we have

$$
\begin{equation*}
\left\|\psi^{m+1}\right\|_{l^{\infty}} \leq C\left\|e^{m+1}\right\|_{H^{1}}+C h^{2-1 / 2}+M_{2} \leq 1+M_{2} \tag{4.56}
\end{equation*}
$$

Combining (4.55) and (4.56) proves (4.53) for $k=m+1$ and thus for all $0 \leq k \leq T / \tau$ by mathematical induction. With the $l^{\infty}$-bound of the numerical solution, the $L^{2}$ estimate of $e^{k}$ follows the proof of Theorem 2.5 by using (4.18) and (4.33), which completes the proof of (2.42).

Remark 4.10. In 2D and 3D, we no longer have $H^{1} \hookrightarrow L^{\infty}$. To obtain the $l^{\infty}$-bound of $\psi^{m+1}$ in (4.56), we use the discrete Sobolev inequalities as in $[5,7,8]$

$$
\|v\|_{l^{\infty}} \leq C|\ln h|\left\|I_{N} v\right\|_{H^{1}}, \quad\|w\|_{l^{\infty}} \leq C h^{-1 / 2}\left\|I_{N} w\right\|_{H^{1}}
$$

where $v$ and $w$ are 2 D and 3 D mesh functions with zero at the boundary, respectively, and the interpolation operator $I_{N}$ can be defined similarly in 2 D and 3 D as in 1D. Thus by requiring that the time step size $\tau$ satisfies the additional assumption (B), we can control the $l^{\infty}$-norm of the numerical solution.
4.5. Proof of (2.43) in Theorem 2.7. In the following, we assume that $1 / 2<$ $\sigma<1, V \in H^{3}(\Omega), \nabla V \in H_{0}^{1}(\Omega), \psi \in C\left([0, T] ; H_{*}^{3}(\Omega)\right) \cap C^{1}\left([0, T] ; H^{1}(\Omega)\right)$ and let

$$
\begin{equation*}
M_{3}:=\max \left\{\|\psi\|_{L^{\infty}\left([0, T] ; H^{3}\right)},\|\psi\|_{L^{\infty}\left([0, T] ; L^{\infty}\right)},\|V\|_{H^{3}}\right\} . \tag{4.57}
\end{equation*}
$$

We first show an analogous result of Lemma 3.5.
Lemma 4.11. Let $\phi \in X_{N}$ such that $\|\phi\|_{H^{3}} \leq M$ and let $0<\tau<1$ and $0<h<1$. Assume that $V \in H^{3}(\Omega)$ and $\nabla V \in H_{0}^{1}(\Omega)$. When $1 / 2<\sigma<1$, we have

$$
\begin{align*}
& \left\|\left(I-e^{i \tau \Delta}\right) P_{N} B(\phi)\right\|_{H^{1}} \leq C_{1}\left(M,\|V\|_{H^{3}}\right) \tau^{\sigma}  \tag{4.58}\\
& \left\|I_{N} B(\phi)-P_{N} B(\phi)\right\|_{H^{1}} \leq C_{2}\left(M,\|V\|_{H^{3}}\right) h^{2 \sigma} \tag{4.59}
\end{align*}
$$

Proof. Similar to (3.21), noting that $V \phi \in H_{*}^{3}(\Omega)$, we have

$$
\begin{align*}
& \left\|\left(I-e^{i \tau \Delta}\right)(V \phi)\right\|_{H^{1}} \lesssim \tau\|V\|_{H^{3}}\|\phi\|_{H^{3}}, \\
& \left\|\left(I_{N}-P_{N}\right)(V \phi)\right\|_{H^{1}} \lesssim h^{2}\|V\|_{H^{3}}\|\phi\|_{H^{3}} . \tag{4.60}
\end{align*}
$$

Following (3.22) and (3.23) with $\|\cdot\|_{H^{1}}$ replacing $\|\cdot\|_{L^{2}}$ and using (2.31), we have

$$
\begin{equation*}
\left\|\left(I-e^{i \tau \Delta}\right)\left(f\left(|\phi|^{2}\right) \phi\right)\right\|_{H^{1}} \leq 2\left\|f\left(|\phi|^{2}\right) \phi-f_{\varepsilon}\left(|\phi|^{2}\right) \phi\right\|_{H^{1}}+C(M) \frac{\tau}{\varepsilon^{2-2 \sigma}} \tag{4.61}
\end{equation*}
$$

By direct calculation, recalling (3.4), one gets

$$
\begin{align*}
& \nabla\left[f\left(|\phi|^{2}\right) \phi-f_{\varepsilon}\left(|\phi|^{2}\right) \phi\right]=\left(f\left(|\phi|^{2}\right)-f_{\varepsilon}\left(|\phi|^{2}\right)\right) \nabla \phi \\
& +\left(f^{\prime}\left(|\phi|^{2}\right)|\phi|^{2}-f_{\varepsilon}^{\prime}\left(|\phi|^{2}\right)|\phi|^{2}\right) \nabla \phi+\left(G(\phi)-f_{\varepsilon}^{\prime}\left(|\phi|^{2}\right) \phi^{2}\right) \nabla \bar{\phi} \tag{4.62}
\end{align*}
$$

Noting that $f^{\prime}\left(|z|^{2}\right)|z|^{2}=f_{\varepsilon}^{\prime}\left(|z|^{2}\right)|z|^{2}, G(z)=f_{\varepsilon}^{\prime}\left(|z|^{2}\right) z^{2}$ when $|z| \geq \varepsilon$ and $f^{\prime}\left(|z|^{2}\right)|z|^{2}+$ $f_{\varepsilon}^{\prime}\left(|z|^{2}\right)|z|^{2}+|G(z)|+\left|f_{\varepsilon}^{\prime}\left(|z|^{2}\right) z^{2}\right| \lesssim \varepsilon^{2 \sigma}$ when $|z|<\varepsilon$, one gets
$\left.\left|f^{\prime}\left(|z|^{2}\right)\right| z\right|^{2}-f_{\varepsilon}^{\prime}\left(|z|^{2}\right)|z|^{2}\left|\lesssim \varepsilon^{2 \sigma} \mathbb{1}_{|z|<\varepsilon}, \quad\right| G(z)-f_{\varepsilon}^{\prime}\left(|z|^{2}\right) z^{2} \mid \lesssim \varepsilon^{2 \sigma} \mathbb{1}_{|z|<\varepsilon}, \quad z \in \mathbb{C}$,
which together with Lemma 2.4 applied to (4.62) yields

$$
\begin{equation*}
\left\|\nabla\left[f\left(|\phi|^{2}\right) \phi-f_{\varepsilon}\left(|\phi|^{2}\right) \phi\right]\right\|_{L^{2}} \lesssim \varepsilon^{2 \sigma}\left\|\nabla \phi \mathbb{1}_{|\phi|<\varepsilon}\right\|_{L^{2}} \leq \varepsilon^{2 \sigma}\|\phi\|_{H^{1}} \tag{4.63}
\end{equation*}
$$

Plugging (4.63) into (4.61), we have

$$
\left\|\left(I-e^{i \tau \Delta}\right)\left(f\left(|\phi|^{2}\right) \phi\right)\right\|_{H^{1}} \leq C(M) \inf _{0<\varepsilon<1}\left(\varepsilon^{2 \sigma}+\frac{\tau}{\varepsilon^{2-2 \sigma}}\right) \leq C(M) \tau^{\sigma}
$$

which combined with (4.60) yields (4.58).
Then we shall show (4.28). Following (3.26) with $\|\cdot\|_{H^{1}}$ replacing $\|\cdot\|_{L^{2}}$, using the standard estimates of $P_{N}$, and (2.31) and (4.63), one gets

$$
\begin{align*}
& \left\|\left(I_{N}-P_{N}\right)\left(f\left(|\phi|^{2}\right) \phi\right)\right\|_{H^{1}} \\
& \leq\left\|I_{N}\left(f\left(|\phi|^{2}\right) \phi-f_{\varepsilon}\left(|\phi|^{2}\right) \phi\right)\right\|_{H^{1}}+\varepsilon^{2 \sigma}\|\phi\|_{H^{1}}+h^{2} \frac{C(M)}{\varepsilon^{2-2 \sigma}} \tag{4.64}
\end{align*}
$$

Using (4.36), one gets

$$
\begin{equation*}
\left\|\nabla I_{N}\left(f\left(|\phi|^{2}\right) \phi-f_{\varepsilon}\left(|\phi|^{2}\right) \phi\right)\right\|_{L^{2}} \lesssim\left\|\delta_{x}^{+}\left(f\left(|\phi|^{2}\right) \phi-f_{\varepsilon}\left(|\phi|^{2}\right) \phi\right)\right\|_{l^{2}} \tag{4.65}
\end{equation*}
$$

Let $\phi_{j}^{\theta}=(1-\theta) \phi_{j}+\theta \phi_{j+1}$ for $0 \leq \theta \leq 1$ and $0 \leq j \leq N-1$, direct calculation gives

$$
\begin{align*}
& \delta_{x}^{+}\left(f\left(\left|\phi_{j}\right|^{2}\right) \phi_{j}-f_{\varepsilon}\left(\left|\phi_{j}\right|^{2}\right) \phi_{j}\right)=\frac{1}{h} \int_{0}^{1} \frac{\mathrm{~d}}{\mathrm{~d} \theta}\left(f\left(\left|\phi_{j}^{\theta}\right|^{2}\right) \phi_{j}^{\theta}-f_{\varepsilon}\left(\left|\phi_{j}^{\theta}\right|^{2}\right) \phi_{j}^{\theta}\right) \mathrm{d} \theta \\
& =\int_{0}^{1}\left[\left(\left(f\left(\left|\phi_{j}^{\theta}\right|^{2}\right)+f^{\prime}\left(\left|\phi_{j}^{\theta}\right|^{2}\right)\left|\phi_{j}^{\theta}\right|^{2}\right)-\left(f_{\varepsilon}\left(\left|\phi_{j}^{\theta}\right|^{2}\right)+f_{\varepsilon}^{\prime}\left(\left|\phi_{j}^{\theta}\right|^{2}\right)\left|\phi_{j}^{\theta}\right|^{2}\right)\right) \delta_{x}^{+} \phi_{j}\right. \\
& \left.\quad+\left(G\left(\phi_{j}^{\theta}\right)-f_{\varepsilon}^{\prime}\left(\left|\phi_{j}^{\theta}\right|^{2}\right)\left(\phi_{j}^{\theta}\right)^{2}\right) \delta_{x}^{+} \overline{\phi_{j}}\right] \mathrm{d} \theta \tag{4.66}
\end{align*}
$$

which implies, similar to the way we obtain (4.63) from (4.62),

$$
\begin{equation*}
\left|\delta_{x}^{+}\left(f\left(\left|\phi_{j}\right|^{2}\right) \phi_{j}-f_{\varepsilon}\left(\left|\phi_{j}\right|^{2}\right) \phi_{j}\right)\right| \lesssim \varepsilon^{2 \sigma}\left|\delta_{x}^{+} \phi_{j}\right| \tag{4.67}
\end{equation*}
$$

From (4.65), using (4.67) and recalling (4.36) and $\phi \in X_{N}$, we obtain

$$
\begin{equation*}
\left\|\nabla I_{N}\left(f\left(|\phi|^{2}\right) \phi-f_{\varepsilon}\left(|\phi|^{2}\right) \phi\right)\right\|_{L^{2}} \lesssim \varepsilon^{2 \sigma}\left\|\delta_{x}^{+} \phi\right\|_{l^{2}} \leq \varepsilon^{2 \sigma}\|\nabla \phi\|_{L^{2}} \tag{4.68}
\end{equation*}
$$

which plugged into (4.64) yields

$$
\left\|\left(I_{N}-P_{N}\right)\left(f\left(|\phi|^{2}\right) \phi\right)\right\|_{H^{1}} \leq C(M) \inf _{0<\varepsilon<1}\left(\varepsilon^{2 \sigma}+\frac{h^{2}}{\varepsilon^{2-2 \sigma}}\right) \leq C(M) h^{2 \sigma}
$$

which combined with (4.60) yields (4.59) and completes the proof.

Proposition 4.12 (local truncation error). Assume that $V \in H^{3}(\Omega), \nabla V \in$ $H_{0}^{1}(\Omega), \psi \in C\left([0, T] ; H_{*}^{3}(\Omega)\right) \cap C^{1}\left([0, T] ; H^{1}(\Omega)\right)$ and $1 / 2<\sigma<1$. For $0 \leq$ $k \leq T / \tau-1$, we have

$$
\left\|P_{N} \psi\left(\cdot, t_{k+1}\right)-\Phi^{\tau}\left(P_{N} \psi\left(\cdot, t_{k}\right)\right)\right\|_{H^{1}(\Omega)} \leq C\left(M_{3}\right) \tau\left(\tau^{\sigma}+h^{2 \sigma}\right)
$$

Proof. Following the proof of Proposition 4.7, we only need to modify the estimate (4.30) and (4.31), which can be easily done by using the assumption $\psi \in$ $C\left([0, T] ; H^{3}\right)$, Lemma 4.11, and the standard estimates of the operators $I_{N}-P_{N}$, $I-P_{N}$ and $I-e^{i \tau \Delta}$.

Proof of (2.43) in Theorem 2.7. Using Proposition 4.12 and (4.34) in (4.52), and noting the $l^{\infty}$-bound of the numerical solution in (2.42), then (2.43) follows from the discrete Gronwall's inequality immediately.

## 5. Numerical results

In this section, we present some numerical examples for the NLSE (1.1) with $0<\sigma<1$ in 1D to confirm our error estimates. Since we are mainly interested in the semi-smooth nonlinearity, we choose $V(x) \equiv 0$, and consider the following two initial set-ups:

Type I: We consider the smooth initial datum

$$
\begin{equation*}
\psi_{0}(x)=x e^{-\frac{x^{2}}{2}}, \quad x \in \Omega=(-16,16) . \tag{5.1}
\end{equation*}
$$

Type II: We consider the initial datum in $H^{2}(\Omega)$ as in [31]

$$
\begin{align*}
& \psi_{0}=\frac{\phi^{(1)}}{\left\|\phi^{(1)}\right\|_{L^{2}}}, \quad \phi^{(1)}(x)=\sum_{l \in \mathcal{T}_{N}} \widetilde{\phi}_{l}^{(1)} \sin \left(\mu_{l}(x-a)\right), \quad x \in \Omega=(-1,1), \\
& \widetilde{\phi}_{l}^{(1)}=\frac{\widetilde{\phi}_{l}}{\left|\mu_{l}\right|^{2.5}}, \quad \widetilde{\phi}_{l}= \begin{cases}\operatorname{rand}(-1,1)+i \operatorname{rand}(-1,1), & l \text { even }, \quad l \in \mathcal{T}_{N} . \\
0, & l \text { odd },\end{cases} \tag{5.2}
\end{align*}
$$

where $\operatorname{rand}(-1,1)$ returns a uniformly distributed random number between -1 and 1.

Note that both Types I and II initial data are chosen as odd functions to demonstrate the influence of the semi-smoothness of $f$ at the origin since with an odd initial datum, the exact solution satisfies $\psi(0, t) \equiv 0$ for all $t \geq 0$. In Figure 5.1 (a), we plot the density of the wave functions at $t=1$ with different $\sigma=0.1,0.25,0.5,1$ and $\beta=-10$ for the Type I initial datum. We observe that the solution of the smooth case $(\sigma=1)$ lies between the solution of the case $\sigma=0.1$ and $\sigma=0.5$, and is close to the solution of the case $\sigma=0.25$. In Figure 5.1 (b), we plot the relative errors of the energy divided by $\tau$ up to $t=8$ for $\sigma=0.1$ and different $\tau=0.05,0.01,0.002$. We see that the relative error of the energy is at $O(\tau)$ with fixed mesh size $h$.

In the following, we shall test the errors of the TSSP in $L^{2}$ - and $H^{1}$-norms. We fix $d=1, T=1$ and $\beta=-1$. The NLSE (1.1) is then solved by the TSSP method on the domain $\Omega$ with Type I and Type II initial setups for different $\sigma>0$. The 'exact' solution is obtained numerically by the Strang splitting sine pseudospectral method with a very fine mesh size $h_{e}=2^{-9}$ and a small time step size $\tau_{e}=10^{-6}$. In our numerical experiments below, when testing the temporal convergence, we


Figure 5.1. (a) density $|\psi(x, 1)|^{2}$ with different $\sigma>0$ and (b) relative errors of the energy divided by $\tau$ up to $t=8$ with $\sigma=0.1$ for the Type I initial datum (5.1) with $\beta=-10$.
always fix the mesh size $h=h_{e}$. To quantify the error, we introduce the following error functions:

$$
e_{L^{2}}^{k}=\left\|\psi\left(\cdot, t_{k}\right)-I_{N} \psi^{k}\right\|_{L^{2}}, \quad e_{H^{1}}^{k}=\left\|\psi\left(\cdot, t_{k}\right)-I_{N} \psi^{k}\right\|_{H^{1}}, \quad 0 \leq k \leq n:=T / \tau
$$

Figure 5.2 exhibits the temporal and spatial errors in $L^{2}$-norm of the TSSP (2.13) for the NLSE (1.1) with Type I initial datum and different $0<\sigma \leq 1 / 2$. Figure 5.2 (a) shows that the temporal convergence is first order in $L^{2}$-norm for all the four $\sigma$, and Figure 5.2 (b) shows the spatial convergence is almost third order in $L^{2}$-norm, which is also increasing with $\sigma$. These results are better than our error estimates in Theorem 2.5 and suggest that first order temporal convergence in $L^{2}$ norm may hold for any $\sigma>0$ and the spatial convergence may be of higher order. Similar results are also observed in our numerical experiments in 2D. However, we remark that it is impossible to obtain the optimal temporal convergence rates and the higher order spatial convergence rates by simply improving the local error estimates in Proposition 3.6, indicating that there must exist error cancellation between different steps, which require new techniques and in-depth analysis to handle. Also, we can observe similar temporal errors as in Figure 5.2 (a) for the Type II initial datum.

Figure 5.3 plots the temporal and spatial errors in $L^{2}$ - and $H^{1}$-norm of the TSSP (2.13) for the NLSE (1.1) with Type II $H^{2}$ initial datum and fixed $\sigma=0.5$. Figure 5.3 (a) shows that the temporal convergence is first order in $L^{2}$-norm and


Figure 5.2. Temporal errors (a) and spatial errors (b) in $L^{2}$-norm for $\sigma=0.1,0.2,0.3,0.4$ with Type I initial datum (5.1).
half order in $H^{1}$-norm, and Figure 5.3 (b) shows the spatial convergence is second order in $L^{2}$-norm and first order in $H^{1}$-norm. These results correspond with our error estimates (2.42) in Theorem 2.7 very well.


Figure 5.3. Temporal errors (a) and spatial errors (b) in $L^{2}$-norm and $H^{1}$-norm for $\sigma=0.5$ with Type II initial data (5.2).

Figure 5.4 displays the temporal and spatial errors in $H^{1}$-norm of the TSSP (2.13) for the NLSE (1.1) with Type I smooth initial datum and different $0<\sigma<1$. Figure 5.4 (a) shows that the temporal convergence in $H^{1}$-norm increases from half order to first order as $\sigma$ increase from 0 to $1 / 2$ and remains first order when $\sigma \geq 1 / 2$. Figure 5.4 (b) shows the spatial convergence is almost 2.5 order in $H^{1}$-norm and is increasing with $\sigma$. Similar to the observation of Figure 5.2, these results are better than our error estimates (2.43) in Theorem 2.7 and suggest that first order temporal convergence in $H^{1}$-norm may hold for any $\sigma \geq 1 / 2$. We would like to comment that the order reduction in $H^{1}$-norm for $0<\sigma<1 / 2$ is indeed resulted from the semi-smoothness of the nonlinearity instead of the regularity of the exact solution. Actually, we numerically checked that with the Type I smooth initial datum, the exact solution is roughly in $H^{3.5+2 \sigma}$.


Figure 5.4. Temporal errors (a) and spatial errors (b) in $H^{1}$ norm for $\sigma=0.1,0.25,0.5,0.75$ with Type I initial datum (5.1).

## 6. Conclusion

Error bounds of the Lie-Trotter splitting sine pseudospectral method for the nonlinear Schrödinger equation (NLSE) with semi-smooth nonlinearity $f(\rho)=\rho^{\sigma}(\sigma>$ 0 ) were established. For $0<\sigma \leq \frac{1}{2}$, we prove error bounds at $O\left(\tau^{\frac{1}{2}+\sigma}+h^{1+2 \sigma}\right)$ in $L^{2}$-norm without any CFL-type time step size restrictions, where $\tau>0$ and $h>0$ are the time step size and mesh size respectively. For $\sigma \geq \frac{1}{2}$, error bounds at $O\left(\tau+h^{2}\right)$ in $L^{2}$-norm and at $O\left(\tau^{\frac{1}{2}}+h\right)$ in $H^{1}$-norm are proved with mild time step size restrictions. In addition, when $\frac{1}{2}<\sigma<1$ and under the assumption of $H^{3}$-solution of the NLSE, we show an error bound at $O\left(\tau^{\sigma}+h^{2 \sigma}\right)$ in $H^{1}$-norm. Numerical results are reported to demonstrate our error estimates.

## Appendix

Proof of (4.49). We shall present the proof in 1D, and one can easily generalize it to higher dimensions. By triangle inequality, recalling that $\phi_{j}=\phi\left(x_{j}\right)$ for $j \in \mathcal{T}_{N}^{0}$,

$$
\begin{aligned}
\left\|\delta_{x}^{+} \phi\right\|_{l^{4}}^{4} & =h \sum_{j=0}^{N-1}\left|\delta_{x}^{+} \phi_{j}\right|^{4}=h \sum_{j=0}^{N-1}\left|\left(\delta_{x}^{+} \phi_{j}\right)^{2}-\left(\delta_{x}^{+} \phi_{0}\right)^{2}+\left(\delta_{x}^{+} \phi_{0}\right)^{2} \| \delta_{x}^{+} \phi_{j}\right|^{2} \\
& \leq h \sum_{j=0}^{N-1}\left|\left(\delta_{x}^{+} \phi_{j}\right)^{2}-\left(\delta_{x}^{+} \phi_{0}\right)^{2} \| \delta_{x}^{+} \phi_{j}\right|^{2}+h \sum_{j=0}^{N-1}\left|\delta_{x}^{+} \phi_{0}\right|^{2}\left|\delta_{x}^{+} \phi_{j}\right|^{2} \\
6.1) \quad & =h \sum_{j=0}^{N-1}\left|\sum_{l=0}^{j-1}\left(\delta_{x}^{+} \phi_{l+1}\right)^{2}-\left(\delta_{x}^{+} \phi_{l}\right)^{2}\right|\left|\delta_{x}^{+} \phi_{j}\right|^{2}+\left|\delta_{x}^{+} \phi_{0}\right|^{2}\left\|\delta_{x}^{+} \phi\right\|_{l^{2}}^{2}=: K_{1}+K_{2} .
\end{aligned}
$$

We have separated the boundary terms $K_{2}$ from $K_{1}$. We start with the estimate of $K_{1}$, which is standard and can be obtained from the proof of the second inequality of (3.3) in [7]. We show it here for the convenience of the reader. Define the central difference operator $\delta_{x}^{2}$ as

$$
\begin{equation*}
\delta_{x}^{2} v_{j}:=\frac{v_{j+1}-2 v_{j}+v_{j-1}}{h^{2}}=\frac{\delta_{x}^{+} v_{j}-\delta_{x}^{+} v_{j-1}}{h}, \quad 1 \leq j \leq N-1, \quad v \in Y_{N} \tag{6.2}
\end{equation*}
$$

For $K_{1}$ defined in (6.1), using triangle inequality and Cauchy inequality, we get

$$
\begin{align*}
K_{1} & \leq h \sum_{j=0}^{N-1} \sum_{l=0}^{N-2}\left|\delta_{x}^{+} \phi_{l+1}+\delta_{x}^{+} \phi_{l}\right|\left|\delta_{x}^{+} \phi_{l+1}-\delta_{x}^{+} \phi_{l}\right|\left|\delta_{x}^{+} \phi_{j}\right|^{2} \\
& \leq h \sum_{j=0}^{N-1}\left|\delta_{x}^{+} \phi_{j}\right|^{2} \sqrt{\sum_{l=0}^{N-2}\left|\delta_{x}^{+} \phi_{l+1}+\delta_{x}^{+} \phi_{l}\right|^{2}} \sqrt{\sum_{l=0}^{N-2}\left|\delta_{x}^{+} \phi_{l+1}-\delta_{x}^{+} \phi_{l}\right|^{2}} \\
& \lesssim\left\|\delta_{x}^{+} \phi\right\|_{l^{2}}^{2} \sqrt{h \sum_{l=0}^{N-1}\left|\delta_{x}^{+} \phi_{l}\right|^{2}} \sqrt{h \sum_{l=1}^{N-1}\left|\delta_{x}^{2} \phi_{l}\right|^{2}}=\left\|\delta_{x}^{+} \phi\right\|_{l^{2}}^{3} \sqrt{h \sum_{l=1}^{N-1}\left|\delta_{x}^{2} \phi_{l}\right|^{2}} \tag{6.3}
\end{align*}
$$

Since $\phi \in X_{N}$, we have

$$
\begin{equation*}
\phi_{j}=\phi\left(x_{j}\right)=\sum_{l=1}^{N-1} \widehat{\phi}_{l} \sin \left(\mu_{l}\left(x_{j}-a\right)\right)=\sum_{l=1}^{N-1} \widehat{\phi}_{l} \sin \left(\mu_{l} j h\right), \quad 0 \leq j \leq N \tag{6.4}
\end{equation*}
$$

which implies, by recalling (6.2),

$$
\begin{equation*}
\delta_{x}^{2} \phi_{j}=\frac{\phi_{j+1}-2 \phi_{j}+\phi_{j-1}}{h^{2}}=-\sum_{l=1}^{N-1} \mu_{l}^{2} \widehat{\phi}_{l}\left|\operatorname{sinc}\left(\mu_{l} h / 2\right)\right|^{2} \sin \left(\mu_{l} j h\right), \tag{6.5}
\end{equation*}
$$

where $\operatorname{sinc}(x)=\sin (x) / x$ for $x \in \mathbb{R}$ with $\operatorname{sinc}(0)=1$. By Parseval's identity, noting (6.5) and $|\operatorname{sinc}(x)| \leq 1$ for $x \in \mathbb{R}$, we get (similar to the proof of (4.36))

$$
\begin{equation*}
h \sum_{j=1}^{N-1}\left|\delta_{x}^{2} \phi_{j}\right|^{2}=\frac{N h}{2} \sum_{l=1}^{N-1} \mu_{l}^{4}\left|\widehat{\phi}_{l}\right|^{2}\left|\operatorname{sinc}\left(\mu_{l} h / 2\right)\right|^{4} \leq \frac{N h}{2} \sum_{l=1}^{N-1} \mu_{l}^{4}\left|\widehat{\phi}_{l}\right|^{2} \leq\|\phi\|_{H^{2}}^{2} \tag{6.6}
\end{equation*}
$$

Plugging (6.6) into (6.3) and using (4.36), we have

$$
\begin{equation*}
K_{1} \lesssim\|\phi\|_{H^{2}}\|\phi\|_{H^{1}}^{3} \leq\|\phi\|_{H^{2}}^{4} \tag{6.7}
\end{equation*}
$$

For $K_{2}$ in (6.1), recalling (6.4) and $|\operatorname{sinc}(x)| \leq 1$ for $x \in \mathbb{R}$, and noting that $\sum_{l=1}^{\infty}\left|\mu_{l}\right|^{-2}<\infty$, we have, by Cauchy inequality,

$$
\left|\delta_{x}^{+} \phi_{0}\right|=\left|\frac{\phi_{1}}{h}\right|=\left|\sum_{l=1}^{N-1} \mu_{l} \widehat{\phi}_{l} \operatorname{sinc}\left(\mu_{l} h\right)\right| \leq \sqrt{\sum_{l=1}^{N-1}\left|\mu_{l}\right|^{4}\left|\widehat{\phi}_{l}\right|^{2}} \sqrt{\sum_{l=1}^{N-1}\left|\mu_{l}\right|^{-2}} \lesssim\|\phi\|_{H^{2}},
$$

which implies, by using (4.36) again,

$$
\begin{equation*}
K_{2}=\left|\delta_{x}^{+} \phi_{0}\right|^{2}\left\|\delta_{x}^{+} \phi\right\|_{l^{2}}^{2} \lesssim\|\phi\|_{H^{2}}^{2}\|\nabla \phi\|_{H^{1}}^{2} \leq\|\phi\|_{H^{2}}^{4} . \tag{6.8}
\end{equation*}
$$

Plugging (6.7) and (6.8) into (6.1) yields the desired result.

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