Uniform Error Estimate of a Nested Picard Integrator Fourier Pseudospectral Method for the Nonlinear Schrödinger Equation with Wave Operator

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Outline

Nonlinear Schrödinger Equation with Wave Operator

Consider nonlinear Schrödinger equation with wave operator (NLSW) in d ($d = 1, 2, 3$) dimensions:

$$\begin{cases} i\partial_t \psi(x,t) - \varepsilon^2 \partial_{tt}\psi(x,t) + \Delta\psi(x,t) + F(|\psi(x,t)|^2)\psi(x,t) = 0, \\ \psi(x,0) = \psi_0(x), \quad \partial_t\psi(x,0) = \psi_1^\varepsilon(x), \quad x \in \mathbb{R}^d, \quad t > 0, \end{cases} \tag{1}$$

$0 < \varepsilon \leq 1$ is a parameter that controls the perturbation operator, $F : [0, +\infty) \to \mathbb{R}$ is a real-valued function.

When $\varepsilon \to 0+$, the solution of (1) will converge to the solution of corresponding nonlinear Schrödinger equation (NLS) (2):

$$\begin{cases} i\partial_t \psi(x,t) + \Delta\psi(x,t) + F(|\psi(x,t)|^2)\psi(x,t) = 0, \\ \psi(x,0) = \psi_0(x), \quad x \in \mathbb{R}^d, \quad t > 0, \end{cases} \tag{2}$$

Initial condition

Assume the initial velocity ψ_1^ε has the form:

$$\psi_1^\varepsilon(x) = i(\Delta\psi_0(x) + F(|\psi_0(x)|^2\psi_0(x))) + \varepsilon^\alpha \omega^\varepsilon(x), \quad \alpha \geq 0, \tag{3}$$

α is describes how close the initial value to NLS case.
$\alpha \geq 2$: well-prepared case, $\partial_{tt}\psi$ is bounded.
$0 \leq \alpha < 2$: ill-prepared case, $\partial_{tt}\psi$ is not bounded.
Asymptotic expansion for the solution $\psi(x,t)$ of NLSW (denote $\psi^s(x,t)$ to be the solution of NLS):

$$\begin{aligned}\psi(x,t) &= \psi^s(x,t) + \varepsilon^2\{\text{no oscillation terms}\} \\ &\quad + \varepsilon^{2+\min\{\alpha,2\}}\Psi(x, \frac{t}{\varepsilon^2}) + \{\text{higher order oscillations}\}.\end{aligned} \tag{4}$$

Previous result

Assume $\psi(\cdot, t) \in H^m(\mathbb{R}^d)$:
Crank-Nicolson finite difference scheme :

$$\begin{cases} O(h^2 + \tau), & \text{well-prepared case,} \\ O(h^2 + \tau^{2/3}), & \text{ill-prepared case.} \end{cases}$$

Exponential wave integrator sine pseudospectral scheme:

$$\begin{cases} O(h^m + \tau^2), & \text{well-prepared case,} \\ O(h^m + \tau), & \text{ill-prepared case.} \end{cases}$$

Our target:

$$O(h^m + \tau^2), \quad \text{uniform for both well-prepared and ill-prepared case.}$$

General idea of NPI

Consider the case where $d = 1$, $F(|\psi|^2) = -|\psi|^2$, truncate the whole space problem (1) onto a bounded interval $\Omega = (a, b)$:

$$\begin{cases} i\partial_t\psi(x,t) - \varepsilon^2\partial_{tt}\psi(x,t) + \Delta\psi(x,t) - |\psi(x,t)|^2\psi(x,t) = 0, \\ \psi(x,0) = \psi_0(x), \quad \partial_t\psi(x,0) = \psi_1^\varepsilon(x), \quad x \in (a,b), \quad t > 0, \\ \psi(a,t) = \psi(b,t), \quad \partial_t\psi(a,t) = \partial_t\psi(b,t), \quad t > 0 \end{cases} \tag{5}$$

Time step $\tau := \Delta t > 0$, $t_n = n\tau$, by variation of constants, from t_n to t_{n+1}, the solution of equation (5) satisfies ($\psi(t_n + s) := \psi(x, t_n + s)$):

$$\begin{aligned} \psi(t_n + s) = {} & e^{i\beta^+ s} h_1(\psi(t_n), \partial_t\psi(t_n)) + e^{i\beta^- s} h_2(\psi(t_n), \partial_t\psi(t_n)) \\ & + i\gamma \int_0^s \kappa(s - w)|\psi(t_n + w)|^2\psi(t_n + w)dw, \quad 0 \le s \le \tau. \end{aligned} \tag{6}$$

$$\beta^+ := \frac{1+\sqrt{1-4\varepsilon^2\Delta}}{2\varepsilon^2} = O(\frac{1}{\varepsilon^2}),$$
$$\beta^- := \frac{1-\sqrt{1-4\varepsilon^2\Delta}}{2\varepsilon^2} = O(1),$$
$$\beta := \beta^+ - \beta^- = \frac{\sqrt{1-4\varepsilon^2\Delta}}{\varepsilon^2},$$
$$\beta^* := \beta^+ - \frac{1}{\varepsilon^2} = \frac{-2\Delta}{1+\sqrt{1-4\varepsilon^2\Delta}} = O(1),$$
$$\gamma := \frac{1}{\varepsilon^2\beta} = \frac{1}{\sqrt{1-4\varepsilon^2\Delta}},$$
$$h_1(\psi(t_n), \partial_t\psi(t_n)) := -\frac{\beta^-\psi(t_n) + i\partial_t\psi(t_n)}{\beta},$$
$$h_2(\psi(t_n), \partial_t\psi(t_n)) := \frac{\beta^+\psi(t_n) + i\partial_t\psi(t_n)}{\beta},$$
$$\kappa(t) := e^{i\beta^+ t} - e^{i\beta^- t} = O(1).$$

General idea of NPI

Our target is to find a uniform 2nd order scheme from formula (6).
By Taylor expansion:

$$
\begin{aligned}
\psi(t_n+s) = {} & e^{i\beta^+ s} h_1(\psi(t_n), \partial_t \psi(t_n)) + e^{i\beta^- s} h_2(\psi(t_n), \partial_t \psi(t_n)) \\
& + i\gamma \int_0^s \kappa(s-w)(|\psi(t_n)|^2 \psi(t_n) \\
& + w(2\partial_t \psi(t_n)|\psi(t_n)|^2 + 2\partial_t \overline{\psi(t_n)} \psi^2(t_n)) \\
& + w^2(4|\psi_t|^2\psi + 2\psi_t^2 \overline{\psi} + 2\psi_{tt}|\psi|^2 + \overline{\psi_{tt}}\psi^2)(t_n + \xi(w)))dw.
\end{aligned}
$$

$\partial_{tt}\psi$ not bounded for ill-prepared case. Using NPI can avoid $\partial_{tt}\psi$ and achieve 2nd order in time.

General idea of NPI

Construct approximation $\psi^{n,k}(s)$ to $\psi(t_n+s)$ recursively:

$$\psi^{n,0}(s) := \psi(t_n)$$
$$\psi_*^{n,k+1}(s) := e^{i\beta^+ s} h_1(\psi(t_n), \partial_t\psi(t_n)) + e^{i\beta^- s} h_2(\psi(t_n), \partial_t\psi(t_n)) + i\gamma\int_0^s \kappa(s-w)|\psi^{n,k}(w)|^2\psi^{n,k}(w)dw, \quad 0\le s\le\tau,$$
$$\psi^{n,k+1}(s) := \psi_*^{n,k+1}(s) - R_{k+1}^n(s), \quad 0\le s\le\tau.$$

If $R_k^n(s) = O(\tau^{k+1})$ for any k, it can be proved

$$\psi(t_n+s) - \psi^{n,k}(s) = O(\tau^{k+1}).$$

Uniform 2nd order scheme: $\psi^{n,2}(s)$.

Compute $\psi^{n,1}(s)$

Denote $h_1^n = h_1(\psi(t_n), \partial_t\psi(t_n))$, $h_2^n = h_2(\psi(t_n), \partial_t\psi(t_n))$,
$f^n = |\psi(t_n)|^2\psi(t_n)$.

$$\psi_*^{n,1}(s) := e^{i\beta^+ s}h_1^n + e^{i\beta^- s}h_2^n + i\gamma\int_0^s \kappa(s-w)f^n dw,$$

$$\psi^{n,1}(s) := e^{i\frac{1}{\varepsilon^2}s}(e^{i\beta^* s}h_1^n + i\gamma p_{-1}(s)f^n) + (e^{i\beta^- s}h_2^n - i\gamma p_0(s)f^n),$$

if we define:

$$p_k(s) := \int_0^s e^{iks_1/\varepsilon^2}ds_1 = O(\tau).$$

Compute $\psi^{n,2}(s)$

$$
\begin{aligned}
|\psi^{n,1}(x,s)|^2 &= F_0^n(s) + p_0(s)F_1^n(s) + p_{-1}(s)F_{-2}^n(s) + p_1(s)F_2^n(s) \\
&\quad + e^{-is/\varepsilon^2}(F_{-3}^n(s) + p_0(s)F_{-4}^n(s) + p_1(s)F_5^n(s)) \\
&\quad + e^{is/\varepsilon^2}(F_3^n(s) + p_0(s)F_4^n(s) + p_{-1}(s)F_{-5}^n(s)) + O(\tau^2), \\
F_0^n(s) &= (e^{i\beta^* s}h_1^n)(e^{-i\beta^* s}\overline{h_1^n}) + (e^{i\beta^- s}h_2^n)(e^{-i\beta^- s}\overline{h_2^n}), \\
F_1^n(s) &= 2\,\mathrm{Re}((i\gamma\overline{f^n})(e^{i\beta^- s}h_2^n)), \\
F_2^n(s) &= (-i\gamma\overline{f^n})(e^{i\beta^* s}h_1^n), \\
F_3^n(s) &= (e^{i\beta^* s}h_1^n)(e^{-i\beta^- s}\overline{h_2^n}), \\
F_4^n(s) &= (i\gamma\overline{f^n})(e^{i\beta^* s}h_1^n), \\
F_5^n(s) &= (-i\gamma\overline{f^n})(e^{i\beta^- s}h_2^n), \\
F_k^n(s) &= \overline{F_{-k}^n(s)}.
\end{aligned}
$$

Compute $\psi^{n,2}(s)$

$$
\begin{aligned}
&|\psi^{n,1}(x,s)|^2\psi^{n,1}(x,s)\\
&\quad= g_0^n(s) + p_0(s)g_1^n(s) + p_1(s)g_2^n(s) + p_{-1}(s)g_3^n(s)\\
&\quad+ e^{-is/\varepsilon^2}(g_4^n(s) + p_0(s)g_5^n(s) + p_1(s)g_6^n(s))\\
&\quad+ e^{is/\varepsilon^2}(g_7^n(s) + p_0(s)g_8^n(s) + p_1(s)g_9^n(s) + p_{-1}(s)g_{10}^n(s))\\
&\quad+ e^{i2s/\varepsilon^2}(g_{11}^n(s) + p_0(s)g_{12}^n(s) + p_{-1}(s)g_{13}^n(s)) + O(\tau^2),
\end{aligned}
$$

$$
\begin{aligned}
g_0^n(s) &= F_{-3}^n(s)e^{i\beta^* s}h_1^n + F_0^n(s)e^{i\beta^- s}h_2^n,\\
g_1^n(s) &= F_{-4}^n(s)e^{i\beta^* s}h_1^n + F_1^n(s)e^{i\beta^- s}h_2^n + F_0^n(s)(-i\gamma f^n),\\
g_2^n(s) &= F_{-5}^n(s)e^{i\beta^* s}h_1^n + F_2^n(s)e^{i\beta^- s}h_2^n,\\
&\cdots
\end{aligned}
$$

Numerical quadrature

$$\psi_*^{n,2}(s) := e^{i\beta^+ s} h_1^n + e^{i\beta^- s} h_2^n + i\gamma \int_0^s \kappa(s-w)|\psi^{n,1}(x,w)|^2 \psi^{n,1}(x,w) dw.$$

Divide the integral term into 3 types:
Type 1: no oscillation term.

$$\int_0^s e^{i\beta^-(s-w)} p_1(w) g_2^n(w) dw = e^{i\beta^- s/2} s p_1(\frac{s}{2}) g_2^n(\frac{s}{2}) + O(\tau^3),$$

by applying midpoint method.

Numerical quadrature

Type 2: highly oscillation term with $O(\tau)$ amplitude.

$$
\begin{aligned}
&\int_0^s e^{-\frac{i}{\varepsilon^2}w} p_1(w) e^{i\beta^*(s-w)} g_2^n(w)\, dw,\\
=&\int_0^s e^{-\frac{i}{\varepsilon^2}w} p_1(w) g_2^n(0)\, dw + O(\tau^3),\\
=&q_{-1,1}(s) g_2^n(0) + O(\tau^3),
\end{aligned}
$$

if we define:

$$
q_{k,l}(s) := \int_0^s \int_0^{s_1} e^{iks_1/\varepsilon^2} e^{ils_2/\varepsilon^2} ds_2 ds_1 = O(\tau^2).
$$

Numerical quadrature

Type 3: highly oscillation term with $O(1)$ amplitude.

$$\begin{aligned}
&\int_0^s e^{i\beta^*(s-w)} e^{-\frac{i}{\varepsilon^2}w} g_0^n(w)dw,\\
=&e^{i\beta^* s}\int_0^s e^{-\frac{i}{\varepsilon^2}w}(g_0^n(0)+w(-i\beta^* g_0^n(0)+\partial_t g_0^n(0)))dw+O(\tau^3),\\
=&e^{i\beta^* s}\int_0^s e^{-\frac{i}{\varepsilon^2}w}(g_0^n(0)+w(-i\frac{\sin(\beta^*\tau)}{\tau} g_0^n(0)+\dot{g}_0^n(0)))dw+O(\tau^3),\\
=&e^{i\beta^* s}(p_{-1}(s)g_0^n(0)+q_{-1,0}(s)(-i\frac{\sin(\beta^*\tau)}{\tau} g_0^n(0)+\dot{g}_0^n(0)))+O(\tau^3).
\end{aligned}$$

Replace unbounded operator β^* with bounded filter $\frac{\sin(\beta^*\tau)}{\tau}$ to achieve uniform accuracy (at the price of higher regularity requirement).
Apply the same replacement to $\partial_t g_0^n(0)$ to compute approximation $\dot{g}_0^n(0)$.

Compute $\psi^{n,2}(s)$

$$
\begin{aligned}
\psi^{n,2}(x,s) &= e^{i\beta^+ s} h_1^n + e^{i\beta^- s} h_2^n \\
&+ i\gamma\big(G_0^n(s) + e^{i\beta^* s/2} G_{*,1}^n(s) + e^{i\beta^* s} G_{*,2}^n(s) \\
&+ e^{i\beta^- s/2} G_{-,1}^n(s) + e^{i\beta^- s} G_{-,2}^n(s)\big), \\
G_{*,1}^n(s) &= e^{is/\varepsilon^2}\big(s g_7^n(s/2) + s^2/2 g_8^n(s/2) + s p_1(s/2) g_9^n(s/2) \\
&+ s p_{-1}(s/2) g_{10}^n(s/2)\big), \\
G_{*,2}^n(s) &= e^{is/\varepsilon^2}\Big(p_{-1}(s) g_0^n(0) + q_{-1,0}(s)\big(-i\frac{\sin(\beta^*\tau)}{\tau} g_0^n(0) + \dot{g}_0^n(0)\big) \\
&+ p_{-2}(s) g_4^n(0) + q_{-2,0}(s)\big(-i\frac{\sin(\beta^*\tau)}{\tau} g_4^n(0) + \dot{g}_4^n(0)\big) \\
&+ p_1(s) g_{11}^n(0) + q_{1,0}(s)\big(-i\frac{\sin(\beta^*\tau)}{\tau} g_{11}^n(0) + \dot{g}_{11}^n(0)\big)\Big).
\end{aligned}
$$

$$
\begin{aligned}
G_0^n(s) = e^{is/\varepsilon^2}(& q_{-1,0}(s)g_1^n(0) + q_{-1,1}(s)g_2^n(0) + q_{-1,-1}(s)g_3^n(0) \\
&+ q_{-2,0}(s)g_5^n(0) + q_{-2,1}(s)g_6^n(0) \\
&+ q_{1,0}(s)g_{12}^n(0) + q_{1,1}(s)g_{13}^n(0)) \\
&+ q_{-1,0}(s)g_5^n(0) + q_{-1,1}(s)g_6^n(0) + q_{-1,-1}(s)g_8^n(0) \\
&+ q_{1,1}(s)g_9^n(0) + q_{1,-1}(s)g_{10}^n(0) \\
&+ q_{2,0}(s)g_{12}^n(0) + q_{2,-1}(s)g_{13}^n(0), \\
G_{-,1}^n(s) = \; & sg_0^n(s/2) + s^2/2g_1^n(s/2) + sp_1(s/2)g_2^n(s/2) \\
&+ sp_{-1}(s/2)g_3^n(s/2), \\
G_{-,2}^n(s) = \; & p_{-1}(s)g_4^n(0) + q_{-1,0}(s)(-i\frac{\sin(\beta^-\tau)}{\tau}g_4^n(0) + \dot{g}_4^n(0)) \\
&+ p_1(s)g_7^n(0) + q_{1,0}(s)(-i\frac{\sin(\beta^-\tau)}{\tau}g_7^n(0) + \dot{g}_7^n(0)) \\
&+ p_2(s)g_{11}^n(0) + q_{2,0}(s)(-i\frac{\sin(\beta^-\tau)}{\tau}g_{11}^n(0) + \dot{g}_{11}^n(0)).
\end{aligned}
$$

Compute $\partial_t \psi^{n,2}(s)$

$$\begin{aligned}\partial_t \psi_*^{n,2}(s) &:= i\beta^+ e^{i\beta^+ s} h_1^n + i\beta^- e^{i\beta^- s} h_2^n \\ &\quad + i\gamma \int_0^s \kappa'(s-w)|\psi^{n,1}(x,w)|^2 \psi^{n,1}(x,w) dw, \\ \kappa'(t) &= i\beta^+ e^{i\beta^+ t} - i\beta^- e^{i\beta^- t}.\end{aligned}$$

Apply similar numerical quadrature:

$$\begin{aligned}\dot{\psi}^{n,2}(x,s) &= i\beta^+ e^{i\beta^+ s} h_1^n + i\beta^- e^{i\beta^- s} h_2^n \\ &\quad + i\gamma(\dot{G}_0^n(s) + e^{i\beta^* s/2} \dot{G}_{*,1}^n(s) + e^{i\beta^* s} \dot{G}_{*,2}^n(s) \\ &\quad + e^{i\beta^- s/2} \dot{G}_{-,1}^n(s) + e^{i\beta^- s} \dot{G}_{-,2}^n(s)).\end{aligned}$$

$$
\begin{aligned}
\dot{G}_0^n(s) &= i\frac{\sin(\beta^*\tau)}{\tau}e^{is/\varepsilon^2}(q_{-1,0}(s)g_1^n(0) + q_{-1,1}(s)g_2^n(0) \\
&\quad + q_{-1,-1}(s)g_3^n(0) + q_{-2,0}(s)g_5^n(0) + q_{-2,1}(s)g_6^n(0) \\
&\quad + q_{1,0}(s)g_{12}^n(0) + q_{1,1}(s)g_{13}^n(0)) \\
&\quad + i\frac{\sin(\beta^-\tau)}{\tau}(q_{-1,0}(s)g_5^n(0) + q_{-1,1}(s)g_6^n(0) \\
&\quad + q_{-1,-1}(s)g_8^n(0) + q_{1,1}(s)g_9^n(0) + q_{1,-1}(s)g_{10}^n(0) \\
&\quad + q_{2,0}(s)g_{12}^n(0) + q_{2,-1}(s)g_{13}^n(0)), \\
\dot{G}_{*,k}^n(s) &= i\frac{\sin(\beta^*\tau)}{\tau}G_{*,k}^n(s), \quad k = 1,2 \\
\dot{G}_{-,k}^n(s) &= i\frac{\sin(\beta^-\tau)}{\tau}G_{-,k}^n(s), \quad k = 1,2.
\end{aligned}
$$

Semi-discretized scheme

$\psi^n(x)$ and $\dot{\psi}^n(x)$ are approximation of $\psi(x,t_n)$ and $\partial_t\psi(x,t_n)$.

$$\psi^0(x) = \psi_0(x), \quad \dot{\psi}^0(x) = \psi_1^\varepsilon(x).$$

Then compute

$$h_1^{[n]} = h_1(\psi^n, \dot{\psi}^n), \quad h_2^{[n]} = h_2(\psi^n, \dot{\psi}^n), \quad f^{[n]} = |\psi^n|^2\psi^n,$$

Submit into the expression:

$$F_0^{[n]}(s) = (e^{i\beta^* s} h_1^{[n]})(e^{-i\beta^* [n]}\overline{h_1^{[n]}}) + (e^{i\beta^- s} h_2^{[n]})(e^{-i\beta^- s}\overline{h_2^{[n]}}),$$

and thereby compute expressions $F_k^{[n]}$, $g_k^{[n]}$, $G_0^{[n]}$, $G_{*,k}^{[n]}$ and $G_{-,k}^{[n]}$.

Given approximation $\psi^n(x)$ and $\dot{\psi}^n(x)$, compute numerical approximation at time $t = t_{n+1}$ by:

$$
\begin{aligned}
\psi^{n+1}(x) &= e^{i\beta^+\tau} h_1^{[n]} + e^{i\beta^-\tau} h_2^{[n]} \\
&\quad + i\gamma\big(G_0^{[n]}(\tau) + e^{i\beta^*\tau/2} G_{*,1}^{[n]}(\tau) + e^{i\beta^*\tau} G_{*,2}^{[n]}(\tau) \\
&\quad + e^{i\beta^-\tau/2} G_{-,1}^{[n]}(\tau) + e^{i\beta^-\tau} G_{-,2}^{[n]}(\tau)\big), \\
\dot{\psi}^{n+1}(x) &= i\beta^+ e^{i\beta^+\tau} h_1^{[n]} + i\beta^- e^{i\beta^-\tau} h_2^{[n]} \\
&\quad + i\gamma\big(\dot{G}_0^{[n]}(\tau) + e^{i\beta^*\tau/2} \dot{G}_{*,1}^{[n]}(\tau) + e^{i\beta^*\tau} \dot{G}_{*,2}^{[n]}(\tau) \\
&\quad + e^{i\beta^-\tau/2} \dot{G}_{-,1}^{[n]}(\tau) + e^{i\beta^-\tau} \dot{G}_{-,2}^{[n]}(\tau)\big).
\end{aligned}
$$

Numerical Implementation

Mesh size $h := \Delta x = \frac{b-a}{M}$. Denote $x_j = a + jh$ to be the grid points, ψ_j^n and $\dot{\psi}_j^n$ to be the numerical approximation of the exact solution $\psi(x_j, t_n)$ and $\partial_t \psi(x_j, t_n)$.
Initially,

$$\psi_j^0 = \psi_0(x_j), \quad \dot{\psi}_j^0 = \psi_1^\varepsilon(x_j).$$

Given approximation ψ_j^n and $\dot{\psi}_j^n$ at time $t = t_n$, to compute the next approximation, starting with $h_{1,j}^{[n]}$, $h_{2,j}^{[n]}$, $f_j^{[n]}$ ($\beta_l^{\pm} = \frac{1 \pm \sqrt{1+4\varepsilon^2\mu_l^2}}{2\varepsilon^2}$):

$$h_{1,j}^{[n]} = \sum_{l=-M/2}^{M/2-1} \left(-\frac{\beta_l^- \widetilde{(\psi^n)}_l + \widetilde{(\dot{\psi}^n)}_l}{\beta_l}\right) e^{i\mu_l(x_j - a)},$$

$$\widetilde{(\psi^n)}_l = \frac{1}{M}\sum_{j=0}^{M-1} \psi_j^n e^{-i\mu_l(x_j-a)}, \quad \widetilde{(\dot{\psi}^n)}_l = \frac{1}{M}\sum_{j=0}^{M-1} \dot{\psi}_j^n e^{-i\mu_l(x_j-a)}.$$

$$
\begin{aligned}
F^{[n]}_{0,j}(0) &= h^{[n]}_{1,j}\overline{h^{[n]}_{1,j}} + h^{[n]}_{2,j}\overline{h^{[n]}_{2,j}},\\
F^{[n]}_{0,j}(\tau/2) &= (e^{i\beta^*\tau/2}h^{[n]}_1)_j(e^{-i\beta^*\tau/2}\overline{h^{[n]}_1})_j\\
&\quad + (e^{i\beta^-\tau/2}h^{[n]}_2)_j(e^{-i\beta^-\tau/2}\overline{h^{[n]}_2})_j,\\
\dot{F}^{n}_{0,j}(0) &= (i\frac{\sin(\beta^*\tau)}{\tau}h^n_1)_j\overline{h^n_{1,j}} + h^n_{1,j}(-i\frac{\sin(\beta^*\tau)}{\tau}\overline{h^n_1})_j\\
&\quad + (i\frac{\sin(\beta^-\tau)}{\tau}h^n_2)_j\overline{h^n_{2,j}} + h^n_{2,j}(-i\frac{\sin(\beta^-\tau)}{\tau}\overline{h^n_2})_j,
\end{aligned}
$$

where $(\beta^*_l = \frac{2\mu_l^2}{1+\sqrt{1+4\varepsilon^2\mu_l^2}},\ \mu_l = \frac{2\pi l}{b-a})$

$$
(e^{i\beta^*\tau/2}h^{[n]}_1)_j = \sum_{l=-M/2}^{M/2-1} e^{i\beta^*_l\tau/2}\widetilde{(h^{[n]}_1)}_l e^{i\mu_l(x_j-a)},
$$

$$
\widetilde{(h^{[n]}_1)}_l = \frac{1}{M}\sum_{j=0}^{M-1} h^{[n]}_{1,j}e^{-i\mu_l(x_j-a)}.
$$

$$
\begin{aligned}
g_{0,j}^{[n]}(0) &= F_{-3,j}^{[n]}(0)h_{1,j}^{[n]} + F_{0,j}^{[n]}(s)h_{2,j}^{[n]}, \\
g_{0,j}^{[n]}(\tau/2) &= F_{-3,j}^{[n]}(0)(e^{i\beta^*\tau/2}h_1^{[n]})_j + F_{0,j}^{[n]}(s)(e^{i\beta^-\tau/2}h_2^{[n]})_j, \\
\dot{g}_{0,j}^{n}(0) &= \dot{F}_{-3,j}^{[n]}(0)h_{1,j}^{[n]} + iF_{-3,j}^{[n]}(0)(\frac{\sin(\beta^*\tau)}{\tau}h_1^n)_j \\
&\quad + \dot{F}_{-0,j}^{[n]}(0)h_{1,j}^{[n]} + iF_{-0,j}^{[n]}(0)(\frac{\sin(\beta^-\tau)}{\tau}h_2^n)_j, \\
\widetilde{(g_0^{[n]})}_l(0) &= \frac{1}{M}\sum_{j=0}^{M-1} g_{0,j}^{[n]}(0)e^{-i\mu_l(x_j-a)}.
\end{aligned}
$$

Similarly compute $\widetilde{(g_k^{[n]})}_l(0)$, $\widetilde{(g_k^{[n]})}_l(\tau/2)$ and $\widetilde{(\dot{g}_k^{[n]})}_l(0)$ for all $k \in \{1, 2, \cdots, 13\}$.

$$
\begin{aligned}
\widetilde{(G_0^{[n]})}_l(\tau) = e^{i\tau/\varepsilon^2}&(q_{-1,0}(\tau)\widetilde{(g_1^{[n]})}_l(0) + q_{-1,1}(\tau)\widetilde{(g_2^{[n]})}_l(0) \\
&+ q_{-1,-1}(\tau)\widetilde{(g_3^{[n]})}_l(0) + q_{-2,0}(\tau)\widetilde{(g_5^{[n]})}_l(0) + q_{-2,1}(\tau)\widetilde{(g_6^{[n]})}_l(0) \\
&+ q_{1,0}(\tau)\widetilde{(g_{12}^{[n]})}_l(0) + q_{1,1}(\tau)\widetilde{(g_{13}^{[n]})}_l(0)) \\
&+ q_{-1,0}(\tau)\widetilde{(g_5^{[n]})}_l(0) + q_{-1,1}(\tau)\widetilde{(g_6^{[n]})}_l(0) + q_{-1,-1}(\tau)\widetilde{(g_8^{[n]})}_l(0) \\
&+ q_{1,1}(\tau)\widetilde{(g_9^{[n]})}_l(0) + q_{1,-1}(\tau)\widetilde{(g_{10}^{[n]})}_l(0) \\
&+ q_{2,0}(\tau)\widetilde{(g_{12}^{[n]})}_l(0) + q_{2,-1}(\tau)\widetilde{(g_{13}^{[n]})}_l(0).
\end{aligned}
$$

and compute $\widetilde{(G_{*,k}^{[n]})}_l(\tau)$, $\widetilde{(G_{-,k}^{[n]})}_l(\tau)$ for $l = -M/2, -M/2+1, \cdots, M/2-1$.

$$
\begin{aligned}
\widetilde{(\psi^{n+1})}_l &= e^{i\beta_l^+\tau}\widetilde{(h_1^{[n]})}_l + e^{i\beta_l^-\tau}\widetilde{(h_2^{[n]})}_l \\
&\quad + i\gamma_l\Big(\widetilde{(G_0^{[n]})}_l(\tau) + e^{i\beta_l^*\tau/2}\widetilde{(G_{*,1}^{[n]})}_l(\tau) + e^{i\beta_l^*\tau}\widetilde{(G_{*,2}^{[n]})}_l(\tau) \\
&\quad + e^{i\beta_l^-\tau/2}\widetilde{(G_{-,1}^{[n]})}_l(\tau) + e^{i\beta_l^-\tau}\widetilde{(G_{-,2}^{[n]})}_l(\tau)\Big), \\
\widetilde{(\dot{\psi}^{n+1})}_l &= i\beta_l^+ e^{i\beta_l^+\tau}\widetilde{(h_1^{[n]})}_l + i\beta_l^- e^{i\beta_l^-\tau}\widetilde{(h_2^{[n]})}_l \\
&\quad + i\gamma_l\Big(\widetilde{(\dot{G}_0^{[n]})}_l(\tau) + e^{i\beta_l^*\tau/2}\widetilde{(\dot{G}_{*,1}^{[n]})}_l(\tau) + e^{i\beta_l^*\tau}\widetilde{(\dot{G}_{*,2}^{[n]})}_l(\tau) \\
&\quad + e^{i\beta_l^-\tau/2}\widetilde{(\dot{G}_{-,1}^{[n]})}_l(\tau) + e^{i\beta_l^-\tau}\widetilde{(\dot{G}_{-,2}^{[n]})}_l(\tau)\Big), \\
\gamma_l &= \frac{1}{\sqrt{1+4\varepsilon^2\mu_l^2}}.
\end{aligned}
$$

Finally the numerical approximation for $t = t_{n+1}$ can be obtained by:

$$\psi_j^{n+1} = \sum_{l=-M/2}^{M/2-1} \widetilde{(\psi^{n+1})}_l e^{i\mu_l(x_j-a)},$$

$$\dot{\psi}_j^{n+1} = \sum_{l=-M/2}^{M/2-1} \widetilde{(\dot{\psi}^{n+1})}_l e^{i\mu_l(x_j-a)}.$$

One time step $t_n \to t_{n+1}$: 37 times FFT/IFFT in $\mathbb{C}^M$ (cost: $O(M \log M)$).

Error estimates

Assume $\psi(x,t)$, solution of NLSW (5) within time $T>0$ satisfies the following:

$$\|\psi\|_{L^\infty([0,T];W^{1,\infty}(\Omega))} + \|\partial_t\psi\|_{L^\infty([0,T];W^{1,\infty}(\Omega))} \lesssim 1,$$
$$\|\psi\|_{L^\infty([0,T];H^2(\Omega)\cap H^m(\Omega))} + \|\partial_t\psi\|_{L^\infty([0,T];H^2(\Omega))} \lesssim 1,$$
$$\psi \text{ and } \partial_t\psi \text{ are perodic on } \Omega.$$

Denote vector space Y_M:

$$Y_M = \{v = (v_0, v_1, \cdots, v_M)^T \in \mathbb{C}^{M+1} | v_0 = v_M\},$$

and interpolation operator $I_M : Y_M \to L^2(\Omega)$ by:

$$(I_M\phi)(x) = \sum_{l=-M/2}^{M/2-1} \tilde{\phi}_l e^{i\mu_l(x-a)},$$
$$\tilde{\phi}_l = \frac{1}{M}\sum_{l=0}^{M-1} \phi_j e^{-i\mu_l(x_j-a)}$$

Error estimates

Theorem

Assume the solution $\psi(x,t)$ satisfies the above assumption, $\psi^n \in Y_M$ and $\dot{\psi}^n$ be the numerical approximation of $\psi(t_n)$ and $\partial_t\psi(t_n)$, and $\psi_I^n(x) = I_M(\psi^n)$, $\dot{\psi}_I^n(x) = I_M(\dot{\psi}^n)$. There exists $0 < \tau_0, h_0$ independent of ε, such that if $0 < h \le h_0$ and $0 < \tau \le \tau_0$, for any $0 < n \le T/\tau$,

$$\|\psi(\cdot,t_n) - \psi_I^n(\cdot)\|_{L^2(\Omega)} + \varepsilon^2\|\partial_t\psi(\cdot,t_n) - \dot{\psi}_I^n(\cdot)\|_{L^2(\Omega)} \lesssim h^m + \tau^2,$$
$$\|\nabla(\psi(\cdot,t_n) - \psi_I^n(\cdot))\|_{L^2(\Omega)} + \varepsilon^2\|\nabla(\partial_t\psi(\cdot,t_n) - \dot{\psi}_I^n(\cdot))\|_{L^2(\Omega)} \lesssim h^{m-1} + \tau^2,$$

and there exists $M > 0$ such that

$$\|\psi_I^n(\cdot)\|_{L^\infty} \le M, \quad \|\dot{\psi}_I^n(\cdot)\|_{L^\infty} \le M,$$
$$\|\psi(\cdot,t_n)\|_{L^\infty} \le M-1, \quad \|\partial_t\psi(\cdot,t_n)\|_{L^\infty} \le M-1,$$

An numerical example

Computation domain: $\Omega = [a, b] = [-16, 16]$, $T = 1$
Initial value:

$$\psi_0(x) = \pi^{-1/4} e^{-x^2/2}, \quad \omega^\varepsilon(x) = e^{-x^2/2}.$$

"Exact" solution: computed with fine mesh $h = 1/64$ and $\tau = 10^{-6}$.
Error function: $e^n(x) = \psi(x, t_n) - \psi_I^n(x)$, measuring the norm $\|e^n(\cdot)\|_{H^1} = \|e^n(\cdot)\|_{L^2} + \|\nabla e^n(\cdot)\|_{L^2}$.
Choose $\alpha = 2$ for well-prepared case and $\alpha = 0$ for ill-prepared case, and compare the error at $T = 1$.

Spatial error

$\|e^n\|_{H^1}$	$h_0 = 2$	$h_0/2$	$h_0/2^2$	$h_0/2^3$
$\varepsilon_0 = 0.5$	1.16E+00	7.81E-02	6.17E-04	2.63E-08
$\varepsilon_0/2$	8.95E-01	8.79E-02	7.56E-04	3.82E-08
$\varepsilon_0/2^2$	9.19E-01	5.26E-02	6.03E-04	3.13E-08
$\varepsilon_0/2^3$	9.58E-01	3.22E-02	4.67E-04	3.33E-08
$\varepsilon_0/2^4$	9.21E-01	5.21E-02	1.29E-04	3.10E-08
$\varepsilon_0/2^5$	9.21E-01	4.74E-02	1.39E-04	2.89E-08
$\varepsilon_0/2^6$	9.25E-01	4.10E-02	1.22E-04	2.87E-08
$\varepsilon_0/2^7$	9.30E-01	3.77E-02	1.17E-04	2.80E-08

Table: Error with different h and ε, $\tau = 10^{-6}$, well-prepared case

$\|e^n\|_{H^1}$	$h_0 = 2$	$h_0/2$	$h_0/2^2$	$h_0/2^3$
$\varepsilon_0 = 0.5$	1.36E+00	9.19E-02	7.25E-04	3.09E-08
$\varepsilon_0/2$	9.94E-01	9.76E-02	8.41E-04	4.24E-08
$\varepsilon_0/2^2$	9.67E-01	5.54E-02	6.34E-04	3.29E-08
$\varepsilon_0/2^3$	9.12E-01	3.07E-02	4.45E-04	3.17E-08
$\varepsilon_0/2^4$	9.21E-01	5.21E-02	1.29E-04	3.10E-08
$\varepsilon_0/2^5$	9.21E-01	4.74E-02	1.39E-04	2.89E-08
$\varepsilon_0/2^6$	9.25E-01	4.10E-02	1.22E-04	2.87E-08
$\varepsilon_0/2^7$	9.30E-01	3.77E-02	1.17E-04	2.80E-08

Table: Error with different h and ε, $\tau = 10^{-6}$, ill-prepared case

Temporal error

$\|e^n\|_{H^1}$	$\tau_0 = 0.1$	$\tau_0/2$	$\tau_0/2^2$	$\tau_0/2^3$	$\tau_0/2^4$	$\tau_0/2^5$	$\tau_0/2^6$	$\tau_0/2^7$
$\varepsilon_0 = 0.5$	1.29E-02	2.02E-03	2.81E-04	3.60E-05	4.45E-06	5.73E-07	7.01E-08	8.98E-09
order	-	2.67	2.85	2.96	3.02	2.96	3.03	2.97
$\varepsilon_0/2$	1.36E-02	2.55E-03	4.22E-04	6.22E-05	8.79E-06	1.18E-06	1.49E-07	1.88E-08
order	-	2.42	2.59	2.76	2.82	2.90	2.98	2.99
$\varepsilon_0/2^2$	5.62E-02	1.22E-02	2.62E-03	4.35E-04	6.47E-05	8.69E-06	1.14E-06	1.47E-07
order	-	2.20	2.22	2.59	2.75	2.90	2.93	2.95
$\varepsilon_0/2^3$	1.60E-01	3.25E-02	7.66E-03	1.78E-03	2.96E-04	4.46E-05	6.30E-06	7.81E-07
order	-	2.30	2.09	2.11	2.59	2.73	2.82	3.01
$\varepsilon_0/2^4$	2.45E-01	6.06E-02	1.49E-02	3.11E-03	6.74E-04	1.19E-04	2.09E-05	3.25E-06
order	-	2.01	2.03	2.26	2.20	2.50	2.51	2.68
$\varepsilon_0/2^5$	4.24E-01	1.06E-01	2.51E-02	5.75E-03	1.33E-03	2.75E-04	5.55E-05	9.71E-06
order	-	2.00	2.07	2.13	2.11	2.27	2.31	2.52
$\varepsilon_0/2^6$	4.08E-01	9.89E-02	2.45E-02	6.04E-03	1.53E-03	3.78E-04	7.57E-05	1.32E-05
order	-	2.04	2.01	2.02	1.98	2.01	2.32	2.53
$\varepsilon_0/2^7$	3.79E-01	9.37E-02	2.50E-02	6.54E-03	1.58E-03	3.76E-04	9.55E-05	2.10E-05
order	-	2.02	1.90	1.94	2.05	2.07	1.98	2.18

Table: Error with different τ and ε, $h = 1/64$, well-prepared case

Temporal error

$\|e^n\|_{H^1}$	$\tau_0 = 0.1$	$\tau_0/2$	$\tau_0/2^2$	$\tau_0/2^3$	$\tau_0/2^4$	$\tau_0/2^5$	$\tau_0/2^6$	$\tau_0/2^7$
$\varepsilon_0 = 0.5$	2.19E-02	3.51E-03	4.91E-04	6.35E-05	8.10E-06	1.01E-06	1.23E-07	1.57E-08
order	-	2.64	2.84	2.95	2.97	3.01	3.04	2.96
$\varepsilon_0/2$	2.41E-02	4.46E-03	7.53E-04	1.04E-04	1.48E-05	1.97E-06	2.54E-07	3.22E-08
order	-	2.43	2.57	2.86	2.80	2.91	2.96	2.98
$\varepsilon_0/2^2$	1.04E-01	2.22E-02	4.58E-03	7.44E-04	1.21E-04	1.52E-05	1.97E-06	2.50E-07
order	-	2.23	2.28	2.62	2.62	3.00	2.95	2.97
$\varepsilon_0/2^3$	2.59E-01	5.78E-02	1.12E-02	2.77E-03	4.57E-04	7.43E-05	1.02E-05	1.33E-06
order	-	2.17	2.37	2.02	2.60	2.62	2.87	2.94
$\varepsilon_0/2^4$	4.19E-01	1.01E-01	2.55E-02	5.31E-03	1.15E-03	2.01E-04	3.58E-05	5.56E-06
order	-	2.05	1.99	2.26	2.20	2.52	2.49	2.68
$\varepsilon_0/2^5$	7.37E-01	1.68E-01	4.06E-02	9.55E-03	2.13E-03	4.54E-04	8.82E-05	1.59E-05
order	-	2.14	2.05	2.09	2.16	2.23	2.37	2.47
$\varepsilon_0/2^6$	6.37E-01	1.45E-01	4.09E-02	9.90E-03	2.45E-03	6.21E-04	1.33E-04	2.25E-05
order	-	2.13	1.83	2.05	2.01	1.98	2.22	2.57
$\varepsilon_0/2^7$	6.35E-01	1.46E-01	3.96E-02	1.00E-02	2.44E-03	5.78E-04	1.52E-04	3.52E-05
Order	-	2.12	1.88	1.99	2.03	2.08	1.93	2.11

Table: Error with different τ and ε, $h = 1/64$, ill-prepared case

Conclusion

The result shows our method is uniformly spectral accurate in mesh size h. For temporal error, the convergence order stays uniformly over 2 for well-prepared and ill-prepared case.
Future study can be focused on proving the error estimation for a wider range of α, (for example $\alpha < 0$) or increasing the number of Picard integration to achieve higher order uniform temporal accuracy.