Error estimates for the long time dynamics of the nonlinear Klein-Gordon equation

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Outline

1. Introduction
2. Numerical methods and error estimates
   - Finite difference time domain (FDTD) methods
   - Exponential wave integrator (EWI) spectral method
   - Time-splitting (TS) spectral method
3. Extension to an oscillatory NKGE
4. Conclusions and future work

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Introduction

Consider the following nonlinear Klein-Gordon equation (NKGE) with a cubic nonlinearity on a torus $\mathbb{T}^d$ $(d = 1, 2, 3)$ as

$$\partial_{tt} u(\mathbf{x}, t) - \Delta u(\mathbf{x}, t) + u(\mathbf{x}, t) + \varepsilon^2 u^3(\mathbf{x}, t) = 0, \ \mathbf{x} \in \mathbb{T}^d, \ t > 0,$$

- Initial data

$$u(\mathbf{x}, 0) = \phi(\mathbf{x}), \quad \partial_t u(\mathbf{x}, 0) = \gamma(\mathbf{x}), \quad \mathbf{x} \in \mathbb{T}^d$$

- $u = u(\mathbf{x}, t)$ real-valued field
- $0 < \varepsilon \leq 1$ a dimensionless parameter
- ϕ and γ given dimensionless real functions, independent of ε

The (nonlinear) Klein-Gordon equation

- Proposed in 1926 by the physicists Oskar Klein and Walter Gordon
- To describe the spinless relativistic particles, like pion
- The discovery of the Higgs boson in 2012 – the first observed ostensibly elementary particle
- A relativistic version of Schrödinger equation
- Applications
  - Propagation of dislocations in crystals
  - Superconducting material, e.g. propagation of magnetic flux in a Josephson junction
  - Universe, e.g. dark matter or black-hole evaporation
  - Nonlinear optics, nonlinear dynamics of DNA chain, ...

Properties of NKGE

- Time symmetric, i.e. unchanged if $t \to -t$
- Hamiltonian (or Energy) conservation

$$
\begin{aligned}
E(t) &:= \int_{\mathbb{T}^d} \left[|\partial_t u(\mathbf{x},t)|^2 + |\nabla u(\mathbf{x},t)|^2 + |u(\mathbf{x},t)|^2 + \frac{\varepsilon^2}{2} |u(\mathbf{x},t)|^4 \right] d\mathbf{x} \\
&\equiv \int_{\mathbb{T}^d} \left[|\gamma(\mathbf{x})|^2 + |\nabla \phi(\mathbf{x})|^2 + |\phi(\mathbf{x})|^2 + \frac{\varepsilon^2}{2} |\phi(\mathbf{x})|^4 \right] d\mathbf{x} \\
&:= E(0) = O(1), \quad t \geq 0.
\end{aligned}
$$

- Two different time regimes
  - $O(1)$-time regime, e.g. $\varepsilon = 1$
  - Long-time regime, e.g. $0 < \varepsilon \ll 1$

Existing results in $O(1)$-time regime

- Analytical results for Cauchy problem, i.e., the existence, uniqueness and regularity of the solutions: Browder, 62'; Segal, 63; Glassey, 73'; Brenner & von Wahl, 81; Klainerman, 85'; Ginibre & Velo, 85' & 89'; Shatah, 85'; Motai, 89'; Simon & Taflin, 93'; Nakamura & Ozawa, 01', ...
- Numerical methods
  - Finite difference time domain (FDTD) methods: Strauss & Vázquez,78'; Li & Vu-Quoc, 95'; Duncan, 97'; Cohen, Hairer & Lubich, 08'; Dehghan, Mohebbi & Asgari, 09', ...
    - Conservative vs non-conservative
    - Implicit vs explicit
  - Spectral methods: Cao & Guo, 93'; Chen, 06',...

Existing results in long-time regime

- Equivalent form
  When $0 < \varepsilon \ll 1$, introducing $w(\mathbf{x}, t) = \varepsilon u(\mathbf{x}, t)$, we obtain the NKGE with small initial data:

$$\partial_{tt} w(\mathbf{x}, t) - \Delta w(\mathbf{x}, t) + w(\mathbf{x}, t) + w^3(\mathbf{x}, t) = 0, \ \mathbf{x} \in \mathbb{T}^d, \ t > 0,$$
$$w(\mathbf{x}, 0) = \varepsilon \phi(\mathbf{x}), \quad \partial_t w(\mathbf{x}, 0) = \varepsilon \gamma(\mathbf{x}), \quad \mathbf{x} \in \mathbb{T}^d.$$

- Lifespan of the solution on a torus: $O(\varepsilon^{-2})$
  Bourgain, 95'; Ozawa, Tsutaya & Tsutsumi, 96; Delort, 96', 97', 98' & 09'; Keel & Tao, 99'; Sunagawa, 03'; Delort & Szeftel, 04', ...

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FDTD methods

- Finite difference discretization operators

$$\delta_t^+ u_j^n = \frac{u_j^{n+1} - u_j^n}{\tau}, \quad \delta_t^- u_j^n = \frac{u_j^n - u_j^{n-1}}{\tau}, \quad \delta_t^2 u_j^n = \frac{u_j^{n+1} - 2u_j^n + u_j^{n-1}}{\tau^2},$$

$$\delta_x^+ u_j^n = \frac{u_{j+1}^n - u_j^n}{h}, \quad \delta_x^- u_j^n = \frac{u_j^n - u_{j-1}^n}{h}, \quad \delta_x^2 u_j^n = \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{h^2}.$$

- The Crank-Nicolson finite difference (CNFD) method

$$\delta_t^2 u_j^n - \frac{1}{2}\delta_x^2 \left(u_j^{n+1} + u_j^{n-1}\right) + \frac{1}{2}\left(u_j^{n+1} + u_j^{n-1}\right) + \varepsilon^2 G\left(u_j^{n+1}, u_j^{n-1}\right) = 0$$

- A semi-implicit energy conservative finite difference (SIFD1) method

$$\delta_t^2 u_j^n - \delta_x^2 u_j^n + \frac{1}{2}\left(u_j^{n+1} + u_j^{n-1}\right) + \varepsilon^2 G\left(u_j^{n+1}, u_j^{n-1}\right) = 0$$

$$G(v,w) = \frac{F(v) - F(w)}{v - w}, \; F(v) = \int_0^v s^3 ds = \frac{v^4}{4}, \; \forall \; v, w \in \mathbb{R}.$$

FDTD methods

- Another semi-implicit finite difference (SIFD2) method

$$\delta_t^2 u_j^n - \frac{1}{2}\delta_x^2\left(u_j^{n+1} + u_j^{n-1}\right) + \frac{1}{2}\left(u_j^{n+1} + u_j^{n-1}\right) + \varepsilon^2\left(u_j^n\right)^3 = 0$$

- The leap-frog finite difference (LFFD) method

$$\delta_t^2 u_j^n - \delta_x^2 u_j^n + u_j^n + \varepsilon^2\left(u_j^n\right)^3 = 0.$$

- The initial and boundary conditions are discretized as

$$u_0^{n+1} = u_M^{n+1}, \quad u_{-1}^{n+1} = u_{M-1}^{n+1}, \quad n \geq 0; \quad u_j^0 = \phi(x_j),\ j = 0, 1, \ldots, M,$$

  and the first step u^1 is updated by

$$u_j^1 = \phi(x_j) + \tau\gamma(x_j) + \frac{\tau^2}{2}\left[\delta_x^2\phi(x_j) - \phi(x_j) - \varepsilon^2\left(\phi(x_j)\right)^3\right],\ j = 0, 1, \ldots, M.$$

Error estimates for FDTD methods

- Define 'error' function $e_j^n = u(x_j, t_n) - u_j^n,\ j = 0, 1, \cdots, M,\ n \geq 0$
- Error bounds of the FDTD methods up to the time at $O(\varepsilon^{-\beta})$ with $0 \leq \beta \leq 2$:

$$\|e^n\|_{l^2} + \|\delta_x^+ e^n\|_{l^2} \lesssim \frac{h^2}{\varepsilon^\beta} + \frac{\tau^2}{\varepsilon^\beta},$$
$$\|u^n\|_{l^\infty} \leq 1 + M_0, \quad 0 \leq n \leq \frac{T_0/\varepsilon^\beta}{\tau}.$$

- Convergence rates for the fixed ε: second order in space & time
- Resolution: $h = O(\varepsilon^{\beta/2}),\ \tau = O(\varepsilon^{\beta/2})$

Numerical results for CNFD with $\beta = 1$

Error bounds: $\|e^n\|_{l^2} + \|\delta_x^+ e^n\|_{l^2} \lesssim \frac{h^2}{\varepsilon} + \frac{\tau^2}{\varepsilon}$

Table: Spatial errors of the CNFD method for the NKGE with $\beta = 1$

$e_{h,\tau_e}(t=1/\varepsilon)$	$h_0=\pi/16$	$h_0/2$	$h_0/2^2$	$h_0/2^3$	$h_0/2^4$	$h_0/2^5$
$\varepsilon_0 = 1$	**3.77E-2**	9.65E-3	2.43E-3	6.09E-4	1.52E-4	3.84E-5
order	-	1.97	1.99	2.00	2.00	1.98
$\varepsilon_0/4$	7.31E-2	**1.77E-2**	4.38E-3	1.09E-3	2.74E-4	7.02E-5
order	-	**2.05**	2.01	2.01	1.99	1.96
$\varepsilon_0/4^2$	6.60E-1	1.71E-1	**4.31E-2**	1.08E-2	2.70E-3	6.91E-4
order	-	1.95	**1.99**	2.00	2.00	1.97
$\varepsilon_0/4^3$	2.78E+0	7.25E-1	1.80E-1	**4.50E-2**	1.13E-2	2.88E-3
order	-	1.94	2.01	**2.00**	1.99	1.97
$\varepsilon_0/4^4$	5.67E+0	8.48E-1	3.96E-1	1.10E-1	**2.81E-2**	7.22E-3
order	-	2.74	1.10	1.85	**1.97**	1.96

Numerical results for CNFD with $\beta = 1$

Error bounds: $\|e^n\|_{l^2} + \|\delta_x^+ e^n\|_{l^2} \lesssim \frac{h^2}{\varepsilon} + \frac{\tau^2}{\varepsilon}$

Table: Temporal errors of the CNFD method for the NKGE with $\beta = 1$

$e_{h_e,\tau}(t=1/\varepsilon)$	$\tau_0 = 0.05$	$\tau_0/2$	$\tau_0/2^2$	$\tau_0/2^3$	$\tau_0/2^4$	$\tau_0/2^5$
$\varepsilon_0 = 1$	**3.27E-2**	8.57E-3	2.19E-3	5.53E-4	1.39E-4	3.48E-5
order	-	1.93	1.97	1.99	1.99	2.00
$\varepsilon_0/4$	4.01E-2	**9.95E-3**	2.49E-3	6.22E-4	1.56E-4	3.89E-5
order	-	**2.01**	2.00	2.00	2.00	2.00
$\varepsilon_0/4^2$	3.45E-1	8.79E-2	**2.21E-2**	5.53E-3	1.38E-3	3.46E-4
order	-	1.97	**1.99**	2.00	2.00	2.00
$\varepsilon_0/4^3$	1.47E+0	3.69E-1	9.19E-2	**2.29E-2**	5.74E-3	1.43E-3
order	-	1.99	2.01	**2.00**	2.00	2.01
$\varepsilon_0/4^4$	8.58E-1	7.05E-1	2.20E-1	5.75E-2	**1.45E-2**	3.64E-3
order	-	0.28	1.68	1.94	**1.99**	1.99

Numerical results for CNFD with $\beta = 2$

Error bounds: $\|e^n\|_{l^2} + \|\delta_x^+ e^n\|_{l^2} \lesssim \frac{h^2}{\varepsilon^2} + \frac{\tau^2}{\varepsilon^2}$

Table: Spatial errors of the CNFD method for the NKGE with $\beta = 2$

$e_{h,\tau_e}(t = 1/\varepsilon^2)$	$h_0 = \pi/16$	$h_0/2$	$h_0/2^2$	$h_0/2^3$	$h_0/2^4$	$h_0/2^5$
$\varepsilon_0 = 1$	**3.77E-2**	9.65E-3	2.43E-3	6.09E-4	1.52E-4	3.84E-5
order	-	1.97	1.99	2.00	2.00	1.98
$\varepsilon_0/2$	3.98E-2	**9.56E-3**	2.39E-3	5.97E-4	1.49E-4	3.81E-5
order	-	**2.06**	2.00	2.00	2.00	1.97
$\varepsilon_0/2^2$	7.17E-1	1.82E-1	**4.55E-2**	1.14E-2	2.85E-3	7.27E-4
order	-	1.98	**2.00**	2.00	2.00	1.97
$\varepsilon_0/2^3$	2.78E+0	6.54E-1	1.58E-1	**3.92E-2**	9.78E-3	2.50E-3
order	-	2.09	2.05	**2.01**	2.00	1.97
$\varepsilon_0/2^4$	3.31E+0	1.78E+0	5.92E-1	1.55E-1	**3.93E-2**	1.01E-2
order	-	0.89	1.59	1.93	**1.98**	1.96

Numerical results for CNFD with $\beta = 2$

Error bounds: $\|e^n\|_{l^2} + \|\delta_x^+ e^n\|_{l^2} \lesssim \frac{h^2}{\varepsilon^2} + \frac{\tau^2}{\varepsilon^2}$

Table: Temporal errors of the CNFD method for the NKGE with $\beta = 2$

$e_{h_e,\tau}(t=1/\varepsilon^2)$	$\tau_0 = 0.05$	$\tau_0/2$	$\tau_0/2^2$	$\tau_0/2^3$	$\tau_0/2^4$	$\tau_0/2^5$
$\varepsilon_0 = 1$	**3.27E-2**	8.57E-3	2.19E-3	5.53E-4	1.39E-4	3.48E-5
order	-	1.93	1.97	1.99	1.99	2.00
$\varepsilon_0/2$	2.56E-2	**6.32E-3**	1.58E-3	3.94E-4	9.86E-5	2.47E-5
order	-	**2.02**	2.00	2.00	2.00	2.00
$\varepsilon_0/2^2$	3.91E-1	9.83E-2	**2.46E-2**	6.16E-3	1.54E-3	3.85E-4
order	-	1.99	**2.00**	2.00	2.00	2.00
$\varepsilon_0/2^3$	1.40E+0	3.32E-1	8.14E-2	**2.03E-2**	5.06E-3	1.26E-3
order	-	2.08	2.03	**2.00**	2.00	2.01
$\varepsilon_0/2^4$	1.81E+0	1.13E+0	3.16E-1	8.07E-2	**2.03E-2**	5.07E-3
order	-	0.68	1.84	1.97	**1.99**	2.00

Exponential wave integrator (EWI) spectral method

$$\partial_{tt}u(x,t) - \partial_{xx}u(x,t) + u(x,t) + \varepsilon^2 u^3(x,t) = 0,\ \ x \in \Omega = (a,b),\ \ t > 0,$$
$$u(x,0) = \phi(x), \quad \partial_t u(x,0) = \gamma(x), \quad x \in \overline{\Omega} = [a,b],$$

- Apply Fourier spectral method for spatial derivatives

  $$\partial_{tt}u_M(x,t) - \partial_{xx}u_M(x,t) + u_M(x,t) + \varepsilon^2 P_M f(u_M(x,t)) = 0,\ \ a \le x \le b,\ \ t \ge 0$$

  with

  $$u_M(x,t) = \sum_{l=-M/2}^{M/2-1} \widehat{(u_M)}_l(t) e^{i\mu_l(x-a)},\ a \le x \le b,\ \mu_l = \frac{2\pi l}{b-a},\ l = -\frac{M}{2}, \cdots, \frac{M}{2} - 1$$

- Take Fourier transform, we get ODEs

  $$\frac{d^2}{dt^2}\widehat{(u_M)}_l(t) + (1 + \mu_l^2)\widehat{(u_M)}_l(t) + \varepsilon^2 \widehat{(f(u_M))}_l(t) = 0$$

Exponential wave integrator (EWI) spectral method

- Analytical solution near $t = t_n$

$$\widehat{(u_M)}_l(t_n+\theta) = c_l^n \cos(\zeta_l^n \theta) + d_l^n \frac{\sin(\zeta_l^n \theta)}{\zeta_l^n} - \frac{\varepsilon^2}{\zeta_l^n} \int_0^\theta \widehat{g}_l^n(\omega) \sin(\zeta_l^n(\theta-\omega)) d\omega,$$

$$\zeta_l^n = \sqrt{1+\mu_l^2+\varepsilon^2\alpha^n}, \quad \widehat{g}_l^n(\theta) = (\widehat{f(u_M)})_l(t_n+\theta) - \alpha^n \widehat{(u_M)}_l(t_n+\theta).$$

- For $n = 0$, letting $\theta = \tau$

$$\widehat{(u_M)}_l(\tau) = \widehat{\phi}_l \cos(\zeta_l^0 \tau) + \widehat{\gamma}_l \frac{\sin(\zeta_l^0 \tau)}{\zeta_l^0} - \frac{\varepsilon^2}{\zeta_l^0} \int_0^\tau \widehat{g}_l^0(\omega) \sin(\zeta_l^0(\tau-\omega)) d\omega$$

- For $n > 0$, letting $\theta = \tau$ and $\theta = -\tau$

$$\begin{aligned}\widehat{(u_M)}_l(t_{n+1}) = &- \widehat{(u_M)}_l(t_{n-1}) + 2\cos(\zeta_l^n \tau)\widehat{(u_M)}_l(t_n) \\ &- \frac{\varepsilon^2}{\zeta_l^n} \int_0^\tau [\widehat{g}_l^n(-\omega) + \widehat{g}_l^n(\omega)] \sin(\zeta_l^n(\tau-\omega)) d\omega\end{aligned}$$

Approximate integral via quadrature

- Gautschi-type quadrature:

Gautschi, 61'; Hochbruck & Lubich, 99'; Hochbruck & Ostermann, 00'; Hairer, Lubich & Wanner, 02'; Grim, 05 &, 06'; Bao & Dong, 12'; ...

$$\int_0^\tau \widehat{g}_l^0(\omega)\sin(\zeta_l^0(\tau-\omega))d\omega \approx \widehat{g}_l^0(0)\int_0^\tau \sin(\zeta_l^0(\tau-\omega))d\omega = \frac{\widehat{g}_l^0(0)}{\zeta_l^0}\left[1-\cos(\tau\zeta_l^0)\right],$$

$$\int_0^\tau \left[\widehat{g}_l^n(-\omega)+\widehat{g}_l^n(\omega)\right]\sin(\zeta_l^n(\tau-\omega))d\omega \approx \frac{2\widehat{g}_l^n(0)}{\zeta_l^n}\left[1-\cos(\tau\zeta_l^n)\right], \quad n \geq 1.$$

- Exponential wave integrator (EWI) in Gautschi-type:

$$\widehat{(u_M^1)}_l = \cos(\zeta_l^0\tau)\widehat{\phi}_l + \frac{\sin(\zeta_l^0\tau)}{\zeta_l^0}\widehat{\gamma}_l + \frac{\varepsilon^2(\cos(\tau\zeta_l^0)-1)}{(\zeta_l^0)^2}\widehat{g}_l^0(0),$$

$$\widehat{(u_M^{n+1})}_l = -\widehat{(u_M^{n-1})}_l + 2\cos(\zeta_l^n\tau)\widehat{(u_M^n)}_l + \frac{2\varepsilon^2(\cos(\tau\zeta_l^n)-1)}{(\zeta_l^n)^2}\widehat{g}_l^n(0), \quad n \geq 1,$$

The EWI-FP method

In practice, it is difficult to compute the Fourier coefficients. We simply replace the projections by the interpolations. Let u_j^n be the approximation of $u(x_j, t_n)$ and denote $u_j^0 = \phi(x_j)$, the exponential wave integrator Fourier pseudospectral (EWI-FP) method for the NKGE is

$$u_j^{n+1} = \sum_{l \in \mathcal{T}_M} \widetilde{u}_l^{n+1} e^{i\mu_l(x_j - a)}, \quad j = 0, 1, \cdots, M,$$

where

$$\widetilde{(u_M^1)}_l = \cos(\zeta_l^0 \tau)\widetilde{\phi}_l + \frac{\sin(\zeta_l^0 \tau)}{\zeta_l^0}\widetilde{\gamma}_l + \frac{\varepsilon^2(\cos(\tau\zeta_l^0) - 1)}{(\zeta_l^0)^2}\widetilde{g}_l^0(0),$$

$$\widetilde{(u_M^{n+1})}_l = -\widetilde{(u_M^{n-1})}_l + 2\cos(\zeta_l^n \tau)\widetilde{(u_M^n)}_l + \frac{2\varepsilon^2(\cos(\tau\zeta_l^n) - 1)}{(\zeta_l^n)^2}\widetilde{g}_l^n(0), \quad n \geq 1,$$

Stability analysis

Let $T_0 > 0$ be a fixed constant, $T_\varepsilon = T_0/\varepsilon^2$ and denote

$$\sigma_{\max} := \max_{0 \le n \le T_\varepsilon/\tau} \|u^n\|_{l^\infty}^2,$$

where $\|u\|_{l^\infty} = \max_{0 \le j \le M-1} |u_j|$.

Lemma

If α^n is chosen such that $\alpha^n \ge \sigma_{\max}$ for $n \ge 0$, the EWI-FP is unconditionally stable for any $h > 0$, $\tau > 0$ and $0 < \varepsilon \le 1$.

In practice, the above lemma suggests that α^n can be chosen as:

$$\alpha^n = \max\left\{\alpha^{n-1}, \max_{u_j^n \ne 0, 0 \le j \le M} \left(u_j^n\right)^2\right\}, \quad n \ge 0, \quad \text{with} \quad \alpha^{-1} = 0.$$

Error bounds for the EWI-FP method

Under the assumptions of the regularity of the exact solution up to the time at $t = T_0/\varepsilon^\beta$ with $0 \le \beta \le 2$ and letting

$$\tau \le \frac{\pi h}{3\sqrt{h^2 + \pi^2 + \varepsilon^2 M_2 h^2}}, \quad 0 < \varepsilon \le 1,$$

we have the following error estimates for the EWI-FS method:

Theorem

Let $u_M^n(x)$ be the approximations obtained from the EWI-FS, under the assumptions, there exist constants $h_0 > 0$ and $\tau_0 > 0$ sufficiently small and independent of ε, such that for any $0 < \varepsilon \le 1$, when $0 < h \le h_0$, $0 < \tau \le \tau_0$, we have

$$\|u(x, t_n) - u_M^n(x)\|_{H^\lambda} \lesssim h^{m_0 - \lambda} + \varepsilon^{2-\beta}\tau^2, \quad \lambda = 0, 1,$$

$$\|u_M^n(x)\|_{L^\infty} \le 1 + M_1, \quad 0 \le n \le \frac{T_0/\varepsilon^\beta}{\tau}.$$

The EWI-FP method for NKGE

- Resolution in long-time regime up to $O(\varepsilon^{-2})$:

$$h = O(1), \quad \tau = O(1)$$

- Properites
  - Explicit - no need to solve any linear system
  - Easy to extend to 2D or 3D
  - Unconditionally stable by adding a proper linear stabilizing term

Numerical results for the EWI-FP method

Table: Spatial errors of the EWI-FP for the NKGE in 1D with different β or ε

	$\|e(\cdot, T_\varepsilon)\|_{H^1}$	$h_0 = \pi/2$	$h_0/2$	$h_0/2^2$	$h_0/2^3$
$\beta = 0$	$\varepsilon_0 = 1$	4.05E-2	8.80E-3	1.53E-4	1.26E-8
	$\varepsilon_0/2$	4.78E-2	8.48E-3	1.58E-4	1.05E-8
	$\varepsilon_0/2^2$	5.17E-2	8.36E-3	1.59E-4	9.92E-9
	$\varepsilon_0/2^3$	5.28E-2	8.33E-3	1.59E-4	9.78E-9
	$\varepsilon_0/2^4$	5.31E-2	8.32E-3	1.59E-4	9.75E-9
$\beta = 1$	$\varepsilon_0 = 1$	4.05E-2	8.80E-3	1.53E-4	1.26E-8
	$\varepsilon_0/2$	3.98E-2	6.27E-3	5.61E-5	1.60E-8
	$\varepsilon_0/2^2$	1.57E-2	8.14E-3	1.33E-4	3.18E-8
	$\varepsilon_0/2^3$	1.02E-2	3.17E-3	2.82E-5	4.61E-9
	$\varepsilon_0/2^4$	6.08E-3	3.44E-3	1.41E-5	1.45E-8
$\beta = 2$	$\varepsilon_0 = 1$	4.05E-2	8.80E-3	1.53E-4	1.26E-8
	$\varepsilon_0/2$	4.04E-2	8.46E-3	1.40E-4	3.21E-8
	$\varepsilon_0/2^2$	6.12E-2	4.18E-3	1.57E-5	1.41E-8
	$\varepsilon_0/2^3$	1.01E-1	3.25E-3	1.45E-4	2.79E-8
	$\varepsilon_0/2^4$	6.05E-2	1.24E-3	1.34E-4	2.83E-8

Temporal errors for EWI-FP with $\beta = 0$

Error bounds: $\|u(x,t_n) - u_M^n(x)\|_{H^\lambda} \lesssim h^{m_0-\lambda} + \varepsilon^2\tau^2$

Table: Temporal errors of the EWI-FP for the NKGE in 1D with $\beta = 0$

$\|e(\cdot,T_\varepsilon)\|_{H^1}$	$\tau_0 = 0.2$	$\tau_0/2$	$\tau_0/2^2$	$\tau_0/2^3$	$\tau_0/2^4$	$\tau_0/2^5$	$\tau_0/2^6$
$\varepsilon_0 = 1$	3.28E-2	8.13E-3	2.03E-3	5.06E-4	1.27E-4	3.16E-5	7.91E-6
order	-	2.01	2.00	2.00	1.99	2.01	2.00
$\varepsilon_0/2$	1.17E-2	2.91E-3	7.25E-4	1.81E-4	4.53E-5	1.13E-5	2.83E-6
order	-	2.01	2.00	2.00	2.00	2.00	2.00
$\varepsilon_0/2^2$	3.25E-3	8.06E-4	2.01E-4	5.02E-5	1.26E-5	3.14E-6	7.85E-7
order	-	2.01	2.00	2.00	1.99	2.00	2.00
$\varepsilon_0/2^3$	8.33E-4	2.07E-4	5.16E-5	1.29E-5	3.22E-6	8.06E-7	2.02E-7
order	-	2.01	2.00	2.00	2.00	2.00	2.00
$\varepsilon_0/2^4$	2.10E-4	5.21E-5	1.30E-5	3.25E-6	8.11E-7	2.03E-7	5.07E-8
order	-	2.01	2.00	2.00	2.00	2.00	2.00
$\varepsilon_0/2^5$	5.25E-5	1.30E-5	3.25E-6	8.13E-7	2.03E-7	5.08E-8	1.27E-8
order	-	2.01	2.00	2.00	2.00	2.00	2.00

Temporal errors for EWI-FP with $\beta = 1$

Error bounds: $\|u(x,t_n) - u_M^n(x)\|_{H^\lambda} \lesssim h^{m_0-\lambda} + \varepsilon\tau^2$

Table: Temporal errors of the EWI-FP for the NKGE in 1D with $\beta = 1$

$\|e(\cdot,T_\varepsilon)\|_{H^1}$	$\tau_0 = 0.2$	$\tau_0/2$	$\tau_0/2^2$	$\tau_0/2^3$	$\tau_0/2^4$	$\tau_0/2^5$	$\tau_0/2^6$
$\varepsilon_0 = 1$	3.28E-2	8.13E-3	2.03E-3	5.06E-4	1.27E-4	3.16E-5	7.91E-6
order	-	2.01	2.00	2.00	1.99	2.01	2.00
$\varepsilon_0/2$	9.66E-3	2.44E-3	6.09E-4	1.52E-4	3.81E-5	9.53E-6	2.38E-6
order	-	1.99	2.00	2.00	2.00	2.00	2.00
$\varepsilon_0/2^2$	5.81E-3	1.44E-3	3.62E-4	9.05E-5	2.26E-5	5.66E-6	1.41E-6
order	-	2.01	1.99	2.00	2.00	2.00	2.01
$\varepsilon_0/2^3$	2.94E-3	7.39E-4	1.85E-4	4.62E-5	1.15E-5	2.89E-6	7.21E-7
order	-	1.99	2.00	2.00	2.01	1.99	2.00
$\varepsilon_0/2^4$	1.66E-3	4.16E-4	1.04E-4	2.60E-5	6.51E-6	1.63E-6	4.07E-7
order	-	2.00	2.00	2.00	2.00	2.00	2.00
$\varepsilon_0/2^5$	5.47E-4	1.37E-4	3.44E-5	8.60E-6	2.15E-6	5.37E-7	1.34E-7
order	-	2.00	1.99	2.00	2.00	2.00	2.00

Temporal errors for EWI-FP with $\beta = 2$

Error bounds: $\|u(x,t_n) - u_M^n(x)\|_{H^\lambda} \lesssim h^{m_0-\lambda} + \tau^2$

Table: Temporal errors of the EWI-FP for the NKGE in 1D with $\beta = 2$

$\|e(\cdot,T_\varepsilon)\|_{H^1}$	$\tau_0 = 0.2$	$\tau_0/2$	$\tau_0/2^2$	$\tau_0/2^3$	$\tau_0/2^4$	$\tau_0/2^5$	$\tau_0/2^6$
$\varepsilon_0 = 1$	3.28E-2	8.13E-3	2.03E-3	5.06E-4	1.27E-4	3.16E-5	7.91E-6
order	-	2.01	2.00	2.00	1.99	2.01	2.00
$\varepsilon_0/2$	1.76E-2	4.45E-3	1.11E-3	2.78E-4	6.96E-5	1.74E-5	4.35E-6
order	-	1.98	2.00	2.00	2.00	2.00	2.00
$\varepsilon_0/2^2$	2.28E-2	5.68E-3	1.42E-3	3.55E-4	8.87E-5	2.22E-5	5.54E-6
order	-	2.01	2.00	2.00	2.00	2.00	2.00
$\varepsilon_0/2^3$	4.68E-2	1.17E-2	2.93E-3	7.33E-4	1.83E-4	4.58E-5	1.15E-5
order	-	2.00	2.00	2.00	2.00	2.00	1.99
$\varepsilon_0/2^4$	3.96E-2	9.94E-3	2.49E-3	6.22E-4	1.56E-4	3.89E-5	9.71E-6
order	-	1.99	2.00	2.00	2.00	2.00	2.00
$\varepsilon_0/2^5$	4.69E-2	1.17E-2	2.93E-3	7.32E-4	1.83E-4	4.57E-5	1.14E-5
order	-	2.00	2.00	2.00	2.00	2.00	2.00

A relativistic NLSE reformulation

$$\partial_{tt}u(x,t) - \partial_{xx}u(x,t) + u(x,t) + \varepsilon^2 u^3(x,t) = 0,\ \ x \in \Omega = (a,b),\ \ t > 0,$$
$$u(x,0) = \phi(x), \quad \partial_t u(x,0) = \gamma(x), \quad x \in \overline{\Omega} = [a,b],$$

A relativistic NLSE reformulation:

- Define the operator $\langle \nabla \rangle = \sqrt{1-\Delta}$
- Denote $\dot{u}(x,t) = \partial_t u(x,t)$ and $\psi(x,t) = u(x,t) - i\langle \nabla \rangle^{-1}\dot{u}(x,t)$
- The NKGE is equivalent to the following NLSE:

$$\begin{cases} i\partial_t \psi(x,t) + \langle \nabla \rangle \psi(x,t) + \varepsilon^2 \langle \nabla \rangle^{-1} f\Big(\frac{1}{2}(\psi + \overline{\psi})\Big)(x,t) = 0, \\ \psi(x,0) = \psi_0(x) := u_0(x) - i\langle \nabla \rangle^{-1} u_1(x), \end{cases}$$

where $f(v) = v^3$ and $\overline{\psi}$ denotes the complex conjugate of ψ.

The second-order Strang splitting

- Step 1: linear part

$$\begin{cases} i\partial_t\psi(x,t) + \langle\nabla\rangle\psi(x,t) = 0, \\ \psi(x,0) = \psi_0(x), \end{cases} \implies \psi(\cdot,t) = \varphi_T^t(\psi_0) := e^{it\langle\nabla\rangle}\psi_0, \quad t \geq 0.$$

- Step 2: nonlinear part

$$\begin{cases} i\partial_t\psi(x,t) + \varepsilon^2\langle\nabla\rangle^{-1} f\big(\frac{1}{2}(\psi+\overline{\psi})\big)(x,t) = 0, \\ \psi(x,0) = \psi_0(x). \end{cases}$$

$$\implies \psi(x,t) = \varphi_V^t(\psi_0) := \psi_0(x) + \varepsilon^2 t F(\psi_0(x)), \quad t \geq 0,$$

with

$$F(\phi) = i\langle\nabla\rangle^{-1}G(\phi), \qquad G(\phi) = f\big(\frac{1}{2}(\phi+\overline{\phi})\big).$$

- The second-order Strang splitting:

$$\psi^{[n+1]} = \mathcal{S}_\tau(\psi^{[n]}) = \varphi_T^{\tau/2} \circ \varphi_V^{\tau} \circ \varphi_T^{\tau/2}(\psi^{[n]}), \quad 0 \leq n \leq \frac{T_0/\varepsilon^2}{\tau} - 1;$$
$$\psi^{[0]} = \psi_0 = u_0 - i\langle\nabla\rangle^{-1}u_1.$$

Time-splitting Fourier spectral (TSFP) method

- Time-splitting Fourier pseudospectral (TSFP) discretization:

$$\psi_j^{(n,1)} = \sum_{l\in\mathcal{T}_N} e^{i\frac{\tau\zeta_l}{2}} \widetilde{(\psi^n)}_l e^{i\mu_l(x_j-a)},$$

$$\psi_j^{(n,2)} = \psi_j^{(n,1)} + \varepsilon^2\tau F_j^n, \quad F_j^n = i\sum_{l\in\mathcal{T}_N} \frac{1}{\zeta_l}\big(\widetilde{G(\psi^{(n,1)})}\big)_l e^{i\mu_l(x_j-a)}$$

$$\psi_j^{n+1} = \sum_{l\in\mathcal{T}_N} e^{i\frac{\tau\zeta_l}{2}} \big(\widetilde{\psi^{(n,2)}}\big)_l e^{i\mu_l(x_j-a)}.$$

- u_j^n and $\dot{u}_j^n$ can be recovered by

$$u_j^{n+1} = \frac{1}{2}\left(\psi_j^{n+1} + \overline{\psi_j^{n+1}}\right), \quad \dot{u}_j^{n+1} = \frac{i}{2}\sum_{l\in\mathcal{T}_N} \zeta_l\left[\widetilde{(\psi^{n+1})}_l - \widetilde{(\overline{\psi^{n+1}})}_l\right] e^{i\mu_l(x_j-a)},$$

Error estimates for the TSFP method

- Assumptions on the exact solution $u(x,t)$ of the NKGE up to the time at $T_\varepsilon = T_0/\varepsilon^\beta$ with $\beta \in [0,2]$:

$$u \in L^\infty\left([0,T_\varepsilon]; H_{\mathrm{p}}^{m+1}\right), \quad \partial_t u \in L^\infty\left([0,T_\varepsilon]; H_{\mathrm{p}}^{m}\right),$$
$$\|u\|_{L^\infty\left([0,T_\varepsilon]; H_{\mathrm{p}}^{m+1}\right)} \lesssim 1, \quad \|\partial_t u\|_{L^\infty\left([0,T_\varepsilon]; H_{\mathrm{p}}^{m}\right)} \lesssim 1,$$

with $m \geq 1$.

Theorem

Let u^n be the numerical approximation obtained from the TSFP. Under the assumption, there exist $h_0 > 0$ and $\tau_0 > 0$ sufficiently small and independent of ε such that, for any $0 < \varepsilon \leq 1$, when $0 < h \leq h_0$ and $0 < \tau \leq \tau_0$, we have the error estimates for $s \in (1/2, m]$

$$\|u(\cdot,t_n) - I_N(u^n)\|_s + \|\partial_t u(\cdot,t_n) - I_N(\dot{u}^n)\|_{s-1} \lesssim h^{1+m-s} + \varepsilon^{2-\beta}\tau^2, \quad 0 \leq n \leq \frac{T_0/\varepsilon^\beta}{\tau}.$$

Moreover, $I_N(u^n)$ and $I_N(\dot{u}^n)$ preserves the regularities, i.e.,

$$I_N(u^n) \in H_{\mathrm{p}}^{m+1}, \quad I_N(\dot{u}^n) \in H_{\mathrm{p}}^{m}.$$

Numerical results for the TSFP with $\beta = 0$

Error bounds: $O(h^{1+m-s} + \varepsilon^2\tau^2)$

Table: Temporal errors of the TSFP method for the NKGE with $\beta = 0$

$\|e(\cdot, T_\varepsilon)\|_1$	$\tau_0 = 0.2$	$\tau_0/2$	$\tau_0/2^2$	$\tau_0/2^3$	$\tau_0/2^4$	$\tau_0/2^5$
$\varepsilon_0 = 1$	2.47E+0	6.08E-1	1.51E-1	3.78E-2	9.45E-3	2.36E-3
order	-	2.02	2.01	2.00	2.00	2.00
$\varepsilon_0/2$	6.29E-1	1.57E-1	3.93E-2	9.82E-3	2.45E-3	6.14E-4
order	-	2.00	2.00	2.00	2.00	2.00
$\varepsilon_0/2^2$	1.55E-1	3.90E-2	9.76E-3	2.44E-3	6.11E-4	1.53E-4
order	-	1.99	2.00	2.00	2.00	2.00
$\varepsilon_0/2^3$	3.85E-2	9.71E-3	2.43E-3	6.09E-4	1.52E-4	3.81E-5
order	-	1.99	2.00	2.00	2.00	2.00
$\varepsilon_0/2^4$	9.61E-3	2.43E-3	6.08E-4	1.52E-4	3.80E-5	9.51E-6
order	-	1.98	2.00	2.00	2.00	2.00
$\varepsilon_0/2^5$	2.40E-3	6.06E-4	1.52E-4	3.80E-5	9.50E-6	2.38E-6
order	-	1.99	2.00	2.00	2.00	2.00
$\varepsilon_0/2^6$	6.00E-4	1.52E-4	3.80E-5	9.50E-6	2.38E-6	5.94E-7
order	-	1.98	2.00	2.00	2.00	2.00

Numerical results for the TSFP with $\beta = 1$

Error bounds: $O(h^{1+m-s} + \varepsilon\tau^2)$

Table: Temporal errors of the TSFP method for the NKGE with $\beta = 1$

$\|e(\cdot, T_\varepsilon)\|_1$	$\tau_0 = 0.2$	$\tau_0/2$	$\tau_0/2^2$	$\tau_0/2^3$	$\tau_0/2^4$	$\tau_0/2^5$
$\varepsilon_0 = 1$	2.47E+0	6.08E-1	1.51E-1	3.78E-2	9.45E-3	2.36E-3
order	-	2.02	2.01	2.00	2.00	2.00
$\varepsilon_0/2$	2.33E+0	5.63E-1	1.40E-1	3.49E-2	8.71E-3	2.18E-3
order	-	2.05	2.01	2.00	2.00	2.00
$\varepsilon_0/2^2$	8.44E-1	2.08E-1	5.19E-2	1.30E-2	3.24E-3	8.10E-4
order	-	2.02	2.00	2.00	2.00	2.00
$\varepsilon_0/2^3$	2.26E-1	5.63E-2	1.41E-2	3.51E-3	8.78E-4	2.19E-4
order	-	2.01	2.00	2.01	2.00	2.00
$\varepsilon_0/2^4$	2.28E-2	5.64E-3	1.41E-3	3.51E-4	8.77E-5	2.19E-5
order	-	2.02	2.00	2.01	2.00	2.00
$\varepsilon_0/2^5$	2.44E-3	5.88E-4	1.46E-4	3.63E-5	9.08E-6	2.27E-6
order	-	2.05	2.01	2.01	2.00	2.00
$\varepsilon_0/2^6$	8.03E-4	1.98E-4	4.93E-5	1.23E-5	3.08E-6	7.67E-7
order	-	2.02	2.01	2.00	2.00	2.01

Numerical results for the TSFP with $\beta = 2$

Error bounds: $O(h^{1+m-s} + \tau^2)$

Table: Temporal errors of the TSFP method for the NKGE with $\beta = 2$

$\|e(\cdot, T_\varepsilon)\|_1$	$\tau_0 = 0.2$	$\tau_0/2$	$\tau_0/2^2$	$\tau_0/2^3$	$\tau_0/2^4$	$\tau_0/2^5$
$\varepsilon_0 = 1$	2.47E+0	6.08E-1	1.51E-1	3.78E-2	9.45E-3	2.36E-3
order	-	2.02	2.01	2.00	2.00	2.00
$\varepsilon_0/2$	2.09E+0	5.06E-1	1.26E-1	3.13E-2	7.83E-3	1.96E-3
order	-	2.04	2.01	2.01	2.00	2.00
$\varepsilon_0/2^2$	2.91E+0	7.18E-1	1.79E-1	4.47E-2	1.12E-2	2.79E-3
order	-	2.02	2.00	2.00	2.00	2.01
$\varepsilon_0/2^3$	1.36E+0	3.39E-1	8.45E-2	2.11E-2	5.28E-3	1.32E-3
order	-	2.00	2.00	2.00	2.00	2.00
$\varepsilon_0/2^4$	5.22E-1	1.30E-1	3.24E-2	8.09E-3	2.02E-3	5.06E-4
order	-	2.01	2.00	2.00	2.00	2.00
$\varepsilon_0/2^5$	7.75E-2	1.93E-2	4.81E-3	1.20E-3	3.00E-4	7.51E-5
order	-	2.01	2.00	2.00	2.00	2.00
$\varepsilon_0/2^6$	1.63E-2	4.06E-3	1.01E-3	2.54E-4	6.38E-5	1.63E-5
order	-	2.01	2.01	1.99	1.99	1.97

Outline

1 Introduction

2 Numerical methods and error estimates
- Finite difference time domain (FDTD) methods
- Exponential wave integrator (EWI) spectral method
- Time-splitting (TS) spectral method

3 Extension to an oscillatory NKGE

4 Conclusions and future work

Extension to an oscillatory NKGE

- Rescaling in time $s = \varepsilon^\beta t$ with $0 \le \beta \le 2$
- Denote $v(\mathbf{x}, s) := u(\mathbf{x}, s/\varepsilon^\beta) = u(\mathbf{x}, t)$
- The oscillatory NKGE

$$\varepsilon^{2\beta}\partial_{ss}v(\mathbf{x}, s) - \Delta v(\mathbf{x}, s) + v(\mathbf{x}, s) + \varepsilon^2 v^3(\mathbf{x}, s) = 0, \;\; x \in \mathbb{T}^d, \;\; s > 0,$$
$$v(\mathbf{x}, 0) = \phi(\mathbf{x}), \quad \partial_s v(\mathbf{x}, 0) = \varepsilon^{-\beta}\gamma(\mathbf{x}), \quad x \in \mathbb{T}^d.$$

- The NKGE with weak nonlinearity/small initial data up to the time T_0/ε^β is equivalent to the oscillatory NKGE up to the fixed time T_0

Extension to an oscillatory NKGE

The solution of the oscillatory NKGE propagates waves with wavelength at $O(1)$ in space and $O(\varepsilon^{\beta})$ in time.

Figure: The solution $v(\pi, s)$ of the oscillatory NKGE with $d = 1$ for different ε and β: (a) $\beta = 1$, (b) $\beta = 2$.

Figure: The solution $v(x, 1)$ of the oscillatory NKGE with $d = 1$ for different ε and β: (a) $\beta = 1$, (b) $\beta = 2$.

Error estimates for the oscillatory NKGE

- FDTD methods
  - Error bounds: $O(\frac{h^2}{\varepsilon^{3\beta}} + \frac{\tau^2}{\varepsilon^{3\beta}})$
  - Resolution: $h = O(\varepsilon^{\beta/2}), \quad \tau = O(\varepsilon^{3\beta/2})$
- EWI-FP method
  - Error bounds: $O(h^m + \varepsilon^{2-3\beta}\tau^2)$
  - Resolution: $h = O(1), \quad \tau = O(\varepsilon^{\alpha^*})$, with $\alpha^* = \max\{0, 3\beta/2 - 1\}$
- TSFP method
  - Error bounds: $O(h^m + \varepsilon^{2-3\beta}\tau^2)$
  - Resolution: $h = O(1), \quad \tau = O(\varepsilon^{\alpha^*})$, with $\alpha^* = \max\{0, 3\beta/2 - 1\}$

Numerical results in the whole space

Consider the following oscillatory NKGE in d-dimensional $(d = 1, 2, 3)$ whole space

$$\varepsilon^{2\beta}\partial_{ss}v(\mathbf{x},s) - \Delta v(\mathbf{x},s) + v(\mathbf{x},s) + \varepsilon^2 v^3(\mathbf{x},s) = 0,\ \ \mathbf{x}\in\mathbb{R}^d,\ \ s>0,$$
$$v(\mathbf{x},0) = \phi(\mathbf{x}),\quad \partial_s v(\mathbf{x},0) = \varepsilon^{-\beta}\gamma(\mathbf{x}),\ \ \mathbf{x}\in\mathbb{R}^d.$$

The solution propagates waves with wave speed in space at $O(\varepsilon^{-\beta})$.

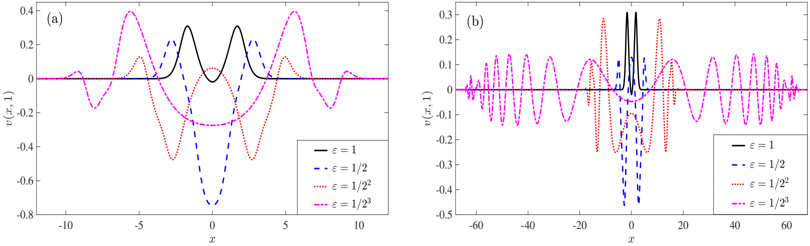

Figure: The solutions $v(x,1)$ of the oscillatory NKGE with $d = 1$ for different ε and β: (a) $\beta = 1$, (b) $\beta = 2$.

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1. Introduction
2. Numerical methods and error estimates
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4. Conclusions and future work

Conclusions and future work

- Conclusions
  - The FDTD, EWI-FP and TSFP methods for the NKGE with weak nonlinearity/small initial data
  - Error bounds of the numerical methods in the long time regime up to $O(\varepsilon^{-2})$
  - Extensions to an oscillatory NKGE
- Future work
  - Design a numerical scheme using large time steps
  - Long-time dynamics for other equations, e.g. Burgers' equation, KdV equation,...

THANK YOU!