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IMPROVED UNIFORM ERROR BOUNDS ON TIME-SPLITTING METHODS FOR LONG-TIME DYNAMICS OF THE NONLINEAR KLEIN–GORDON EQUATION WITH WEAK NONLINEARITY*

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Abstract. We establish improved uniform error bounds on a second-order Strang time-splitting method which is equivalent to an exponential wave integrator for the long-time dynamics of the nonlinear Klein–Gordon equation (NKGE) with weak cubic nonlinearity, whose strength is characterized by ε^2 with $0 < \varepsilon \leq 1$ a dimensionless parameter. Actually, when $0 < \varepsilon \ll 1$, the NKGE with $O(\varepsilon^2)$ nonlinearity and $O(1)$ initial data is equivalent to that with $O(1)$ nonlinearity and small initial data, the amplitude of which is at $O(\varepsilon)$. We begin with a semidiscretization of the NKGE by the second-order time-splitting method and derive a full-discretization by the Fourier spectral method in space. Employing the regularity compensation oscillation technique which controls the high frequency modes by the regularity of the exact solution and analyzes the low frequency modes by phase cancellation and energy method, we carry out the improved uniform error bounds at $O(\varepsilon^2\tau^2)$ and $O(h^m + \varepsilon^2\tau^2)$ for the second-order semidiscretization and full-discretization up to the long time $T_\varepsilon = T/\varepsilon^2$ with T fixed, respectively. Extensions to higher-order time-splitting methods and the case of an oscillatory complex NKGE are also discussed. Finally, numerical results are provided to confirm the improved error bounds and to demonstrate that they are sharp.

Key words. nonlinear Klein–Gordon equation, long-time dynamics, time-splitting methods, improved uniform error bounds, regularity compensation oscillation

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1. Introduction.

In this paper, we consider the following nonlinear Klein–Gordon equation (NKGE) [13, 30, 31, 34, 46]:

$$\begin{cases}\partial_{tt}u(\mathbf{x},t) - \Delta u(\mathbf{x},t) + u(\mathbf{x},t) + \varepsilon^2 u^3(\mathbf{x},t) = 0, & \mathbf{x}\in\Omega, \quad t>0,\\ u(\mathbf{x},0) = u_0(\mathbf{x}), \quad \partial_t u(\mathbf{x},0) = u_1(\mathbf{x}), & \mathbf{x}\in\Omega.\end{cases} \tag{1.1}$$

Here, t is time, $\mathbf{x}$ is the spatial coordinate, Δ is the Laplace operator, $u := u(\mathbf{x},t)$ is a real-valued scalar field, $\varepsilon \in (0,1]$ is a dimensionless parameter used to characterize the nonlinearity strength, and $\Omega = \prod_{i=1}^{d}(a_i,b_i) \subset \mathbb{R}^d$ $(d = 1,2,3)$ is a bounded domain equipped with periodic boundary conditions. The initial data $u_0(\mathbf{x})$ and $u_1(\mathbf{x})$ are two given real-valued functions independent of ε.

When $0 < \varepsilon \ll 1$, by introducing $w(\mathbf{x},t) = \varepsilon u(\mathbf{x},t)$, the NKGE (1.1) with weak nonlinearity and $O(1)$ initial data can be reformulated into the following NKGE with

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small initial data and $O(1)$ nonlinearity:

$$\begin{cases}\partial_{tt}w(\mathbf{x},t) - \Delta w(\mathbf{x},t) + w(\mathbf{x},t) + w^3(\mathbf{x},t) = 0, & \mathbf{x}\in\Omega, \quad t>0,\\ w(\mathbf{x},0) = \varepsilon u_0(\mathbf{x}), \quad \partial_t w(\mathbf{x},0) = \varepsilon u_1(\mathbf{x}), & \mathbf{x}\in\Omega.\end{cases} \tag{1.2}$$

In fact, the long-time dynamics of the NKGE (1.2) with small initial data and $O(1)$ nonlinearity is equivalent to that of the NKGE (1.1) with weak nonlinearity and $O(1)$ initial data.

The NKGE as a relativistic wave equation has a prominent place in quantum mechanics to describe spinless particles [42, 45]. Especially, the NKGE with cubic nonlinearity serves as a model for polymers, the relativistic Bose gas, and order-disorder transitions in solids [21, 32]. From both analytical and numerical perspectives, the NKGE has been extensively investigated [3, 6, 7, 11, 16, 20, 33, 41, 42, 45, 47]. Recently, the long-time dynamics of the NKGE (1.1) in the weak nonlinearity regime (or (1.2) with small initial data) has attracted much attention. According to the analytical results, the life span of a smooth solution to the NKGE (1.1) (or (1.2)) is at least up to the time at $O(\varepsilon^{-2})$ [9, 17, 18, 19, 22, 34]. For the long-time dynamics, near-conservation (or approximate preservation) of energy, momentum, and harmonic actions have been established for the semidiscretization and full-discretization of the NKGE (1.2) with small initial data via the technique of modulated Fourier expansions [14, 15, 29]. In our recent work, long-time error bounds have been rigorously established for the finite difference time domain methods [4, 24], the exponential wave integrator Fourier pseudospectral method [26], and the time-splitting Fourier pseudospectral (TSFP) method [5, 25]. In the numerical simulations, we surprisingly found the improved uniform error bounds for the TSFP method which are better than the analytical results [5]. For the long-time dynamics of the Schrödinger/nonlinear Schrödinger equation, a new technique of the *regularity compensation oscillation* (RCO) has been introduced to establish the improved uniform error bounds for the TSFP method in the long-time regime [1]. Different from the nonlinear Schrödinger equation case, the second-order time-splitting method for NKGE is equivalent to a Deuflhard exponential wave integrator [8], and as far as we know, improved uniform error bounds have not been proven on time-splitting methods or exponential integrators for the long-time dynamics of the NKGE. The aim of this paper is to analyze the errors of time-splitting methods carefully and to carry out improved uniform error bounds on semidiscretization and full-discretization for the long-time dynamics of the NKGE with the help of the RCO technique. For the refined analysis, we first reformulate the NKGE into a relativistic nonlinear Schrödinger equation (NLSE), where the nonlinear term involving a pseudodifferential operator is more difficult to analyze than the cubic nonlinearity. It is a consequence of the special structure of the relativistic NLSE that the first-order and second-order time-splitting schemes are equivalent to the corresponding exponential integrators, which is quite different from the classical cubic NLSE. To overcome the difficulty caused by the nonlinearity, we divide it into four parts and rigorously carry out the improved uniform error bounds. In addition, the relativistic NLSE involves a pseudodifferential operator, of which the spectral analysis is more complicated and is not periodic even in one dimension (1D). Based on the RCO approach, we choose a frequency cutoff parameter τ_0 and control the high frequency modes ($> 1/\tau_0$) by the smoothness of the exact solution and analyze the low frequency modes ($\leq 1/\tau_0$) by phase cancellation and energy method.

The rest of the paper is organized as follows: in section 2, we adopt the time-splitting method to discretize the NKGE in time and establish the improved uniform error bounds for the semidiscretization up to the time at $O(1/\varepsilon^2)$. In particular, the time-splitting methods are equivalent to the corresponding exponential integrators for solving NKGE. In section 3, the full-discretization by the Fourier spectral method in space is shown with the proof of improved uniform error bounds. Extensions to the complex NKGE with a general power nonlinearity and an oscillatory complex NKGE are presented in section 4. Numerical results for the long-time dynamics and the oscillatory complex NKGE are shown in section 5. Finally, some conclusions are drawn in section 6. Throughout this paper, the notation $A \lesssim B$ is used to represent that there exists a generic constant $C > 0$ independent of the mesh size h, time step τ, ε, and τ_0 such that $|A| \le CB$.

2. Semidiscretization and improved uniform error bounds. In this section, we utilize the time-splitting method to discretize the NKGE (1.1) in time and establish the improved uniform error bounds up to the time at $O(1/\varepsilon^2)$, while we notice that the time-splitting schemes can be also viewed as a class of exponential integrators. For the simplicity of presentation, we only present the numerical schemes and corresponding results in 1D. Generalization to higher dimensions is straightforward, and results remain valid without modifications. In 1D, the NKGE (1.1) with periodic boundary conditions on the domain $\Omega = (a,b)$ reduces to

$$\begin{cases} \partial_{tt}u(x,t) - \partial_{xx}u(x,t) + u(x,t) + \varepsilon^2 u^3(x,t) = 0, & a < x < b,\ t > 0, \\ u(x,0) = u_0(x),\ \partial_t u(x,0) = u_1(x), & x \in \overline{\Omega} = [a,b], \end{cases} \tag{2.1}$$

with boundary conditions as $u(a,t) = u(b,t),\ \partial_x u(a,t) = \partial_x u(b,t)$ for $t > 0$.

For an integer $m \ge 0$, we denote by $H^m(\Omega)$ the space of functions $u(x) \in L^2(\Omega)$ with finite H^m-norm $\|\cdot\|_m$ given by

$$\|u\|_m^2 = \sum_{l\in\mathbb{Z}} (1+\mu_l^2)^m |\widehat{u}_l|^2 \quad \text{for} \quad u(x) = \sum_{l\in\mathbb{Z}} \widehat{u}_l e^{i\mu_l(x-a)}, \quad \mu_l = \frac{2\pi l}{b-a}, \tag{2.2}$$

where $\widehat{u}_l$ ($l \in \mathbb{Z}$) is the Fourier coefficients of the function $u(x)$ [2, 5]. In fact, the space $H^m(\Omega)$ is the subspace of classical Sobolev space $W^{m,2}(\Omega)$, which consists of functions with derivatives of order up to $m-1$ being $(b-a)$-periodic. Since we consider periodic boundary conditions, the above space $H^m(\Omega)$ is suitable. In addition, the space is $L^2(\Omega)$ for $m = 0$, and the corresponding norm is denoted as $\|\cdot\|$. Here, the space $H^s(\Omega)$ with $s \in \mathbb{R}$ is also well defined consisting of functions with finite norm $\|\cdot\|_s$ [43].

Denote $X_N := \{u = (u_0, u_1, \ldots, u_N)^T \in \mathbb{C}^{N+1} \mid u_0 = u_N\}$, $C_{\rm per}(\Omega) = \{u \in C(\overline{\Omega}) \mid u(a) = u(b)\}$, and

$$Y_N := \text{span}\left\{e^{i\mu_l(x-a)},\ x \in \overline{\Omega},\ l \in \mathcal{T}_N\right\},\ \mathcal{T}_N = \left\{l \mid l = -\frac{N}{2}, -\frac{N}{2}+1, \ldots, \frac{N}{2}-1\right\}.$$

For any $u(x) \in C_{\rm per}(\Omega)$ and a vector $u \in X_N$, let $P_N : L^2(\Omega) \to Y_N$ be the standard L^2-projection operator onto Y_N and $I_N : C_{\rm per}(\Omega) \to Y_N$ or $I_N : X_N \to Y_N$ be the trigonometric interpolation operator [43], i.e.,

$$P_N u(x) = \sum_{l\in\mathcal{T}_N} \widehat{u}_l e^{i\mu_l(x-a)}, \qquad I_N u(x) = \sum_{l\in\mathcal{T}_N} \widetilde{u}_l e^{i\mu_l(x-a)}, \qquad x \in \overline{\Omega}, \tag{2.3}$$

where

$$\widehat{u}_l = \frac{1}{b-a}\int_a^b u(x)e^{-i\mu_l(x-a)}dx, \quad \widetilde{u}_l = \frac{1}{N}\sum_{j=0}^{N-1} u_j e^{-i\mu_l(x_j-a)}, \quad l \in \mathcal{T}_N, \tag{2.4}$$

with u_j interpreted as $u(x_j)$ when involved.

Define the operator $\langle\nabla\rangle = \sqrt{1-\Delta}$ through its action in the Fourier space by [5, 8, 23]

$$\langle\nabla\rangle u(x) = \sum_{l\in\mathbb{Z}} \sqrt{1+\mu_l^2}\,\widehat{u}_l e^{i\mu_l(x-a)} \quad \text{for} \quad u(x) = \sum_{l\in\mathbb{Z}} \widehat{u}_l e^{i\mu_l(x-a)}, \quad x \in \overline{\Omega},$$

and the inverse operator $\langle\nabla\rangle^{-1}$ as $\langle\nabla\rangle^{-1}u(x) = \sum_{l\in\mathbb{Z}} \frac{\widehat{u}_l}{\sqrt{1+\mu_l^2}} e^{i\mu_l(x-a)}$, which leads to $\|\langle\nabla\rangle^{-1}u\|_s = \|u\|_{s-1} \le \|u\|_s$.

Introduce $v(x,t) = \partial_t u(x,t)$ and

$$\psi(x,t) = u(x,t) - i\langle\nabla\rangle^{-1}v(x,t), \quad x \in \overline{\Omega}, \quad t \ge 0; \tag{2.5}$$

then the NKGE (2.1) can be reformulated into the following relativistic NLSE for $\psi := \psi(t) = \psi(x,t)$ (spatial variable x may be omitted for brevity):

$$\begin{cases} i\partial_t\psi(x,t) + \langle\nabla\rangle\psi(x,t) + \dfrac{\varepsilon^2}{8}\langle\nabla\rangle^{-1}\left(\psi+\overline{\psi}\right)^3(x,t) = 0, \quad x\in\Omega,\ t>0, \\ \psi(a,t) = \psi(b,t), \quad \partial_x\psi(a,t) = \partial_x\psi(b,t), \quad t\ge 0, \\ \psi(x,0) = \psi_0(x) := u_0(x) - i\langle\nabla\rangle^{-1}u_1(x), \quad x\in\overline{\Omega}, \end{cases} \tag{2.6}$$

where $\overline{\psi}$ denotes the complex conjugate of ψ. According to (2.5), the solution of the NKGE (2.1) can be recovered by

$$u(x,t) = \frac{1}{2}\left(\psi(x,t) + \overline{\psi}(x,t)\right), \qquad v(x,t) = \frac{i}{2}\langle\nabla\rangle\left(\psi(x,t) - \overline{\psi}(x,t)\right). \tag{2.7}$$

2.1. The time-splitting method. By the splitting technique [35, 36], the relativistic NLSE (2.6) is split into the linear part and the nonlinear part. The evolution operator for the linear part $\partial_t\psi(x,t) = i\langle\nabla\rangle\psi(x,t)$ with initial data $\psi(x,0) = \psi_0(x)$ is given by

$$\psi(\cdot,t) = \varphi_T^t(\psi_0) := e^{it\langle\nabla\rangle}\psi_0, \quad t \ge 0, \tag{2.8}$$

and the nonlinear part $\partial_t\psi(x,t) = F(\psi(x,t))$ with initial data $\psi(x,0) = \psi_0(x)$ can be integrated exactly in time as

$$\psi(x,t) = \varphi_V^t(\psi_0) := \psi_0 + \varepsilon^2 t F(\psi_0), \quad t \ge 0, \tag{2.9}$$

where the nonlinear operator F is given by

$$F(\phi) = i\langle\nabla\rangle^{-1}G(\phi), \quad G(\phi) = \frac{1}{8}\left(\phi+\overline{\phi}\right)^3. \tag{2.10}$$

Let $\tau > 0$ be the time step size and $t_n = n\tau$ $(n = 0, 1, \ldots)$ as the time steps. Denote $\psi^{[n]} := \psi^{[n]}(x)$ as the approximation of $\psi(x,t_n)$; then the second-order discrete-in-time–splitting method via the Strang splitting for the relativistic NLSE (2.6) can be written as [44]

$$\psi^{[n+1]} = \mathcal{S}_\tau(\psi^{[n]}) = \varphi_T^{\frac{\tau}{2}} \circ \varphi_V^{\tau} \circ \varphi_T^{\frac{\tau}{2}}(\psi^{[n]}) = e^{i\tau\langle\nabla\rangle}\psi^{[n]} + \varepsilon^2\tau e^{i\frac{\tau\langle\nabla\rangle}{2}} F(e^{i\frac{\tau\langle\nabla\rangle}{2}}\psi^{[n]}), \tag{2.11}$$

with $\psi^{[0]} = \psi_0 = u_0 - i\langle\nabla\rangle^{-1}u_1$. Noticing (2.7), the semidiscretization of the NKGE (2.1) is given by

$$u^{[n]} = \frac{1}{2}\left(\psi^{[n]} + \overline{\psi^{[n]}}\right), \quad v^{[n]} = \frac{i}{2}\langle\nabla\rangle\left(\psi^{[n]} - \overline{\psi^{[n]}}\right), \quad n = 0, 1, \dots, \tag{2.12}$$

where $u^{[n]} := u^{[n]}(x)$ and $v^{[n]} := v^{[n]}(x)$ are the approximations of $u(x, t_n)$ and $\partial_t u(x, t_n)$, respectively.

Remark 2.1. The split-steps (2.8) and (2.9) are equivalent to the splitting of NKGE (2.1) (in terms of u and $v = \partial_t u$), respectively, as

$$\partial_t \begin{bmatrix} u \\ v \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ \partial_{xx} - 1 & 0 \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix}, \quad \partial_t \begin{bmatrix} u \\ v \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ -\varepsilon^2 u^2 & 0 \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix}. \tag{2.13}$$

It is easy to check that the second-order time-splitting scheme (2.11) is also a symmetric second-order exponential integrator of Deuflhard type.

2.2. Improved uniform error bounds. According to discussions in [5, 18, 22] and the references therein, we make the following assumptions on the exact solution $u := u(x, t)$ of the NKGE (2.1) up to the time at $T_\varepsilon = T/\varepsilon^2$ with $T > 0$ fixed:

$$\text{(A)} \qquad \|u\|_{L^\infty([0,T_\varepsilon];H^{m+1})} \lesssim 1, \qquad \|\partial_t u\|_{L^\infty([0,T_\varepsilon];H^m)} \lesssim 1, \quad m \geq 1.$$

Let $u^{[n]}$ and $v^{[n]}$ be the numerical approximations obtained from the Strang splitting method (2.11) with (2.12). According to the analysis in [5], under the assumption (A), for sufficiently small $0 < \tau \leq \tau_c$ (τ_c is a constant), there exists a constant $M > 0$ depending on T, $\|u_0\|_{m+1}$, $\|u_1\|_m$, $\|u\|_{L^\infty([0,T_\varepsilon];H^m)}$, and $\|\partial_t u\|_{L^\infty([0,T_\varepsilon];H^m)}$ such that

$$\|u^{[n]}\|_{m+1}^2 + \|v^{[n]}\|_m^2 \leq M \text{or equivalently } \|\psi^{[n]}\|_{m+1}^2 \leq M, \quad 0 \leq n \leq \frac{T/\varepsilon^2}{\tau}. \tag{2.14}$$

The main result of this work is to establish the following improved uniform error bounds for the Strang splitting method up to the long time T_ε.

Theorem 2.2. *Under the assumption* (A), *for* $0 < \tau_0 \leq 1$ *sufficiently small and independent of* ε *such that, when* $0 < \tau < \alpha \frac{\pi(b-a)\tau_0}{2\sqrt{\tau_0^2(b-a)^2 + 4\pi^2(1+\tau_0^2)}}$ *for a fixed constant* $\alpha \in (0, 1)$, *we have the following improved uniform error bounds:*

$$\|u(\cdot, t_n) - u^{[n]}\|_1 + \|\partial_t u(\cdot, t_n) - v^{[n]}\| \lesssim \varepsilon^2\tau^2 + \tau_0^{m+1}, \quad 0 \leq n \leq \frac{T/\varepsilon^2}{\tau}. \tag{2.15}$$

In particular, if the exact solution is sufficiently smooth, e.g., $u, \partial_t u \in H^\infty$, *the last term* τ_0^{m+1} *decays exponentially fast* ($\sim e^{-c/\tau_0}$) *and can be ignored practically for small enough* τ_0, *and the improved uniform error bounds for sufficiently small* τ *are*

$$\|u(\cdot, t_n) - u^{[n]}\|_1 + \|\partial_t u(\cdot, t_n) - v^{[n]}\| \lesssim \varepsilon^2\tau^2, \quad 0 \leq n \leq \frac{T/\varepsilon^2}{\tau}. \tag{2.16}$$

Remark 2.3. $\tau_0 \in (0, 1)$ is a cutoff parameter introduced in the analysis, and the requirement on τ (essentially $\tau \lesssim \tau_0$) enables the improved estimates on the low Fourier modes $|l| \leq 1/\tau_0$, where the constant in front of $\varepsilon^2\tau^2$ depends on α. The high Fourier modes $|l| > 1/\tau_0$ are treated by Fourier projection. τ_0 can be arbitrary as long as the assumed relation between τ and τ_0 holds; i.e., τ_0 can be fixed or depend on τ, e.g., $\tau_0 = \frac{2\sqrt{8\pi^2 + (b-a)^2}}{\alpha(b-a)\pi}\tau$.

Remark 2.4. Compared to the previous uniform estimates $\|u(\cdot,t_n)-u^{[n]}\|_1+\|\partial_t u(\cdot,t_n)-v^{[n]}\|\lesssim\tau^2$ established in [5], our estimates are improved in the sense that the leading error term as $\tau\to 0^+$ is now $\varepsilon^2\tau^2$, which was numerically observed in [5]. The estimates in Theorem 2.2 hold for higher-order norms $\|\cdot\|_s$ $(s\le m)$, and the proof remains the same. The results are valid in higher dimensions $d=2,3$, independent of the aspect ratio of the rectangular domain Ω.

Remark 2.5. The second-order Strang splitting method is adopted to discretize the NKGE (2.1), and it is straightforward to design the first-order Lie–Trotter splitting method [48] and fourth-order partitioned Runge–Kutta (PRK4) splitting method [10, 27]. Under appropriate assumptions on the exact solution, the improved uniform error bounds can be extended to the first-order Lie–Trotter splitting and the PRK4 splitting method with improved uniform error bounds at $\varepsilon^2\tau$ and $\varepsilon^2\tau^4$, respectively. Using the properties of the subproblems (2.8)–(2.9), the Lie–Trotter and PRK4 splitting methods are equivalent to a certain type of exponential integrators, which implies the improved uniform error bounds hold true for a class of exponential integrators (see also Remark 2.7 for more discussion).

2.3. Proof for Theorem 2.2. The assumption (A) is equivalent to the regularity of $\psi(x,t)$ as $\|\psi\|_{L^\infty([0,T_\varepsilon];H^{m+1})}\lesssim 1$. Let

$$F_t:\ \phi\mapsto e^{-it\langle\nabla\rangle}F\big(e^{it\langle\nabla\rangle}\phi\big),\quad t\in\mathbb{R}; \tag{2.17}$$

we have the following estimates by the standard analysis for the local truncation error [1, 5].

LEMMA 2.6. *For $0<\varepsilon\le 1$, the local error of the Strang splitting* (2.11) *can be written as*

$$\mathcal{E}^n:=\mathcal{S}_\tau(\psi(t_n))-\psi(t_{n+1})=\mathcal{F}(\psi(t_n))+\mathcal{R}^n,\quad n=0,1,\ldots, \tag{2.18}$$

where

$$\mathcal{F}(\psi(t_n))=\varepsilon^2 e^{i\tau\langle\nabla\rangle}\left(\tau F_{\tau/2}(\psi(t_n))-\int_0^\tau F_\theta(\psi(t_n))d\theta\right), \tag{2.19}$$

and the following error bounds hold under the assumption (A) with $m\ge 1$:

$$\|\mathcal{F}(\psi(t_n))\|_1\lesssim\varepsilon^2\tau^3,\quad \|\mathcal{R}^n\|_1\lesssim\varepsilon^4\tau^3. \tag{2.20}$$

Under the assumption (A), for $0<\tau\le\tau_c$, we have the estimates (2.14) on the numerical solution $\psi^{[n]}$, which provide control on the nonlinearity. Thus, we focus on the refined estimates in Theorem 2.2.

Introduce the numerical error function $e^{[n]}:=e^{[n]}(x)$ $(n=0,1,\ldots)$ by

$$e^{[n]}:=\psi^{[n]}-\psi(t_n); \tag{2.21}$$

then, from (2.11) and (2.18),we have the following error equation:

$$e^{[n+1]}=\mathcal{S}_\tau(\psi^{[n]})-\mathcal{S}_\tau(\psi(t_n))+\mathcal{E}^n=e^{i\tau\langle\nabla\rangle}e^{[n]}+W^n+\mathcal{E}^n,\quad n\ge 0, \tag{2.22}$$

where $W^n:=W^n(x)$ $(n=0,1,\ldots)$ is given by

$$W^n(x)=\varepsilon^2\tau e^{i\frac{\tau}{2}\langle\nabla\rangle}\left(F\left(e^{i\frac{\tau}{2}\langle\nabla\rangle}\psi^{[n]}\right)-F\left(e^{i\frac{\tau}{2}\langle\nabla\rangle}\psi(t_n)\right)\right).$$

Under the assumption (A), we have from (2.10) and the estimates on $\psi^{[n]}$ in (2.14) that

$$\|W^n(x)\|_1 \lesssim \varepsilon^2\tau \left\|F\left(e^{i\frac{\tau}{2}\langle\nabla\rangle}\psi^{[n]}\right) - F\left(e^{i\frac{\tau}{2}\langle\nabla\rangle}\psi(t_n)\right)\right\|_1 \lesssim \varepsilon^2\tau\left\|e^{[n]}\right\|_1. \tag{2.23}$$

Based on (2.22), we obtain

$$e^{[n+1]} = e^{i(n+1)\tau\langle\nabla\rangle}e^{[0]} + \sum_{k=0}^{n} e^{i(n-k)\tau\langle\nabla\rangle}\left(W^k(x) + \mathcal{E}^k\right), \quad 0 \le n \le T_\varepsilon/\tau - 1. \tag{2.24}$$

Noticing $e^{[0]} = 0$, (2.18), (2.20), and (2.23), we have the estimates for $0 \le n \le T_\varepsilon/\tau - 1$,

$$\left\|e^{[n+1]}\right\|_1 \lesssim \varepsilon^2\tau^2 + \varepsilon^2\tau\sum_{k=0}^{n}\left\|e^{[k]}\right\|_1 + \left\|\sum_{k=0}^{n} e^{i(n-k)\tau\langle\nabla\rangle}\mathcal{F}(\psi(t_k))\right\|_1. \tag{2.25}$$

Direct applications of (2.20) and the Gronwall inequality lead to the uniform error estimates $\|e^{[n+1]}\|_1 \lesssim \tau^2$ $(0 \le n \le T_\varepsilon/\tau - 1)$ as shown in [8]. To analyze the error more carefully, we shall employ the RCO technique [1] to deal with the last term on the right-hand side (RHS) of (2.25). The key idea is a summation-by-parts procedure combined with spectrum cutoff and phase cancellation.

The first step is a spectral projection on $\psi(t_k)$ such that only finite Fourier modes of $\psi(t_k)$ need to be considered and the projection error can be controlled by the regularity of $\psi(t_k)$. The second step is to apply the summation-by-parts formula for the low Fourier modes in a proper way such that the phase can be canceled for small τ (the terms of the type $\sum_{k=0}^{n} e^{i(n-k)\tau\langle\nabla\rangle}$) and an extra order of ε^2 can be gained from the terms like $\mathcal{F}(\psi(t_k)) - \mathcal{F}(\psi(t_{k+1}))$.

Now, we demonstrate our strategy in detail. From the relativistic NLSE (2.6), we find that $\partial_t\psi(x,t) - i\langle\nabla\rangle\psi(x,t) = i\varepsilon^2 F(\psi(x,t)) = O(\varepsilon^2)$. Thus, in order to gain an extra order of ε^2, instead of $\psi(x,t)$, it is natural to consider the "twisted variable" given by

$$\phi(x,t) = e^{-it\langle\nabla\rangle}\psi(x,t), \quad t \ge 0, \tag{2.26}$$

which satisfies the equation $\partial_t\phi(x,t) = \varepsilon^2 e^{-it\langle\nabla\rangle}F(e^{it\langle\nabla\rangle}\phi(x,t))$. Under the assumption (A), we have $\|\phi\|_{L^\infty([0,T_\varepsilon];H^{m+1})} \lesssim 1$ and $\|\partial_t\phi\|_{L^\infty([0,T_\varepsilon];H^{m+1})} \lesssim \varepsilon^2$ with

$$\|\phi(t_{n+1}) - \phi(t_n)\|_{m+1} \lesssim \varepsilon^2\tau, \quad 0 \le n \le T_\varepsilon/\tau - 1. \tag{2.27}$$

The RCO technique will be used to force $\partial_t\phi(t)$ to appear with a gain of order $O(\varepsilon^2)$ for the summation-by-parts procedure in $\sum_{k=0}^{n} e^{i(n-k)\tau\langle\nabla\rangle}\mathcal{F}(\psi(t_k))$. Then, small τ is required to control the accumulation of the frequency of the type $e^{i(n-k)\tau\langle\nabla\rangle}$.

Step 1. As introduced in [1], we start with the choice of the cutoff parameter on the Fourier modes. Let $\tau_0 \in (0,1)$, and choose $N_0 = 2\lceil 1/\tau_0\rceil \in \mathbb{Z}^+$ ($\lceil\cdot\rceil$ is the ceiling function) with $1/\tau_0 \le N_0/2 < 1 + 1/\tau_0$. Recalling F_t from (2.17) as

$$\begin{aligned} F_t(\phi) &= e^{-it\langle\nabla\rangle}F\left(e^{it\langle\nabla\rangle}\phi\right) \\ &= \frac{i}{8}e^{-it\langle\nabla\rangle}\langle\nabla\rangle^{-1}\left(e^{it\langle\nabla\rangle}\phi + e^{-it\langle\nabla\rangle}\overline{\phi}\right)^3, \end{aligned}$$

under the assumption (A) and properties of operators $e^{-it\langle\nabla\rangle}$ and $\langle\nabla\rangle^{-1}$, we have

$$\|F_t(e^{it_k\langle\nabla\rangle}\phi(t_k))\|_{m+2} \lesssim \|\phi(t_k)\|_{m+1}^3 \lesssim 1, \quad t \in \mathbb{R}, \quad 0 \le k \le \frac{T_\varepsilon}{\tau}, \tag{2.28}$$

and the following estimates hold by the standard Fourier projection properties for $s \in [0, m+1]$:

$$\|F_t(\phi(t_k)) - P_{N_0}F_t(\phi(t_k))\|_s + \tau_0\|\phi(x,t_k) - P_{N_0}\phi(x,t_k)\|_s \lesssim \tau_0^{m+2-s}. \tag{2.29}$$

Combining the above estimates, (2.10), (2.19), and assumption (A), we derive, for $0 \le k \le T_\varepsilon/\tau$,

$$\begin{aligned}&\|P_{N_0}\mathcal{F}(e^{it_k\langle\nabla\rangle}(P_{N_0}\phi(t_k))) - \mathcal{F}(e^{it_k\langle\nabla\rangle}\phi(t_k))\|_1\\ &\lesssim \varepsilon^2\tau\tau_0^{m+1} + \varepsilon^2\tau\|P_{N_0}\phi(t_k) - \phi(t_k)\| \lesssim \varepsilon^2\tau\tau_0^{m+1}.\end{aligned} \tag{2.30}$$

Since $e^{i\tau\langle\nabla\rangle}$ preserves the H^1-norm, multiplying the last term in (2.25) by $e^{i(n-1)\tau\langle\nabla\rangle}$, we obtain, for $0 \le n \le T_\varepsilon/\tau - 1$,

$$\left\|e^{[n+1]}\right\|_1 \lesssim \tau_0^{m+1} + \varepsilon^2\tau^2 + \varepsilon^2\tau\sum_{k=0}^{n}\left\|e^{[k]}\right\|_1 + \|\mathcal{L}^n\|_1, \tag{2.31}$$

where

$$\mathcal{L}^n = \sum_{k=0}^{n} e^{-i(k+1)\tau\langle\nabla\rangle}P_{N_0}\mathcal{F}(e^{it_k\langle\nabla\rangle}(P_{N_0}\phi(t_k))). \tag{2.32}$$

Step 2. Now, we concentrate on the low Fourier modes term $\mathcal{L}^n$. Recalling the nonlinear function $F(\cdot)$, we have the decomposition

$$F(\phi) = \sum_{q=1}^{4} F^q(\phi), \quad F^q(\phi) = i\langle\nabla\rangle^{-1}G^q(\phi), \quad q = 1,2,3,4, \tag{2.33}$$

with $G^1(\phi) = \frac{1}{8}\phi^3$, $G^2(\phi) = \frac{3}{8}\bar\phi\phi^2$, $G^3(\phi) = \frac{3}{8}\bar\phi^2\phi$, $G^4(\phi) = \frac{1}{8}\bar\phi^3$. For $\theta \in \mathbb{R}$ and $q = 1,2,3,4$, introducing $F_\theta^q(\psi(t_k)) = e^{-i\theta\langle\nabla\rangle}F^q(e^{i\theta\langle\nabla\rangle}\psi(t_k))$ and

$$\mathcal{F}^q(\psi(t_k)) = \varepsilon^2 e^{i\tau\langle\nabla\rangle}\left(\tau F_{\tau/2}^q(\psi(t_n)) - \int_0^\tau F_\theta^q(\psi(t_n))d\theta\right) \tag{2.34}$$

and recalling (2.17) and (2.19), we have

$$\mathcal{L}^n = \sum_{q=1}^{4}\mathcal{L}_q^n, \quad \mathcal{L}_q^n = \sum_{k=0}^{n} e^{-i(k+1)\tau\langle\nabla\rangle}P_{N_0}\mathcal{F}^q(e^{it_k\langle\nabla\rangle}(P_{N_0}\phi(t_k))),\ 1 \le q \le 4. \tag{2.35}$$

Since the estimates on $\mathcal{L}_q^n$ $(q = 1,2,3,4)$ are the same, we only present the case for $\mathcal{L}_1^n$ $(0 \le n \le T_\varepsilon/\tau - 1)$. For $l \in \mathcal{T}_{N_0}$, define the index set $\mathcal{I}_l^{N_0}$ associated to l as

$$\mathcal{I}_l^{N_0} = \{(l_1,l_2,l_3) \mid l_1 + l_2 + l_3 = l,\ l_1,l_2,l_3 \in \mathcal{T}_{N_0}\}; \tag{2.36}$$

then, the following expansion holds in view of $P_{N_0}\phi(t_k) = \sum_{l\in\mathcal{T}_{N_0}}\widehat{\phi}_l(t_k)e^{i\mu_l(x-a)}$:

$$\begin{aligned}&e^{-it_{k+1}\langle\nabla\rangle}P_{N_0}(e^{i\tau\langle\nabla\rangle}F_\theta^1(e^{it_k\langle\nabla\rangle}P_{N_0}\phi(t_k)))\\ &= \sum_{l\in\mathcal{T}_{N_0}}\sum_{(l_1,l_2,l_3)\in\mathcal{I}_l^{N_0}}\frac{i}{8\delta_l}\mathcal{G}_{l,l_1,l_2,l_3}^k(\theta)e^{i\mu_l(x-a)},\end{aligned}$$

where the coefficients $\mathcal{G}^k_{l,l_1,l_2,l_3}(\theta)$ are functions of $\theta \in \mathbb{R}$ defined as

$$\mathcal{G}^k_{l,l_1,l_2,l_3}(\theta) = e^{-i(t_k+\theta)\delta_{l,l_1,l_2,l_3}} \widehat{\overline{\phi_{l_1}}}(t_k)\widehat{\phi}_{l_2}(t_k)\widehat{\phi}_{l_3}(t_k) \tag{2.37}$$

with $\delta_{l,l_1,l_2,l_3} = \delta_l - \delta_{l_1} - \delta_{l_2} - \delta_{l_3}$ and $\delta_l = \sqrt{1+\mu_l^2}$ for $l \in \mathcal{T}_{N_0}$. Thus, we have

$$\mathcal{L}_1^n = \frac{i\varepsilon^2}{8} \sum_{k=0}^{n} \sum_{l\in\mathcal{T}_{N_0}} \sum_{(l_1,l_2,l_3)\in\mathcal{I}_l^{N_0}} \frac{1}{\delta_l} \Lambda^k_{l,l_1,l_2,l_3} e^{i\mu_l(x-a)}, \tag{2.38}$$

where

$$\Lambda^k_{l,l_1,l_2,l_3} = -\tau \mathcal{G}^k_{l,l_1,l_2,l_3}(\tau/2) + \int_0^\tau \mathcal{G}^k_{l,l_1,l_2,l_3}(\theta)\, d\theta = r_{l,l_1,l_2,l_3} e^{-it_k\delta_{l,l_1,l_2,l_3}} c^k_{l,l_1,l_2,l_3}, \tag{2.39}$$

with coefficients c^k_{l,l_1,l_2,l_3} and r_{l,l_1,l_2,l_3} given by

$$c^k_{l,l_1,l_2,l_3} = \widehat{\overline{\phi}}_{l_1}(t_k)\widehat{\phi}_{l_2}(t_k)\widehat{\phi}_{l_3}(t_k), \tag{2.40}$$

$$r_{l,l_1,l_2,l_3} = -\tau e^{-i\tau\delta_{l,l_1,l_2,l_3}/2} + \int_0^\tau e^{-i\theta\delta_{l,l_1,l_2,l_3}}\, d\theta = O\left(\tau^3(\delta_{l,l_1,l_2,l_3})^2\right). \tag{2.41}$$

We only need to consider the case $\delta_{l,l_1,l_2,l_3} \neq 0$ as $r_{l,l_1,l_2,l_3} = 0$ if $\delta_{l,l_1,l_2,l_3} = 0$. For $l \in \mathcal{T}_{N_0}$ and $(l_1,l_2,l_3) \in \mathcal{I}_l^{N_0}$, we have

$$|\delta_{l,l_1,l_2,l_3}| \le 4\delta_{N_0/2} = 4\sqrt{1+\mu^2_{N_0/2}} < 4\sqrt{1+\frac{4\pi^2(1+\tau_0)^2}{\tau_0^2(b-a)^2}}, \tag{2.42}$$

which implies

$$\frac{\tau}{2}|\delta_{l,l_1,l_2,l_3}| \le \alpha\pi, \tag{2.43}$$

if $0 < \tau \le \alpha\frac{\pi(b-a)\tau_0}{2\sqrt{\tau_0^2(b-a)^2+4\pi^2(1+\tau_0)^2}} := \tau_0^\alpha$ $(0 < \tau_0, \alpha < 1)$. Denoting $S^n_{l,l_1,l_2,l_3} = \sum_{k=0}^n e^{-it_k\delta_{l,l_1,l_2,l_3}}$ $(n \ge 0)$, for $0 < \tau \le \tau_0^\alpha$, we then obtain

$$|S^n_{l,l_1,l_2,l_3}| \le \frac{1}{|\sin(\tau\delta_{l,l_1,l_2,l_3}/2)|} \le \frac{C}{\tau|\delta_{l,l_1,l_2,l_3}|}, \quad C = \frac{2\alpha\pi}{\sin(\alpha\pi)} \quad \forall n \ge 0. \tag{2.44}$$

Using summation-by-parts, we find from (2.39) that

$$\sum_{k=0}^n \Lambda^k_{l,l_1,l_2,l_3} = r_{l,l_1,l_2,l_3}\left[\sum_{k=0}^{n-1} S^k_{l,l_1,l_2,l_3}(c^k_{l,l_1,l_2,l_3} - c^{k+1}_{l,l_1,l_2,l_3}) + S^n_{l,l_1,l_2,l_3} c^n_{l,l_1,l_2,l_3}\right], \tag{2.45}$$

with

$$\begin{aligned} c^k_{l,l_1,l_2,l_3} - c^{k+1}_{l,l_1,l_2,l_3} &= (\widehat{\overline{\phi}}_{l_1}(t_k) - \widehat{\overline{\phi}}_{l_1}(t_{k+1}))\widehat{\phi}_{l_2}(t_k)\widehat{\phi}_{l_3}(t_k) + \widehat{\overline{\phi}}_{l_1}(t_{k+1})(\widehat{\phi}_{l_2}(t_k) - \widehat{\phi}_{l_2}(t_{k+1}))\widehat{\phi}_{l_3}(t_k) \\ &\quad + \widehat{\overline{\phi}}_{l_1}(t_{k+1})\widehat{\phi}_{l_2}(t_{k+1})(\widehat{\phi}_{l_3}(t_k) - \widehat{\phi}_{l_3}(t_{k+1})). \end{aligned} \tag{2.46}$$

Combining (2.41), (2.44), (2.45), and (2.46), we have

$$\begin{aligned}\left|\sum_{k=0}^{n}\Lambda^k_{l,l_1,l_2,l_3}\right| \lesssim \tau^2|\delta_{l,l_1,l_2,l_3}|\sum_{k=0}^{n-1}\bigg(&\left|\widehat{\phi}_{l_1}(t_k)-\widehat{\phi}_{l_1}(t_{k+1})\right|\left|\widehat{\phi}_{l_2}(t_k)\right|\left|\widehat{\phi}_{l_3}(t_k)\right|\\ &+\left|\widehat{\phi}_{l_1}(t_{k+1})\right|\left|\widehat{\phi}_{l_2}(t_k)-\widehat{\phi}_{l_2}(t_{k+1})\right|\left|\widehat{\phi}_{l_3}(t_k)\right|\\ &+\left|\widehat{\phi}_{l_1}(t_{k+1})\right|\left|\widehat{\phi}_{l_2}(t_{k+1})\right|\left|\widehat{\phi}_{l_3}(t_k)-\widehat{\phi}_{l_3}(t_{k+1})\right|\bigg)\\ &+\tau^2|\delta_{l,l_1,l_2,l_3}|\left|\widehat{\phi}_{l_1}(t_n)\right|\left|\widehat{\phi}_{l_2}(t_n)\right|\left|\widehat{\phi}_{l_3}(t_n)\right|.\end{aligned}\tag{2.47}$$

For $l\in\mathcal{T}_{N_0}$ and $(l_1,l_2,l_3)\in\mathcal{I}_l^{N_0}$, we see that there holds

$$|\delta_{l,l_1,l_2,l_3}|\le\left(1+\left(\sum_{j=1}^{3}\mu_{l_j}\right)^2\right)^{1/2}+\sum_{j=1}^{3}\sqrt{1+\mu_{l_j}^2}\lesssim\prod_{j=1}^{3}\sqrt{1+\mu_{l_j}^2}.\tag{2.48}$$

Based on (2.38), (2.47), (2.48), and noticing $\delta_l=\sqrt{1+\mu_l^2}$, we have

$$\begin{aligned}&\|\mathcal{L}_1^n\|_1^2\\ &=\varepsilon^4\sum_{l\in\mathcal{T}_{N_0}}\left|\sum_{(l_1,l_2,l_3)\in\mathcal{I}_l^{N_0}}\sum_{k=0}^{n}\Lambda^k_{l,l_1,l_2,l_3}\right|^2\\ &\lesssim\varepsilon^4\tau^4\left\{\sum_{l\in\mathcal{T}_{N_0}}\left(\sum_{(l_1,l_2,l_3)\in\mathcal{I}_l^{N_0}}\left|\widehat{\phi}_{l_1}(t_n)\right|\left|\widehat{\phi}_{l_2}(t_n)\right|\left|\widehat{\phi}_{l_3}(t_n)\right|\prod_{j=1}^{3}\sqrt{1+\mu_{l_j}^2}\right)^2\right.\\ &\quad+n\sum_{k=0}^{n-1}\sum_{l\in\mathcal{T}_{N_0}}\left[\left(\sum_{(l_1,l_2,l_3)\in\mathcal{I}_l^{N_0}}\left|\widehat{\phi}_{l_1}(t_k)-\widehat{\phi}_{l_1}(t_{k+1})\right|\left|\widehat{\phi}_{l_2}(t_k)\right|\left|\widehat{\phi}_{l_3}(t_k)\right|\prod_{j=1}^{3}\sqrt{1+\mu_{l_j}^2}\right)^2\right.\\ &\quad+\left(\sum_{(l_1,l_2,l_3)\in\mathcal{I}_l^{N_0}}\left|\widehat{\phi}_{l_1}(t_{k+1})\right|\left|\widehat{\phi}_{l_2}(t_k)-\widehat{\phi}_{l_2}(t_{k+1})\right|\left|\widehat{\phi}_{l_3}(t_k)\right|\prod_{j=1}^{3}\sqrt{1+\mu_{l_j}^2}\right)^2\\ &\quad\left.\left.+\left(\sum_{(l_1,l_2,l_3)\in\mathcal{I}_l^{N_0}}\left|\widehat{\phi}_{l_1}(t_{k+1})\right|\left|\widehat{\phi}_{l_2}(t_{k+1})\right|\left|\widehat{\phi}_{l_3}(t_k)-\widehat{\phi}_{l_3}(t_{k+1})\right|\prod_{j=1}^{3}\sqrt{1+\mu_{l_j}^2}\right)^2\right]\right\}.\end{aligned}\tag{2.49}$$

In order to estimate the sum on the RHS of the above inequality, e.g. for the first term, on the RHS, we use the auxiliary function $\xi(x)=\sum_{l\in\mathbb{Z}}\sqrt{1+\mu_{l_j}^2}|\widehat{\phi}_l(t_n)|e^{i\mu_l(x-a)}$, where $\xi(x)\in H^m(\Omega)$ is implied by assumption (A) and $\|\xi\|_{H^s}\lesssim\|\phi(t_n)\|_{H^{s+1}}$ ($s\le m$). Expanding $(\xi(x))^3=\sum_{l\in\mathbb{Z}}\sum_{l_1+l_2+l_3=l,l_j\in\mathbb{Z}}\prod_{j=1}^{3}(\sqrt{1+\mu_{l_j}^2}|\widehat{\phi}_{l_j}(t_n)|)e^{i\mu_l(x-a)}$, we obtain

$$\sum_{l\in\mathcal{T}_{N_0}}\left(\sum_{(l_1,l_2,l_3)\in\mathcal{I}_l^{N_0}}\left|\widehat{\phi}_{l_1}(t_n)\right|\left|\widehat{\phi}_{l_2}(t_n)\right|\left|\widehat{\phi}_{l_3}(t_n)\right|\prod_{j=1}^{3}\sqrt{1+\mu_{l_j}^2}\right)^2$$
$$\leq \left\|\xi^3(x)\right\|^2 \lesssim \|\xi(x)\|_1^6 \lesssim \|\phi(t_n)\|_2^6 \lesssim 1. \tag{2.50}$$

Thus, in light of (2.27), we estimate each term in (2.49) similarly as

$$\|\mathcal{L}_1^n\|_1^2 \lesssim \varepsilon^4\tau^4\left[\|\phi(t_n)\|_2^6 + n\sum_{k=0}^{n-1}\|\phi(t_k)-\phi(t_{k+1})\|_2^2\left(\|\phi(t_k)\|_2+\|\phi(t_{k+1})\|_2\right)^4\right]$$
$$\lesssim \varepsilon^4\tau^4 + n^2\varepsilon^4\tau^4(\varepsilon^2\tau)^2 \lesssim \varepsilon^4\tau^4, \quad 0\leq n\leq T_\varepsilon/\tau-1. \tag{2.51}$$

The same estimates can be established for $\mathcal{L}_q^n$ $(q=2,3,4)$, and (2.31) together with (2.35) implies

$$\left\|e^{[n+1]}\right\|_1 \lesssim \tau_0^{m+1} + \varepsilon^2\tau^2 + \varepsilon^2\tau\sum_{k=0}^{n}\left\|e^{[k]}\right\|_1, \quad 0\leq n\leq T_\varepsilon/\tau-1. \tag{2.52}$$

The discrete Gronwall inequality yields

$$\left\|e^{[n+1]}\right\|_1 \lesssim \varepsilon^2\tau^2 + \tau_0^{m+1}, \quad 0\leq n\leq T_\varepsilon/\tau-1, \tag{2.53}$$

and the error bound (2.15) follows in view of (2.7) and (2.12).

Remark 2.7. Similar results to Theorem 2.2 have been previously obtained for time-splitting methods applied to the long-time dynamics of the NLSE with weak nonlinearity [12], where the periodicity of the free Schrödinger operator plays an important role and the time step size has to be an integer fraction of the period. Thus, the results and analysis in [12] are difficult to extend to a higher dimensional rectangular domain with irrational aspect ratio and/or general time step sizes. The presented RCO-based approach does not depend on the periodicity of the free relativistic Schrödinger operator. It is easy to check that our analysis works for higher dimensional cases and allows general time step sizes. Furthermore, recalling that (2.11) is also an exponential integrator of Deuflhardtype, we could find that the improved uniform error bounds hold for the second-order Deuflhard exponential integrator. Numerical examples in section 5 show that the exponential integrators of Gautschi type do not have improved error bounds. More precisely, recalling the Duhamel principle for the relativistic NLSE (2.6),

$$\psi(t_n+\tau) = e^{i\tau\langle\nabla\rangle}\psi(t_n) + \varepsilon^2\int_0^\tau e^{i(\tau-s)\langle\nabla\rangle}F(\psi(t_n+s))\,ds,$$

if the integral term is treated by approximating $e^{-is\langle\nabla\rangle}F(\psi(t_n+s))$ as a whole (like the second-order Deuflhard integrator, i.e., TSFP (2.11)), we have the improved uniform error bounds. On the other hand, if the integral is treated by approximating $F(\psi(t_n+s))$ (e.g., by interpolation in time) and then integrating in time exactly (like the Gautschi-type integrator), we do not observe improved uniform error bounds.

3. Full-discretization and improved uniform error bounds. In this section, we present the practical full-discretization for the NKGE (2.1) by the Fourier pseudospectral method in space and establish the improved uniform error bounds.

3.1. Full-discretization by Fourier pseudospectral method. Let N be an even positive integer, and define the spatial mesh size $h = (b-a)/N$; then the grid points are chosen as

$$x_j := a + jh, \quad j \in \mathcal{T}_N^0 = \{j \mid j = 0, 1, \ldots, N\}. \tag{3.1}$$

Let ψ_j^n be the numerical approximation of $\psi(x_j, t_n)$ for $j \in \mathcal{T}_N^0$, and $n \geq 0$ and denote $\psi^n = (\psi_0^n, \psi_1^n, \ldots, \psi_N^n)^T \in \mathbb{C}^{N+1}$ for $n = 0, 1, \ldots$. Then, a TSFP method for discretizing the relativistic NLSE (2.6) via (2.11) with a Fourier pseudospectral discretization in space is given as

$$\begin{aligned}
&\psi_j^{(1)} = \sum_{l \in \mathcal{T}_N} e^{i\frac{\tau\delta_l}{2}} \, \widetilde{(\psi^n)}_l \, e^{i\mu_l(x_j-a)}, \\
&\psi_j^{(2)} = \psi_j^{(1)} + \varepsilon^2 \tau \, F_j^n, \qquad F_j^n = i \sum_{l \in \mathcal{T}_N} \frac{1}{\delta_l} \big(\widetilde{G(\psi^{(1)})}\big)_l \, e^{i\mu_l(x_j-a)}, \\
&\psi_j^{n+1} = \sum_{l \in \mathcal{T}_N} e^{i\frac{\tau\delta_l}{2}} \, \big(\widetilde{\psi^{(2)}}\big)_l \, e^{i\mu_l(x_j-a)}, \quad j \in \mathcal{T}_N^0, \quad n = 0, 1, \ldots,
\end{aligned} \tag{3.2}$$

where $\delta_l = \sqrt{1+\mu_l^2}$ for $l \in \mathcal{T}_N$, $\psi^{(k)} = (\psi_0^{(k)}, \psi_1^{(k)}, \ldots, \psi_N^{(k)})^T \in \mathbb{C}^{N+1}$ for $k = 1, 2$, $G(\psi^{(1)}) := (G(\psi_0^{(1)}), G(\psi_2^{(1)}), \ldots, G(\psi_N^{(1)}))^T \in \mathbb{R}^{N+1}$, and

$$\psi_j^0 = u_0(x_j) - i \sum_{l \in \mathcal{T}_N} \frac{\widetilde{(u_1)}_l}{\delta_l} e^{i\mu_l(x_j-a)}, \quad j \in \mathcal{T}_N^0.$$

Let u_j^n and v_j^n be the approximations of $u(x_j, t_n)$ and $v(x_j, t_n)$, respectively, for $j \in \mathcal{T}_N^0$ and $n \geq 0$, and denote $u^n = (u_0^n, u_1^n, \ldots, u_N^n)^T \in \mathbb{R}^{N+1}$ and $v^n = (v_0^n, v_1^n, \ldots, v_N^n)^T \in \mathbb{R}^{N+1}$ for $n = 0, 1, \ldots$. Combining (2.12) and (3.2), we obtain the full-discretization of the NKGE (2.1) by the TSFP method as

$$\left.\begin{aligned}
&u_j^{n+1} = \frac{1}{2}\left(\psi_j^{n+1} + \overline{\psi_j^{n+1}}\right), \\
&v_j^{n+1} = \frac{i}{2} \sum_{l \in \mathcal{T}_N} \delta_l \left[\widetilde{(\psi^{n+1})}_l - \left(\widetilde{\overline{\psi^{n+1}}}\right)_l\right] \, e^{i\mu_l(x_j-a)},
\end{aligned}\right. \qquad j \in \mathcal{T}_N^0, \quad n \geq 0, \tag{3.3}$$

with $u_j^0 = u_0(x_j)$ and $v_j^0 = u_1(x_j)$ for $j \in \mathcal{T}_N^0$.

3.2. Improved uniform error bounds. Let u^n and v^n be the numerical approximations obtained from the TSFP (3.2)–(3.3). According to the analysis in [5], under the assumption (A), for $0 < \tau \leq \tau_c, 0 < h \leq h_c$ (τ_c, h_c are constants independent of ε), there exists a constant $M > 0$ depending on T, $\|u_0\|_{m+1}$, $\|u_1\|_m$, $\|u\|_{L^\infty([0,T_\varepsilon];H^m)}$, and $\|\partial_t u\|_{L^\infty([0,T_\varepsilon];H^m)}$ such that the numerical solution satisfies

$$\|I_N u^n\|_{m+1}^2 + \|I_N v^n\|_m^2 \leq M \text{ or equivalently } \|I_N \psi^n\|_{m+1}^2 \leq M, \; 0 \leq n \leq \frac{T_\varepsilon}{\tau}. \tag{3.4}$$

Then, we have the improved uniform error bounds for the full-discretization.

THEOREM 3.1. *Under the assumption* (A), *there exist* $h_0 > 0$ *and* $0 < \tau_0 < 1$ *sufficiently small and independent of* ε *such that, for any* $0 < \varepsilon \leq 1$, *when* $0 < h \leq h_0$

and $0 < \tau < \alpha \frac{\pi(b-a)\tau_0}{2\sqrt{\tau_0^2(b-a)^2+4\pi^2(1+\tau_0^2)}}$ *for a fixed constant* $\alpha \in (0,1)$*, we have the following improved uniform error estimates:*

$$\|u(\cdot,t_n) - I_N u^n\|_1 + \|\partial_t u(\cdot,t_n) - I_N v^n\| \lesssim h^m + \varepsilon^2\tau^2 + \tau_0^{m+1},\ 0 \le n \le \frac{T/\varepsilon^2}{\tau}. \tag{3.5}$$

In particular, if the exact solution is sufficiently smooth, e.g., $u, \partial_t u \in H^\infty$*, the improved uniform error bounds for sufficiently small* τ *are*

$$\|u(\cdot,t_n) - I_N u^n\|_1 + \|\partial_t u(\cdot,t_n) - I_N v^n\| \lesssim h^m + \varepsilon^2\tau^2,\ 0 \le n \le \frac{T/\varepsilon^2}{\tau}. \tag{3.6}$$

Proof. It suffices to consider the numerical approximation ψ^n to the solution of the relativistic NLSE (2.6). Recalling the semidiscrete-in-time approximation $\psi^{[n]}$ ($0 \le n \le \frac{T/\varepsilon^2}{\tau}$) given by the scheme (2.11)–(2.12), under the assumptions of Theorem 3.1, we have the estimates in Theorem 2.2, (2.14), and (3.4), which directly yield

$$\left\|\psi^{[n]} - P_N\psi^{[n]}\right\|_1 \lesssim h^m, \quad \left\|\psi(\cdot,t_n) - \psi^{[n]}\right\|_1 \lesssim \varepsilon^2\tau^2 + \tau_0^{m+1}, \quad 0 \le n \le \frac{T/\varepsilon^2}{\tau}. \tag{3.7}$$

Since $\psi(\cdot,t_n) - I_N\psi^n = \psi(\cdot,t_n) - \psi^{[n]} + \psi^{[n]} - P_N\psi^{[n]} + P_N\psi^{[n]} - I_N\psi^n$, we derive that

$$\|\psi(\cdot,t_n) - I_N\psi^n\|_1 \le \|P_N\psi^{[n]} - I_N\psi^n\|_1 + C_1(\varepsilon^2\tau^2 + \tau_0^{m+1} + h^m). \tag{3.8}$$

As a result, it remains to establish the estimates on the error function $e^n := e^n(x) \in Y_N$ given as

$$e^n := P_N\psi^{[n]} - I_N\psi^n, \quad 0 \le n \le \frac{T/\varepsilon^2}{\tau}.$$

From (2.11) and (3.2), we get

$$\begin{aligned} I_N\psi^{n+1} &= e^{i\tau\langle\nabla\rangle} I_N\psi^n + i\varepsilon^2\tau\langle\nabla\rangle^{-1} e^{i\tau\langle\nabla\rangle/2} I_N(G(e^{i\tau\langle\nabla\rangle/2} I_N\psi^n)),\\ P_N\psi^{[n+1]} &= e^{i\tau\langle\nabla\rangle} P_N\psi^{[n]} + i\varepsilon^2\tau\langle\nabla\rangle^{-1} e^{i\tau\langle\nabla\rangle/2} P_N(G(e^{i\tau\langle\nabla\rangle/2}\psi^{[n]})), \end{aligned}$$

which lead to

$$e^{n+1} = e^{i\tau\langle\nabla\rangle} e^n + i\varepsilon^2\tau\langle\nabla\rangle^{-1} e^{i\tau\langle\nabla\rangle/2}\left(P_N G(\psi^{\langle 1\rangle}) - I_N G(\psi^{(1)})\right), \tag{3.9}$$

with $\psi^{\langle 1\rangle} = e^{i\tau\langle\nabla\rangle/2}\psi^{[n]}$ and $\psi^{(1)} = e^{i\tau\langle\nabla\rangle/2} I_N\psi^n$. Hence, combining the bounds (2.14) and (3.4), we have $\|G(\psi^{\langle 1\rangle})\|_{m+1} + \|G(\psi^{(1)})\|_{m+1} \lesssim 1$ and

$$\|G(\psi^{\langle 1\rangle}) - G(\psi^{(1)})\| \lesssim \|\psi^{\langle 1\rangle} - \psi^{(1)}\| \lesssim \|\psi^{[n]} - I_N\psi^n\| \lesssim h^{m+1} + \|e^n\|. \tag{3.10}$$

To summarize, noticing $\|P_N G(\psi^{\langle 1\rangle}) - I_N G(\psi^{(1)})\| \le \|P_N(G(\psi^{(1)})) - I_N(G(\psi^{(1)}))\| + \|P_N(G(\psi^{\langle 1\rangle})) - P_N(G(\psi^{(1)}))\| \lesssim h^{m+1} + \|G(\psi^{\langle 1\rangle}) - G(\psi^{(1)})\|$, we obtain from (3.9) that

$$\begin{aligned} \|e^{n+1}\|_1 \le& \|e^n\|_1 + \varepsilon^2\tau\|P_N G(\psi^{\langle 1\rangle}) - I_N G(\psi^{(1)})\|\\ \le& \|e^n\|_1 + C_1\varepsilon^2\tau h^{m+1} + C_2\varepsilon^2\tau\|e^n\|, \quad 0 \le n \le T_\varepsilon/\tau - 1, \end{aligned}$$

where C_1, C_2 are constants independent of $\varepsilon, h, \tau, n, \tau_0$. Since $e^0 = P_N u_0 - I_N u_0 - i\langle\nabla\rangle^{-1}(P_N u_1 - I_N u_1)$, we have $\|e^0\|_1 \lesssim h^m$, and the discrete Gronwall inequality implies $\|e^{n+1}\|_1 \lesssim h^m$ $(0 \le n \le T_\varepsilon/\tau - 1)$. Combining the above estimtates with (3.8), we derive

$$\|\psi(\cdot, t_n) - I_N\psi^n\|_1 \lesssim h^m + \varepsilon^2\tau^2 + \tau_0^{m+1}, \quad 0 \le n \le T_\varepsilon/\tau.$$

Recalling (3.3), we obtain error bounds for u^n and v^n $(0 \le n \le T_\varepsilon/\tau)$ as

$$\begin{aligned}\|u(\cdot, t_n) - I_N u^n\|_1 &= \frac{1}{2}\left\|\psi(\cdot, t_n) + \overline{\psi(\cdot, t_n)} - I_N\psi^n - I_N\overline{\psi^n}\right\|_1 \\ &\le \|\psi(\cdot, t_n) - I_N\psi^n\|_1 \lesssim h^m + \varepsilon^2\tau^2 + \tau_0^{m+1}, \\ \|v(\cdot, t_n) - I_N v^n\| &= \frac{1}{2}\left\|\langle\nabla\rangle(\psi(\cdot, t_n) - \overline{\psi(\cdot, t_n)}) - \langle\nabla\rangle(I_N\psi^n - I_N\overline{\psi^n})\right\| \\ &\le \|\psi(\cdot, t_n) - I_N\psi^n\|_1 \lesssim h^m + \varepsilon^2\tau^2 + \tau_0^{m+1},\end{aligned}$$

which show (3.5), and the proof for Theorem 3.1 is completed. □

Remark 3.2. Through the proof of Theorem 3.1, it is not difficult to see that the spatial error estimates of $u(\cdot, t_n) - I_N u^n$ in L^2-norm can be improved to h^{m+1}.

4. Extensions. In this section, we discuss the extensions of the time-splitting method and corresponding error estimates to the complex NKGE with a general power nonlinearity and an oscillatory complex NKGE which propagates waves with wavelength at $O(\varepsilon^{2p})$ in time.

4.1. The complex NKGE with a general power nonlinearity. Consider the following complex NKGE with a general power nonlinearity:

$$\begin{cases}\partial_{tt}u(\mathbf{x}, t) - \Delta u(\mathbf{x}, t) + u(\mathbf{x}, t) + \varepsilon^{2p}|u(\mathbf{x}, t)|^{2p}u(\mathbf{x}, t) = 0, \quad \mathbf{x} \in \Omega, \quad t > 0, \\ u(\mathbf{x}, 0) = u_0(\mathbf{x}), \quad \partial_t u(\mathbf{x}, 0) = u_1(\mathbf{x}), \quad \mathbf{x} \in \Omega.\end{cases} \tag{4.1}$$

Here, $u := u(\mathbf{x}, t)$ is a complex-valued scalar field, $p \in \mathbb{N}^+$ is the power index, and the initial data $u_0(\mathbf{x})$ and $u_1(\mathbf{x})$ are two given complex-valued functions which are independent of ε. The domain Ω and periodic boundary conditions are as in (1.1). The local/global well-posedness and scattering properties of the Cauchy problem (4.1) have been widely studied in the literature and the references therein [28, 31, 37, 38, 39, 40, 47]. From the analytical results, the life span of a smooth solution to the complex NKGE (4.1) is at least $O(\varepsilon^{-2p})$.

For simplicity of notations, we only show the numerical scheme in 1D under periodic boundary conditions. Similarly, introducing $v(x, t) = \partial_t u(x, t)$ and

$$\eta_\pm(x, t) = u(x, t) \mp i\ \langle\nabla\rangle^{-1}v(x, t), \qquad a \le x \le b, \quad t \ge 0, \tag{4.2}$$

and denoting $f(\varphi) = |\varphi|^{2p}\varphi$, then the complex NKGE (4.1) can be reformulated into the following coupled relativistic NLSEs:

$$\begin{cases} i\partial_t\eta_\pm \pm \langle\nabla\rangle\eta_\pm \pm \varepsilon^{2p}\langle\nabla\rangle^{-1}f\left(\frac{1}{2}\eta_+ + \frac{1}{2}\eta_-\right) = 0, \\ \eta_\pm(t = 0) = u_0 \mp i\ \langle\nabla\rangle^{-1}v_0.\end{cases} \tag{4.3}$$

Let $\eta^n_{\pm,j}$ be the approximations of $\eta_\pm(x_j, t_n)$ for $j \in \mathcal{T}_N^0$ and $n \ge 0$, and denote $\eta^n_\pm = (\eta^n_{\pm,0}, \eta^n_{\pm,1}, \ldots, \eta^n_{\pm,N})^T \in \mathbb{C}^{n+1}$ as the solution at $t_n = n\tau$. Similar to the NKGE with cubic nonlinearity, the second-order TSFP discretization for the relativistic NLSE (4.3) is given by

$$\eta^{(1)}_{\pm,j} = \sum_{l\in\mathcal{T}_N} e^{\pm\, i\frac{\tau\delta_l}{2}}\, \widetilde{(\eta^n_\pm)}_l\, e^{i\mu_l(x_j-a)},$$

$$\eta^{(2)}_{\pm,j} = \eta^{(1)}_{\pm,j} \pm \varepsilon^{2p}\tau f^n_j, \qquad j\in\mathcal{T}^0_N, \quad n\ge 0, \tag{4.4}$$

$$\eta^{n+1}_{\pm,j} = \sum_{l\in\mathcal{T}_N} e^{\pm\, i\frac{\tau\delta_l}{2}}\, \widetilde{(\eta^{(2)}_\pm)}_l\, e^{i\mu_l(x_j-a)},$$

with

$$\eta^0_{\pm,j} = u_0(x_j)\mp i\sum_{l\in\mathcal{T}_N}\frac{1}{\delta_l}\widetilde{(v_0)}_l e^{i\mu_l(x_j-a)}, \quad f^n_j = i\sum_{l\in\mathcal{T}_N}\frac{1}{\delta_l}\left(\widetilde{f\left(\left(\eta^n_+ + \eta^n_-\right)/2\right)}\right)_l e^{i\mu_l(x_j-a)}.$$

Then u^{n+1}_j and v^{n+1}_j ($j\in\mathcal{T}^0_N, n\ge 0$) which are approximations of $u(x_j,t_{n+1})$ and $v(x_j,t_{n+1})$, respectively, can be recovered by

$$u^{n+1}_j = \frac{1}{2}\left(\eta^{n+1}_{+,j}+\eta^{n+1}_{-,j}\right),\ v^{n+1}_j = \frac{i}{2}\sum_{l\in\mathcal{T}_N}\delta_l\Big(\widetilde{(\eta^{n+1}_+)}_l - \widetilde{(\eta^{n+1}_-)}_l\Big)e^{i\mu_l(x_j-a)}. \tag{4.5}$$

We assume existence of the exact solution $u := u(x,t)$ of the NKGE (4.1) up to the time $T_{\varepsilon,p} = T/\varepsilon^{2p}$ ($T>0$ fixed) and

$$\text{(B)} \qquad \|u\|_{L^\infty([0,T_{\varepsilon,p}];H^{m+1})}\lesssim 1, \qquad \|\partial_t u\|_{L^\infty([0,T_{\varepsilon,p}];H^m)}\lesssim 1, \quad m\ge 1;$$

then the following improved uniform error bounds for the TSFP method (4.4)–(4.5) can be established up to the time $T_{\varepsilon,p}$.

THEOREM 4.1. *Let u^n and v^n be the numerical approximations obtained from the TSFP* (4.4)–(4.5)*. Under the assumption* (B)*, there exist $h_0>0$ and $0<\tau_0<1$ sufficiently small and independent of ε such that, for any $0<\varepsilon\le 1$, when $0<h\le h_0$ and $0<\tau\le\alpha\tau_0$ for some fixed constant $\alpha>0$, we have the following improved uniform error estimates:*

$$\|u(\cdot,t_n)-I_N u^n\|_1 + \|\partial_t u(\cdot,t_n) - I_N v^n\| \lesssim h^m + \varepsilon^{2p}\tau^2 + \tau_0^{m+1},\ 0\le n\le \frac{T/\varepsilon^{2p}}{\tau}. \tag{4.6}$$

In particular, if the exact solution is sufficiently smooth, e.g., $u,\partial_t u\in H^\infty$, the uniform improved error bounds for sufficiently small τ are

$$\|u(\cdot,t_n)-I_N u^n\|_1 + \|\partial_t u(\cdot,t_n) - I_N v^n\| \lesssim h^m + \varepsilon^{2p}\tau^2,\ 0\le n\le \frac{T/\varepsilon^{2p}}{\tau}. \tag{4.7}$$

Remark 4.2. The above second-order time-splitting method is equivalent to the Deuflhard-type exponential wave integrator (EWI) method for discretizing the NKGE (4.1). For the Gautschi-type EWI method [26], we only have uniform error bounds (see also numerical results in Figure 5.6)

$$\|u(\cdot,t_n)-I_N u^n\|_1 \lesssim h^m + \tau^2, \quad 0\le n\le\frac{T/\varepsilon^{2p}}{\tau}. \tag{4.8}$$

As a result, the second-order time-splitting method/Deuflhard-type EWI performs better than the Gautschi-type EWI discretization for the NKGE (4.1) up to the time at $O(1/\varepsilon^{2p})$.

Remark 4.3. The NKGE (4.1) conserves the energy as [4, 8]

$$\begin{aligned} E(t) &:= \int_\Omega \left[|\partial_t u(x,t)|^2 + |\nabla u(x,t)|^2 + |u(x,t)|^2 + \frac{\varepsilon^{2p}}{p+1}|u(x,t)|^{2p+2}\right] dx \\ &\equiv \int_\Omega \left[|u_1(x)|^2 + |\nabla u_0(x)|^2 + |u_0(x)|^2 + \frac{\varepsilon^{2p}}{p+1}|u_0(x)|^{2p+2}\right] dx \\ &= E(0), \quad t \geq 0. \end{aligned}$$

Introducing the discrete energy at $t = t_n$ with the mesh size h as

$$E_h^n = h \sum_{j=0}^{N-1} \left[|v_j^n|^2 + |(\partial_x u)_j^n|^2 + |u_j^n|^2 + \frac{\varepsilon^{2p}}{p+1}|u_j^n|^{2p+2}\right], \tag{4.9}$$

where

$$(\partial_x u)_j^n = i \sum_{l\in\mathcal{T}_N} \mu_l \widetilde{(u^n)}_l e^{i\mu_l(x_j-a)}, \quad j = 0, 1, \ldots, N-1, \tag{4.10}$$

we have the following estimates for the discrete energy:

$$|E_h^n - E_h^0| \lesssim h^m + \varepsilon^{2p}\tau^2 + \tau_0^{m+1}, \quad 0 \leq n \leq \frac{T/\varepsilon^{2p}}{\tau}. \tag{4.11}$$

In addition, if the exact solution is sufficiently smooth, e.g., $u, \partial_t u \in H^\infty$, the estimate for the discrete energy for sufficiently small τ is

$$|E_h^n - E_h^0| \lesssim h^m + \varepsilon^{2p}\tau^2, \quad 0 \leq n \leq \frac{T/\varepsilon^{2p}}{\tau}. \tag{4.12}$$

4.2. An oscillatory complex NKGE. Introducing a rescale in time

$$t = \frac{r}{\varepsilon^{2p}} \Leftrightarrow r = \varepsilon^{2p} t, \quad \nu(\mathbf{x}, r) = u(\mathbf{x}, t), \tag{4.13}$$

the NKGE (4.1) can be reformulated into the following oscillatory complex NKGE:
(4.14)

$$\begin{cases} \varepsilon^{2p}\partial_{rr}\nu(\mathbf{x},r) - \dfrac{1}{\varepsilon^{2p}}\Delta\nu(\mathbf{x},r) + \dfrac{1}{\varepsilon^{2p}}\nu(\mathbf{x},r) + |\nu(\mathbf{x},r)|^{2p}\nu(\mathbf{x},r) = 0, \ \mathbf{x}\in\Omega, \ r > 0, \\ \nu(\mathbf{x},0) = u_0(\mathbf{x}), \quad \partial_r\nu(\mathbf{x},0) = \dfrac{1}{\varepsilon^{2p}}u_1(\mathbf{x}), \quad \mathbf{x}\in\Omega. \end{cases}$$

The solution of the oscillatory NKGE (4.14) propagates waves with amplitude at $O(1)$, wavelength at $O(1)$ and $O(\varepsilon^{2p})$ in space and time, respectively, and wave velocity at $O(\varepsilon^{-2p})$. Denote $\mu(\mathbf{x}, r) = \partial_r\nu(\mathbf{x}, r)$; by taking the time step $\kappa = \varepsilon^{2p}\tau$, the improved error bounds on the time-splitting methods (see Remark 2.1) for the long-time problem can be extended to the oscillatory complex NKGE (4.14) up to the fixed time T.

THEOREM 4.4. *Let ν^n and μ^n be the numerical approximations obtained from the TSFP method. Assume the exact solution ν of the oscillatory complex NKGE* (4.14) *satisfies for some $m \geq 1$*

$$\begin{aligned} &\nu \in L^\infty\left([0,T]; H^{m+1}\right), \quad \partial_r\nu \in L^\infty\left([0,T]; H^m\right), \\ &\|\nu\|_{L^\infty([0,T];H^{m+1})} \lesssim 1, \qquad \|\partial_r\nu\|_{L^\infty([0,T];H^m)} \lesssim \frac{1}{\varepsilon^{2p}}; \end{aligned}$$

then, there exist $h_0 > 0$ and $0 < \kappa_0 < 1$ sufficiently small and independent of ε such that, for any $0 < \varepsilon \le 1$, when the mesh size $0 < h \le h_0$ and the time step $0 < \kappa \le \alpha\kappa_0\varepsilon^{2p}$ for a fixed constant $\alpha > 0$, we have the following improved error estimates:

$$\|\nu(\cdot, r_n) - I_N\nu^n\|_1 + \varepsilon^{2p}\|\partial_r\nu(\cdot, r_n) - I_N\mu^n\| \lesssim h^m + \frac{\kappa^2}{\varepsilon^{2p}} + \kappa_0^{m+1},\ 0 \le n \le \frac{T}{\kappa}. \tag{4.15}$$

In particular, if the exact solution is sufficiently smooth, e.g., $\nu, \partial_r\nu \in H^\infty$, the improved error bounds for sufficiently small κ are

$$\|\nu(\cdot, r_n) - I_N\nu^n\|_1 + \varepsilon^{2p}\|\partial_r\nu(\cdot, r_n) - I_N\mu^n\| \lesssim h^m + \kappa^2/\varepsilon^{2p},\ 0 \le n \le \frac{T}{\kappa}. \tag{4.16}$$

Remark 4.5. Under the assumption of Theorem 4.4, direct error analysis for time-splitting schemes [5, 35] would lead to the error estimates as $\|\nu(\cdot, r_n) - I_N\nu^n\|_1 + \varepsilon^{2p}\|\partial_r\nu(\cdot, r_n) - I_N\mu^n\| \lesssim h^m + \frac{\kappa^2}{\varepsilon^{4p}}$. Our results are improved in the sense that the error bound $\frac{\kappa^2}{\varepsilon^{4p}}$ is now $\frac{\kappa^2}{\varepsilon^{2p}}$.

Remark 4.6. The proof of the improved error bounds for the oscillatory complex NKGE in Theorem 4.4 is similar to the long-time problem, and we omit the details for brevity. We will provide an example in section 5 to confirm the improved error bounds for the oscillatory complex NKGE and to demonstrate that they are sharp.

5. Numerical results.

In this section, we present some numerical examples in 1D and two dimensions (2D) to validate our improved uniform error bounds on the time-splitting methods for the long-time dynamics of the NKGE with weak nonlinearity and the improved error bounds for the oscillatory complex NKGE.

5.1. The long-time dynamics in 1D.

First, we test the long-time errors of the TSFP (4.4)–(4.5) for the NKGE (4.1) in 1D with $p = 2$ and real-valued initial data as

$$u_0(x) = \frac{3}{2 + \cos^2(x)}, \quad u_1(x) = \frac{3}{4 + \cos^2(x)}, \quad x \in \Omega = (0, 2\pi). \tag{5.1}$$

The numerical "exact" solution is computed by the TSFP (4.4)–(4.5) with a very fine mesh size $h_e = \pi/60$ and time step $\tau_e = 10^{-4}$. To quantify the error, we introduce the following error functions:

$$e_1(t_n) = \|u(x, t_n) - I_N u^n\|_1, \quad e_{1,\max}(t_n) = \max_{0\le q\le n} e_1(t_q). \tag{5.2}$$

In the rest of the paper, the spatial mesh size is always chosen sufficiently small such that the spatial errors can be neglected when considering the long-time temporal errors.

Figure 5.1 displays the long-time errors of the TSFP (4.4)–(4.5) for the NKGE (4.1) with $p = 2$, the fixed time step τ, and different ε, which confirms the improved uniform error bounds in H^1-norm at $O(\varepsilon^4\tau^2)$ up to time at $O(1/\varepsilon^4)$. Figure 5.2 and Figure 5.3 depict the spatial and temporal errors of the TSFP (4.4)–(4.5) for the NKGE (4.1) with $p = 2$ at $t = 1/\varepsilon^4$, respectively. Figure 5.2 indicates the spectral accuracy of the TSFP (4.4)–(4.5) for the NKGE (4.1) in space, and the spatial errors are independent of the small parameter ε. Each line in Figure 5.3(a) corresponds to a fixed ε and shows the global errors in H^1-norm versus the time step τ, which confirms the second-order convergence of the TSFP (4.4)–(4.5) for the NKGE (4.1) in time.

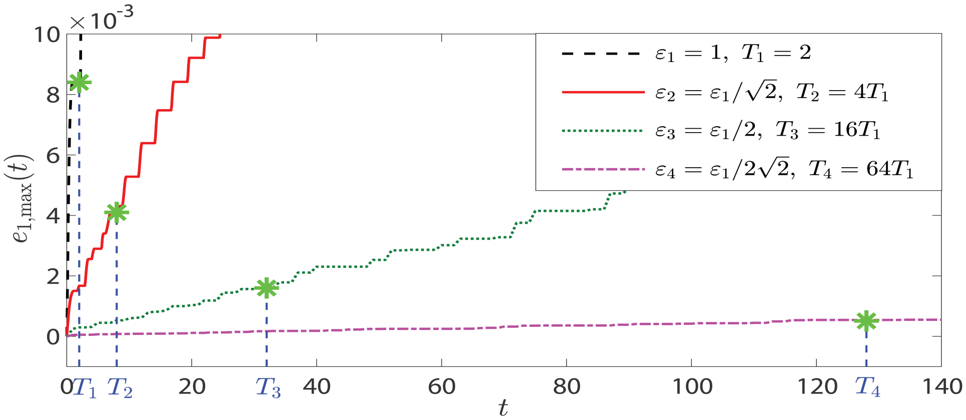

FIG. 5.1. *Long-time temporal errors of the TSFP* (4.4)–(4.5) *for the NKGE* (4.1) *with* $p = 2$ *and different* ε *in* 1*D.*

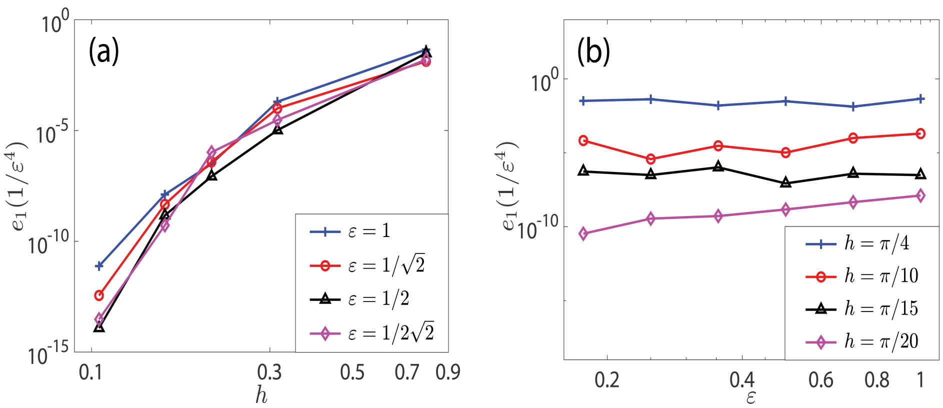

FIG. 5.2. *Long-time spatial errors of the TSFP* (4.4)–(4.5) *for the NKGE* (4.1) *with* $p = 2$ *in* 1*D at* $t = 1/\varepsilon^4$.

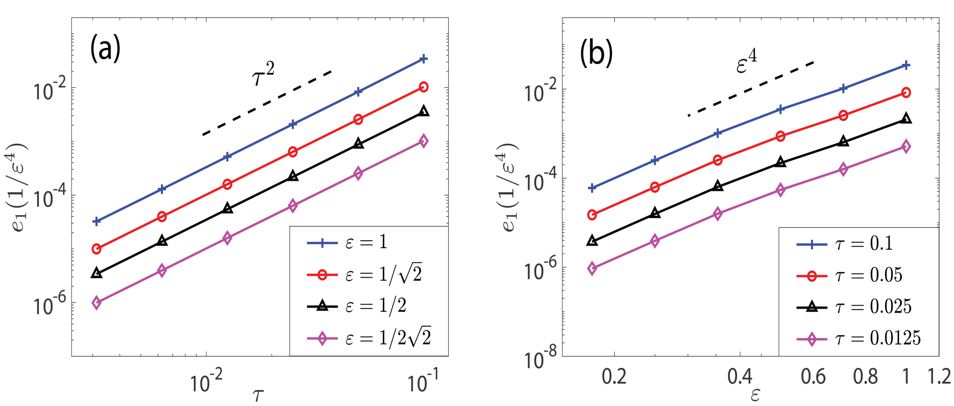

FIG. 5.3. *Long-time temporal errors of the TSFP* (4.4)–(4.5) *for the NKGE* (4.1) *with* $p = 2$ *in* 1*D at* $t = 1/\varepsilon^4$.

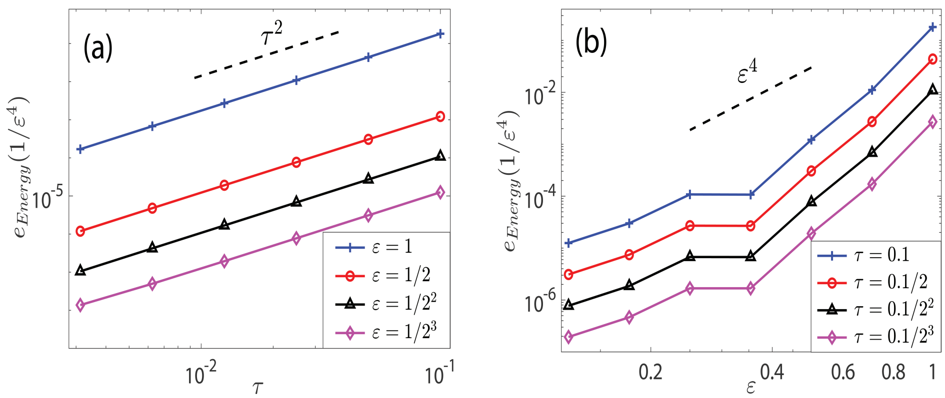

FIG. 5.4. *Long-time errors for the discrete energy of the TSFP* (4.4)–(4.5) *for the NKGE* (4.1) *with* $p = 2$ *in* 1D *at* $t = 1/\varepsilon^4$.

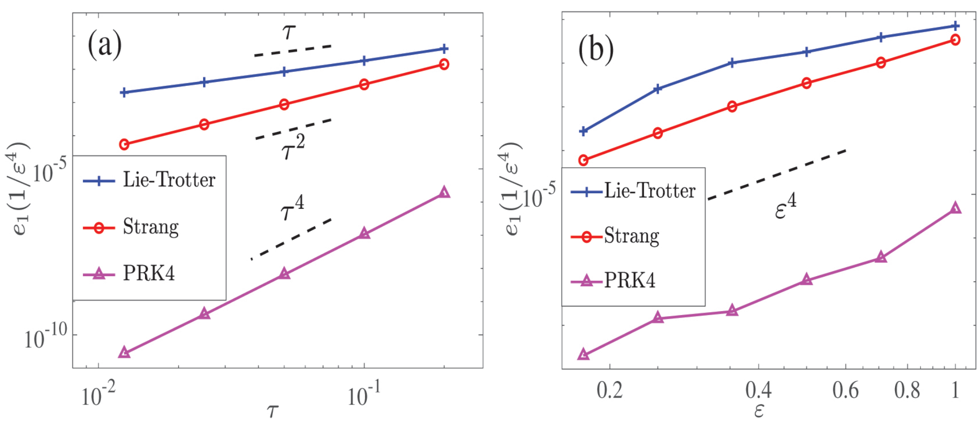

FIG. 5.5. *Comparisons of the first-, second-, and fourth-order splitting methods for the NKGE* (4.1) *with* $p = 2$ *in* 1D *at* $t = 1/\varepsilon^4$*:* (a) *convergence in terms of* τ *for fixed* $\varepsilon = 1/2$ *(left);* (b) *convergence in terms of* ε *for fixed* $\tau = 0.1$ *(right).*

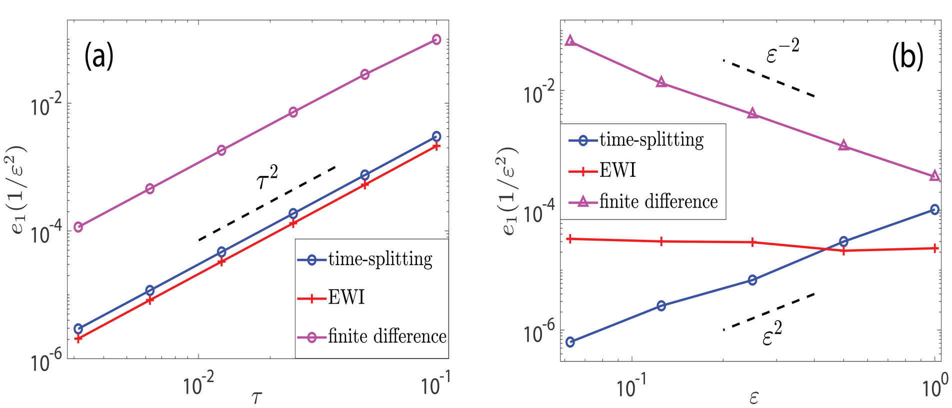

FIG. 5.6. *Comparisons of the finite difference, Gautschi-type EWI, and time-splitting methods for the NKGE* (1.1) *in* 1D *at* $t = 1/\varepsilon^2$*:* (a) *convergence in terms of* τ *for fixed* $\varepsilon = 1/2$ *(left);* (b) *convergence in terms of* ε *for fixed* $\tau = 0.01$ *(right).*

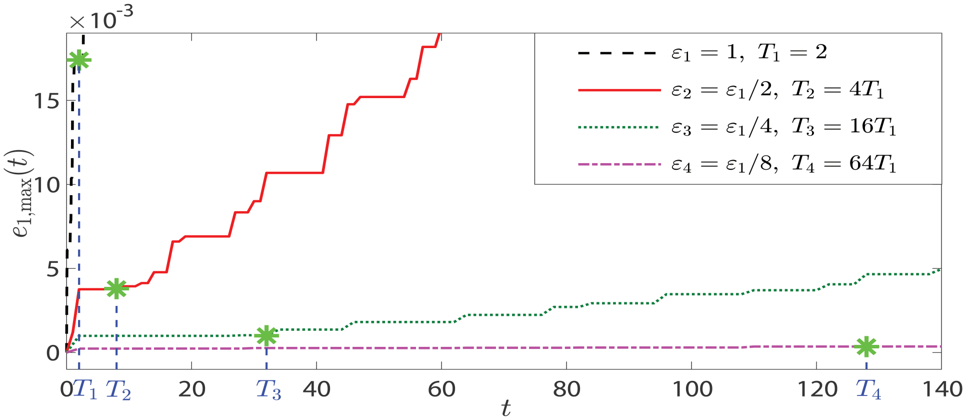

FIG. 5.7. *Long-time temporal errors of the TSFP method for the NKGE in 2D with different ε.*

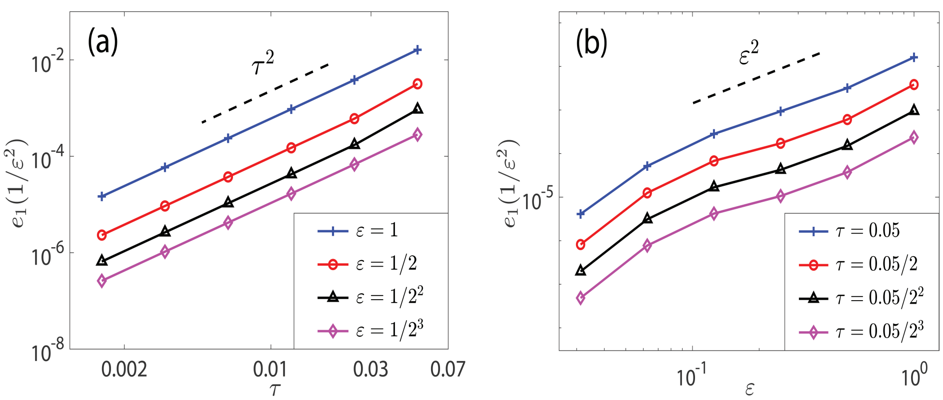

FIG. 5.8. *Long-time temporal errors of the TSFP method for the NKGE in 2D at $t = 1/\varepsilon^2$.*

Figure 5.3(b) again validates that the global errors in H^1-norm behave like $O(\varepsilon^4\tau^2)$ up to the time at $O(1/\varepsilon^4)$. Figure 5.4 shows the long-time errors for the discrete energy of the TSFP (4.4)–(4.5) for the NKGE (4.1) with $p = 2$ at $t = 1/\varepsilon^4$, which verifies the improved uniform error bounds for the discrete energy (4.11).

For comparisons, we present the temporal errors of the first-, Second-, and fourth-order splitting methods. In space, we use the Fourier pseudospectral method with a very fine mesh size such that the spatial errors are negligible.

Figure 5.5(a) depicts the temporal errors of three splitting methods with $\varepsilon = 1/2$, which indicates that the higher-order splitting method not only has higher order convergence rate but also achieves better accuracy under the same time step size. Figure 5.5(b) shows the temporal errors of three splitting methods for the fixed time step $\tau = 0.1$ and confirms the improved uniform error bounds for all the three splitting methods up to the time at $O(1/\varepsilon^4)$.

Figure 5.6 compares the second-order semiimplicit finite difference method [4], second-order Gautschi-type EWI method [26], and time-splitting method (2.11) for the long-time dynamics of the NKGE. Figure 5.6(a) depicts temporal errors of these three methods with $\varepsilon = 1/2$, which indicates that they are all second-order methods

TABLE 5.1
Temporal errors of the TSFP method for the oscillatory complex NKGE (4.14) in 1D.

$e_1(r=1)$	$\kappa_0 = 0.05$	$\kappa_0/4$	$\kappa_0/4^2$	$\kappa_0/4^3$	$\kappa_0/4^4$
$\varepsilon_0 = 1$	**1.11E-2**	6.90E-4	4.31E-5	2.69E-6	1.68E-7
order	**-**	2.00	2.00	2.00	2.00
$\varepsilon_0/2$	6.25E-2	**3.45E-3**	2.14E-4	1.34E-5	8.35E-7
order	-	**2.09**	2.01	2.00	2.00
$\varepsilon_0/2^2$	8.26E-1	1.89E-2	**1.11E-3**	6.93E-5	4.33E-6
order	-	2.72	**2.04**	2.00	2.00
$\varepsilon_0/2^3$	1.54	3.19E-1	1.62E-2	**1.01E-3**	6.29E-5
order	-	1.14	2.15	**2.00**	2.00
$\varepsilon_0/2^4$	2.09	3.82	7.90E-2	4.26E-3	**2.64E-4**
order	-	-0.44	2.80	2.11	**2.01**

for fixed ε. Figure 5.6(b) shows that just the time-splitting method has improved uniform error bounds at $O(\varepsilon^2)$ for fixed time step $\tau = 0.01$, while the Gautschi-type EWI method is uniform and the finite difference method performs like $O(1/\varepsilon^2)$ up to the time at $O(1/\varepsilon^2)$.

5.2. The long-time dynamics in 2D. In this subsection, we show an example in 2D with the irrational aspect ratio of the domain $(x, y) \in \Omega = (0, 1) \times (0, 2\pi)$. In the numerical experiment, we choose $p = 1$ and the initial data as

$$u_0(x, y) = \frac{2}{1 + \cos^2(2\pi x + y)}, \quad u_1(x) = \frac{3}{2 + 2\cos^2(2\pi x + y)}.$$

Figure 5.7 presents the long-time errors of the TSFP method for the NKGE in 2D with a fixed time step τ and different ε, which confirms that the improved uniform error bounds at $O(\varepsilon^2\tau^2)$ up to the time at $O(1/\varepsilon^2)$ are also suitable for the domain with irrational aspect ratio. Figure 5.8 depicts the temporal errors for the TSFP method for the NKGE in 2D at $t = 1/\varepsilon^2$, which again indicates that the TSFP method is second-order in time and validates the improved uniform error bounds up to the time at $O(1/\varepsilon^2)$.

5.3. The oscillatory complex NKGE. In this subsection, we present the numerical result for the oscillatory complex NKGE (4.15) in 1D to confirm the improved error bound (4.14). We choose $p = 1$ and the complex-valued initial data as

$$u_0(x) = x^2(x-1)^2 + 3, \quad u_1(x) = x(x-1)(2x-1) + 3i\cos(2\pi x), \quad x \in \Omega = (0, 1).$$

The regularity is enough to ensure the improved error bound in H^1-norm.

Table 5.1 lists the temporal errors of the TSFP method for the oscillatory NKGE (4.14) in 1D, which indicates that the second-order convergence can only be observed when $\kappa \lesssim \varepsilon^2$ (cf. the upper triangle above the diagonal with bold letters, and the boldface text stands for $\kappa/\varepsilon^2 = 0.05$), and the temporal errors in H^1-norm behave like $O(\kappa^2/\varepsilon^2)$ to confirm the improved error bound (4.15) and to demonstrate that they are sharp.

6. Conclusions. Improved uniform error bounds on the time-splitting methods for the long-time dynamics of the NKGE with weak cubic nonlinearity were rigorously established. By employing the technique of RCO, the improved uniform error bounds for the second-order semidiscretization and full-discretization up to the time at $O(1/\varepsilon^2)$ were carried out at $O(\varepsilon^2\tau^2)$ and $O(h^m + \varepsilon^2\tau^2)$, respectively. The improved error bounds are extended to the complex NKGE with a general power nonlinearity in the long-time regime and the oscillatory complex NKGE up to the fixed time T. Numerical results in 1D and 2D were presented to confirm the improved error bounds and to demonstrate that they are sharp. The equivalence between the time-splitting methods and the Deuflhard-type EWIs for NKGE implies the improved error bounds hold for a class of exponential integrators, which would be the object of future study.

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