ESAIM: M2AN 57 (2023) 899–919
https://doi.org/10.1051/m2an/2022096

ESAIM: Mathematical Modelling and Numerical Analysis
www.esaim-m2an.org

A SECOND-ORDER LOW-REGULARITY CORRECTION OF LIE SPLITTING FOR THE SEMILINEAR KLEIN–GORDON EQUATION

Buyang Li[1,*], Katharina Schratz[2] and Franco Zivcovich[2]

Abstract. The numerical approximation of nonsmooth solutions of the semilinear Klein–Gordon equation in the d-dimensional space, with $d = 1, 2, 3$, is studied based on the discovery of a new cancellation structure in the equation. This cancellation structure allows us to construct a low-regularity correction of the Lie splitting method (*i.e.*, exponential Euler method), which can significantly improve the accuracy of the numerical solutions under low-regularity conditions compared with other second-order methods. In particular, the proposed time-stepping method can have second-order convergence in the energy space under the regularity condition $(u, \partial_t u) \in L^\infty(0, T; H^{1+\frac{d}{4}} \times H^{\frac{d}{4}})$. In one dimension, the proposed method is shown to have almost $\frac{4}{3}$-order convergence in $L^\infty(0, T; H^1 \times L^2)$ for solutions in the same space, *i.e.*, no additional regularity in the solution is required. Rigorous error estimates are presented for a fully discrete spectral method with the proposed low-regularity time-stepping scheme. The numerical experiments show that the proposed time-stepping method is much more accurate than previously proposed methods for approximating the time dynamics of nonsmooth solutions of the semilinear Klein–Gordon equation.

Mathematics Subject Classification. 65M12, 65M15, 76D05.

Received May 2, 2022. Accepted November 22, 2022.

1. Introduction

We consider the following initial-boundary value problem of the semilinear Klein–Gordon equation:

$$\begin{cases} \partial_{tt} u - \Delta u = f(u) & \text{in } \Omega \times (0, T], \\ u = 0 & \text{on } \partial\Omega \times (0, T], \\ u|_{t=0} = u^0 \ \text{ and } \ \partial_t u|_{t=0} = v^0 & \text{in } \Omega, \end{cases} \tag{1.1}$$

in a rectangular domain $\Omega \subset \mathbb{R}^d$ under the homogeneous Dirichlet boundary condition, where $f : \mathbb{R} \to \mathbb{R}$ is a given nonlinear function. For example, equation (1.1) is often referred to as the sine–Gordon equation in the case $f(u) = \sin(u)$, which arises in many physical applications, such as magnetic-flux propagation in Josephson

Keywords and phrases. Semilinear Klein–Gordon equation, wave equation, energy space, low regularity, second order, error estimates.

[1] Department of Applied Mathematics, The Hong Kong Polytechnic University, Hung Hom, Hong Kong

[2] Laboratoire Jacques-Louis Lions, Sorbonne Université, Bureau 16-26-315, 4 place Jussieu, Paris, France.

[*]Corresponding author: `buyang.li@polyu.edu.hk`; `libuyang@gmail.com`

junctions, bloch-wall dynamics in magnetic crystals, propagation of dislocation in solid and liquid crystals, propagation of ultra-short optical pulses in two-level media; see [3].

The numerical approximation of semilinear Klein–Gordon equations in the form of (1.1) has been extensively studied in computational mathematics. A large variety of numerical schemes for approximating the time dynamics of the semilinear Klein–Gordon equation has been proposed and analyzed, including trigonometric/exponential integrators that are based on the variation-of-constants formula (*e.g.*, see [5, 11, 13, 18, 34]), splitting methods (*e.g.*, see [1, 2, 5, 12, 16, 29]), symplectic methods [7, 8, 14], and finite difference methods (such as the Crank–Nicolson, Runge–Kutta and Newmark methods, see [6, 17, 20–22, 25, 28, 30, 33]).

The analyses in these articles (*e.g.*, [5, 11, 18, 34]) have shown that for initial data (u^0, v^0) in the physically natural energy space $H^1(\Omega)\times L^2(\Omega)$, so that the solution $(u, \partial_t u)$ is bounded in the energy space $H^1(\Omega)\times L^2(\Omega)$ uniformly for $t \in [0, T]$, the classical time-stepping methods such as splitting methods, trigonometric integrators, and averaged exponential integrators, can approximate the solution $(u, \partial_t u)$ with second-order convergence in the weaker space $L^2(\Omega)\times H^{-1}(\Omega)$, but only with first-order convergence in the energy space $H^1(\Omega)\times L^2(\Omega)$ itself. Moreover, the second-order approximation to $(u, \partial_t u)$ in the energy space $H^1(\Omega) \times L^2(\Omega)$ generally requires the initial data to be in the stronger space $H^2(\Omega) \times H^1(\Omega)$. Since every two temporal derivatives in the solution of the wave equation can be converted to two spatial derivatives in the solution, the finite difference time-stepping methods generally require more regularity of the solution according to the analyses in the literature.

The only method which breaks this order barrier is the low-regularity integrator proposed in [31], which can have second-order convergence in the energy space $H^1(\Omega) \times L^2(\Omega)$ under the weaker regularity condition $(u^0, v^0) \in H^{\frac{7}{4}}(\Omega)\times H^{\frac{3}{4}}(\Omega)$; see Corollary 5.7 of [31]. This low-regularity integrator is based on the reformulation of (1.1) into the first-order equation

$$i\partial_t w = -(-\Delta)^{\frac{1}{2}} w + (-\Delta)^{-\frac{1}{2}} f\left(\frac{w+\bar{w}}{2}\right) \tag{1.2}$$

through the transformation $w = u - i(-\Delta)^{-\frac{1}{2}}\partial_t u$, which is then discretized by the low-regularity integrators proposed in [31] for first-order semilinear evolution equations. Such low-regularity types of numerical schemes have recently gained a lot of attention in particular in the context of the nonlinear Schrödinger equation (see, *e.g.*, [4, 26, 27, 31]), KdV equation (see, *e.g.*, [19, 23, 36, 37]), and the Navier–Stokes equations [24]. Second-order approximations to the solutions of these equations in the H^s norm generally require the solutions to be bounded in $H^s(\Omega)$ for $s > d/2 + 1$.

In this article, we construct a new time-stepping method for the semilinear Klein–Gordon equation based on the discovery of a new cancellation structure in the equation, which allows us to find a low-regularity correction of the Lie splitting method, *i.e.*,

$$\begin{pmatrix} u^{n+1} \\ v^{n+1} \end{pmatrix} = \underbrace{\mathrm{e}^{\tau L}\begin{pmatrix} u^{n} \\ v^{n} \end{pmatrix} + \tau \mathrm{e}^{\tau L}\begin{pmatrix} 0 \\ f(u^{n}) \end{pmatrix}}_{\text{Lie splitting}} + \underbrace{\tau^2 \mathrm{e}^{\tau L}\varphi_2(-2\tau L)\begin{pmatrix} -f(u^{n}) \\ f'(u^{n})v^n \end{pmatrix}}_{\text{low-regularity correction}} \tag{1.3}$$

where $(u^n, v^n)^\top$ is an approximation to $(u(t_n), \partial_t u(t_n))^\top$, and L is a linear anti-symmetric partial differential operator defined by

$$L = \begin{pmatrix} 0 & 1 \\ \Delta & 0 \end{pmatrix} : \left[H^2(\Omega) \cap H^1_0(\Omega)\right] \times H^1(\Omega) \to H^1_0(\Omega) \times L^2(\Omega). \tag{1.4}$$

The last term in (1.3), which contains the operator $\varphi_2(-2\tau L) := (2\tau L)^{-2}\big(\mathrm{e}^{-2\tau L} + 2\tau L - I\big)$, is a low-regularity correction term for the Lie splitting, *i.e.*, it improves the Lie splitting method to second order under low-regularity conditions, without requiring second-order partial derivatives of the solution. Theoretically, we prove that the new time-stepping method can achieve second-order convergence in the energy space $H^1(\Omega) \times L^2(\Omega)$ under the regularity condition $(u^0, v^0) \in H^{1+\frac{d}{4}}(\Omega) \times H^{\frac{d}{4}}(\Omega)$ for spatial dimension $d = 1, 2, 3$; see Theorem 3.1. In the one-dimension case, the proposed method is shown to have a convergence order arbitrarily close to

$\frac{4}{3}$ in the energy space $H^1(\Omega) \times L^2(\Omega)$ for solutions in the same space, *i.e.*, no additional regularity in the solution is required. The numerical experiments in this article show that the proposed method is practically higher-order than the previously proposed methods for approximating nonsmooth solutions in the energy space $H^1(\Omega) \times L^2(\Omega)$.

The following convergence results are proved in this article.

Theorem 1.1. *Let $f : \mathbb{R} \to \mathbb{R}$ be a given nonlinear function satisfying the following Lipschitz continuity condition (for some constants C_1):*

$$|f'(s)| \le C_1 \quad \text{and} \quad |f''(s)| \le C_1 \quad \text{for } s \in \mathbb{R}. \tag{1.5}$$

Then, for $d = 1, 2, 3$ and $(u^0, v^0) \in [H^{1+\frac{d}{4}}(\Omega) \cap H_0^1(\Omega)] \times H^{\frac{d}{4}}(\Omega)$, the numerical solution given by (1.3) has the following error bound:

$$\max_{0 \le n \le T/\tau} \Big(\|u^n - u(t_n)\|_{H^1(\Omega)} + \|v^n - \partial_t u(t_n)\|_{L^2(\Omega)} \Big) \le C_2 \tau^2, \tag{1.6}$$

where C_2 is some positive constant independent of the stepsize τ (but may depend on T).

Moreover, for $d = 1$ and $(u^0, v^0) \in H_0^1(\Omega) \times L^2(\Omega)$, the numerical solution given by (1.3) has the following error bound:

$$\max_{0 \le n \le T/\tau} \Big(\|u^n - u(t_n)\|_{H^1(\Omega)} + \|v^n - \partial_t u(t_n)\|_{L^2(\Omega)} \Big) \le C_3 \tau^{\frac{4}{3} - \epsilon}, \tag{1.7}$$

where $\epsilon \in (0, 1)$ is an arbitrary fixed small constant, and C_3 is some positive constant independent of the stepsize τ (but may depend on T).

Remark 1.2. The order of convergence in (1.7) is higher than 1 without requiring additional regularity in the solution. The error estimate in (1.5) shows that second-order convergence is achieved with a regularity condition weaker than $H^2(\Omega) \times H^1(\Omega)$. These results not only have theoretical value but also affect the accuracy in the practical computation, as reflected in the numerical experiments in Section 4, *i.e.*, the proposed time-stepping method is much more accurate (with higher-order convergence) than the other methods for approximating nonsmooth solutions of the semilinear Klein–Gordon equation.

Remark 1.3. The consistency errors of the numerical method actually only contain first-order partial derivatives of the solution, instead of $1+\frac{d}{4}$ order partial derivatives. The regularity condition $H^{1+\frac{d}{4}}(\Omega) \times H^{\frac{d}{4}}(\Omega)$ arises from the use of Sobolev embedding $H^{1+\frac{d}{4}}(\Omega) \hookrightarrow W^{1,4}(\Omega)$ in the error estimation. In the one-dimensional numerical experiments (see Fig. 1 in Sect. 4), we observe second-order convergence of the method for $H^1(\Omega) \times L^2(\Omega)$ initial data.

Remark 1.4. The Lipschitz continuity condition in (1.5) can be removed in the case $d = 1$, as the L^∞ bound of the numerical solution u^n can be proved by using its convergence in H^1. For $d = 2, 3$ this Lipschitz continuity condition is needed for a general nonlinear function $f(u)$, but is still possible to be removed for some special nonlinear functions such as $f(u) = u^3$. Since such analysis requires different treatments for different nonlinearities and $d = 1, 2, 3$ (see [35] for the excellent treatment of the case $f(u) = u^3$ in one dimension), we focus on the construction of the low-regularity integrator in the general case $d = 1, 2, 3$ with a general nonlinear function under the Lipschitz continuity condition.

The rest of this article is devoted to the construction of the method and the proof of the theorem. In Section 2 we construct the second-order low-regularity integrator by analyzing the consistency errors in approximating the semilinear Klein–Gordon equation. In Section 3 we present error estimates for a fully discrete spectral method with the time-stepping scheme in (1.3) (see Thm. 3.1 and Rem. 3.3), which imply Theorem 1.1 by passing to the limit $N \to \infty$, where N^d denotes the degrees of freedom in the spatial discretization. The numerical experiments are presented in Section 4 to show the favorable error behaviour of the new scheme for both nonsmooth and smooth initial data.

2. Construction of the low-regularity integrators

We rewrite the semilinear Klein–Gordon equation into the following first-order system, *i.e.*,

$$\begin{cases} \partial_t U - LU = F(U) & \text{in } \Omega \times (0,T], \\ U(t_n) = U^0 & \text{in } \Omega, \end{cases} \tag{2.1}$$

where

$$U = \begin{pmatrix} u \\ \partial_t u \end{pmatrix}, \quad U^0 = \begin{pmatrix} u^0 \\ v^0 \end{pmatrix} \quad \text{and} \quad F(U) = \begin{pmatrix} 0 \\ f(u) \end{pmatrix}, \tag{2.2}$$

and L is defined in (1.4). Under the Lipschitz continuity condition (1.5), it is well known that problem (2.1) has a unique energy solution $U \in L^\infty(0,T; H_0^1(\Omega) \times L^2(\Omega))$ satisfying the following variation-of-constants formula:

$$U(t+s) = \mathrm{e}^{sL} U(t) + \int_0^s \mathrm{e}^{(s-\sigma)L} F(U(t+\sigma))\,\mathrm{d}\sigma \quad \text{for } t, s \geq 0, \tag{2.3}$$

where e^{tL} is the continuous semigroup on $H_0^1(\Omega) \times L^2(\Omega)$ generated by the anti-symmetric partial differential operator L.

For the simplicity of notation, we denote by $A \lesssim B$ the statement "$A \leq CB$ for some constant C which is independent of the stepsize τ (or the degrees of freedom N in the case there is spatial discretization)".

For the error analysis we define the energy norm $|W|_1 = \left(\|\nabla w_1\|^2_{L^2(\Omega)} + \|w_2\|^2_{L^2(\Omega)}\right)^{\frac{1}{2}}$ and the following non-energy norms:

$$\begin{aligned} \|W\|_0 &= \left(\|w_1\|^2_{L^2(\Omega)} + \|w_2\|^2_{H^{-1}(\Omega)}\right)^{\frac{1}{2}}, \\ \|W\|_1 &= \left(\|w_1\|^2_{H^1(\Omega)} + \|w_2\|^2_{L^2(\Omega)}\right)^{\frac{1}{2}}, \\ \|W\|_2 &= \left(\|w_1\|^2_{H^2(\Omega)} + \|w_2\|^2_{H^1(\Omega)}\right)^{\frac{1}{2}}. \end{aligned}$$

It is known that the semigroup e^{tL} satisfies the energy conservation $|\mathrm{e}^{tL} W|_1 = |W|_1$ for $W \in H_0^1(\Omega) \times L^2(\Omega)$, and the following estimates:

$$\begin{aligned} &\|\mathrm{e}^{tL} W\|_0 \lesssim \|W\|_0 \quad \forall\, W \in L^2(\Omega) \times H^{-1}(\Omega), \\ &\|\mathrm{e}^{tL} W\|_1 \lesssim \|W\|_1 \quad \forall\, W \in H_0^1(\Omega) \times L^2(\Omega), \\ &\|\mathrm{e}^{tL} W\|_2 \lesssim \|W\|_2 \quad \forall\, W \in [H^2(\Omega) \cap H_0^1(\Omega)] \times L^2(\Omega). \end{aligned} \tag{2.4}$$

Moreover, the nonlinear function $F(U)$ defined in (2.2) satisfies the following estimate:

$$\|F(U)\|_1 \lesssim \|f(u)\|_{L^2} \lesssim \|U\|_0. \tag{2.5}$$

In the following two subsections, we study the consistency errors in approximating formula (2.3). We begin with a first-order approximation in the next subsection, which provides insights for us for the construction of the second-order low-regularity integrator.

2.1. First-order approximation

Let $t_n = n\tau$, $n = 0, 1, \ldots, [T/\tau]$, be a sequence of discrete time levels with stepsize τ, and consider the variation-of-constant formula:

$$U(t_n+s) = \mathrm{e}^{sL} U(t_n) + \int_0^s \mathrm{e}^{(s-\sigma)L} F(U(t_n+\sigma))\,\mathrm{d}\sigma \quad \text{for } s \in [0,\tau], \tag{2.6}$$

which implies that

$$U(t_{n+1}) = \mathrm{e}^{\tau L}U(t_n) + \int_0^\tau \mathrm{e}^{(\tau-s)L}F(U(t_n+s))\,\mathrm{d}s. \tag{2.7}$$

Substituting (2.6) into the right-hand side of (2.7) yields

$$U(t_{n+1}) = \mathrm{e}^{\tau L}U(t_n) + \int_0^\tau \mathrm{e}^{(\tau-s)L}F\big(\mathrm{e}^{sL}U(t_n)\big)\,\mathrm{d}s + R_1(t_n), \tag{2.8}$$

where the remainder $R_1(t_n)$ is given by

$$R_1(t_n) = \int_0^\tau \mathrm{e}^{(\tau-s)L}\big[F(U(t_n+s)) - F\big(\mathrm{e}^{sL}U(t_n)\big)\big]\,\mathrm{d}s. \tag{2.9}$$

For the simplicity of notation, we denote by $\tilde{u}(t_n+s)$ and $\tilde{v}(t_n+s)$ the two functions defined by

$$\begin{pmatrix} \tilde{u}(t_n+s) \\ \tilde{v}(t_n+s) \end{pmatrix} = \mathrm{e}^{sL}\begin{pmatrix} u(t_n) \\ \partial_t u(t_n) \end{pmatrix} = \mathrm{e}^{sL}U(t_n).$$

Then the remainder $R_1(t_n)$ defined in (2.9) satisfies the following estimate in view of (2.6):

$$\begin{aligned}
\|R_1(t_n)\|_1 &\lesssim \int_0^\tau \big\|F(U(t_n+s)) - F\big(\mathrm{e}^{sL}U(t_n)\big)\big\|_1\,\mathrm{d}s \\
&= \int_0^\tau \|f(u(t_n+s)) - f(\tilde{u}(t_n+s))\|_{L^2(\Omega)}\,\mathrm{d}s \\
&\lesssim \int_0^\tau \|u(t_n+s) - \tilde{u}(t_n+s)\|_{L^2(\Omega)}\,\mathrm{d}s \\
&\lesssim \int_0^\tau \big\|U(t_n+s) - \mathrm{e}^{sL}U(t_n)\big\|_0\,\mathrm{d}s \\
&\lesssim \int_0^\tau \int_0^s \Big\|\mathrm{e}^{(s-\sigma)L}F(U(t_n+\sigma))\Big\|_0\,\mathrm{d}\sigma\,\mathrm{d}s \\
&\lesssim \int_0^\tau \int_0^s \|F(U(t_n+\sigma))\|_0\,\mathrm{d}\sigma\,\mathrm{d}s \\
&\lesssim \tau^2 \max_{\sigma\in[0,\tau]} \|f(u(t_n+\sigma))\|_{H^{-1}}.
\end{aligned}$$

Since $H_0^1(\Omega) \hookrightarrow L^6(\Omega)$, it follows that $L^{\frac{6}{5}}(\Omega) = L^6(\Omega)' \hookrightarrow H_0^1(\Omega)' = H^{-1}(\Omega)$ and therefore

$$\begin{aligned}
\|f(u(t_n+\sigma))\|_{H^{-1}} &\le \|f(u(t_n+\sigma))\|_{L^{6/5}} \\
&\le \|f(u(t_n+\sigma))\|_{L^2} \\
&\le \|f(0)\|_{L^2} + \|f(u(t_n+\sigma)) - f(0)\|_{L^2} \\
&\le \|f(0)\|_{L^2} + \|u(t_n+\sigma)\|_{L^2} \\
&\le \|f(0)\|_{L^2} + \|U(t_n+\sigma)\|_0.
\end{aligned}$$

The two estimates above imply the following estimate for the remainder $R_1(t_n)$:

$$\|R_1(t_n)\|_1 \lesssim \tau^2\Big(1 + \max_{\sigma\in[t_n,t_{n+1}]} \|U(t)\|_0\Big). \tag{2.10}$$

Freezing the variable s at 0 in (2.8) would yield

$$U(t_{n+1}) = \mathrm{e}^{\tau L}U(t_n) + \tau \mathrm{e}^{\tau L}F(U(t_n)) + R_1(t_n) + R_2(t_n), \tag{2.11}$$

with an additional remainder

$$\begin{aligned} R_2(t_n) &= \int_0^\tau \mathrm{e}^{\tau L}[\mathrm{e}^{-sL}F\big(\mathrm{e}^{sL}U(t_n)\big) - F(U(t_n))]\,\mathrm{d}s \\ &= \int_0^\tau \mathrm{e}^{\tau L}\int_0^s \frac{\mathrm{d}}{\mathrm{d}\sigma}\mathrm{e}^{-\sigma L}F\big(\mathrm{e}^{\sigma L}U(t_n)\big)\,\mathrm{d}\sigma\,\mathrm{d}s. \end{aligned} \tag{2.12}$$

By using the chain rule of differentiation, it is straightforward to verify that

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}\sigma}\mathrm{e}^{-\sigma L}F\big(\mathrm{e}^{\sigma L}U(t_n)\big) &= \frac{\mathrm{d}}{\mathrm{d}\sigma}\mathrm{e}^{-\sigma L}F\big(\mathrm{e}^{\sigma L}U(t_n)\big) \\ &= -\mathrm{e}^{-\sigma L}LF\big(\mathrm{e}^{\sigma L}U(t_n)\big) + \mathrm{e}^{-\sigma L}F'\big(\mathrm{e}^{\sigma L}U(t_n)\big)\mathrm{e}^{\sigma L}LU(t_n) \\ &= -\mathrm{e}^{-\sigma L}\begin{pmatrix} 0 & 1 \\ \Delta & 0 \end{pmatrix}\begin{pmatrix} 0 \\ f(\tilde{u}(t_n+\sigma)) \end{pmatrix} + \mathrm{e}^{-\sigma L}\begin{pmatrix} 0 & 0 \\ f'(\tilde{u}(t_n+\sigma)) & 0 \end{pmatrix}\left[\begin{pmatrix} 0 & 1 \\ \Delta & 0 \end{pmatrix}\mathrm{e}^{\sigma L}\begin{pmatrix} u(t_n) \\ \partial_t u(t_n) \end{pmatrix}\right] \\ &= -\mathrm{e}^{-\sigma L}\begin{pmatrix} 0 & 1 \\ \Delta & 0 \end{pmatrix}\begin{pmatrix} 0 \\ f(\tilde{u}(t_n+\sigma)) \end{pmatrix} + \mathrm{e}^{-\sigma L}\begin{pmatrix} 0 & 0 \\ f'(\tilde{u}(t_n+\sigma)) & 0 \end{pmatrix}\begin{pmatrix} \tilde{v}(t_n+\sigma) \\ \Delta\tilde{u}(t_n+\sigma) \end{pmatrix} \\ &= \mathrm{e}^{-\sigma L}\begin{pmatrix} -f(\tilde{u}(t_n+\sigma)) \\ f'(\tilde{u}(t_n+\sigma))\tilde{v}(t_n+\sigma) \end{pmatrix}. \end{aligned} \tag{2.13}$$

Therefore,

$$\begin{aligned} \left\| \frac{\mathrm{d}}{\mathrm{d}\sigma}\mathrm{e}^{-\sigma L}F\big(\mathrm{e}^{\sigma L}U(t_n)\big)\right\|_1 &\lesssim \left\| \begin{pmatrix} -f(\tilde{u}(t_n+\sigma)) \\ f'(\tilde{u}(t_n+\sigma))\tilde{v}(t_n+\sigma) \end{pmatrix}\right\|_1 \\ &\lesssim (1 + \|\tilde{u}(t_n+\sigma)\|_{H^1(\Omega)}) + \|\tilde{v}(t_n+\sigma)\|_{L^2(\Omega)} \\ &\lesssim 1 + \|U(t_n)\|_1. \end{aligned} \tag{2.14}$$

By utilizing this result, from (2.12) we obtain

$$\|R_2(t_n)\| \lesssim \tau^2(1 + \|U(t_n)\|_1). \tag{2.15}$$

By dropping the remainders R_1 and R_2 in (2.11), we obtain the following time-stepping method:

$$U^{n+1} = \mathrm{e}^{\tau L}U^n + \tau\mathrm{e}^{\tau L}F(U^n). \tag{2.16}$$

In view of the two estimates (2.10) and (2.15), the method in (2.16) should have first-order convergence in the energy space $H_0^1(\Omega)\times L^2(\Omega)$ under the regularity condition

$$U \in L^\infty\big(0,T; H_0^1(\Omega)\times L^2(\Omega)\big).$$

This is the same regularity condition in [11, 18, 34] for first-order convergence in the energy space. This condition is required in (2.14) in estimating the remainder $R_2(t_n)$, which involves $\frac{\mathrm{d}}{\mathrm{d}\sigma}\mathrm{e}^{-\sigma L}F\big(\mathrm{e}^{\sigma L}U(t_n)\big)$.

From the analysis above we can see that, in order to have higher-order convergence in the energy space, higher-order approximations of $F(U(t_n+s))$ should be used in approximating (2.7). This is considered in the next subsection.

In the construction of a second-order method, the remainder which involves the term $\frac{\mathrm{d}}{\mathrm{d}\sigma}\mathrm{e}^{-\sigma L}F\big(\mathrm{e}^{\sigma L}U(t_n)\big)$ will require the solution to be in $H^2(\Omega)\times H^1(\Omega)$. We shall construct a second-order approximation by eliminating this part of the remainder, thus significantly improves the order of convergence without requiring additional regularity of the solution.

2.2. Second-order approximation

By using the Taylor expansion of $F(U)$ at $U = \mathrm{e}^{sL}U(t_n)$, we have

$$\begin{aligned} F(U(t_n+s)) &= F\big(\mathrm{e}^{sL}U(t_n)\big) + \int_0^1 F'\big((1-\theta)\mathrm{e}^{sL}U(t_n) + \theta U(t_n+s)\big)\big(U(t_n+s) - \mathrm{e}^{sL}U(t_n)\big)\,\mathrm{d}\theta \\ &= F\big(\mathrm{e}^{sL}U(t_n)\big) + F'\big(\mathrm{e}^{sL}U(t_n)\big)(U(t_n+s) - \mathrm{e}^{sL}U(t_n)) \\ &\quad + R_F(s)(U(t_n+s) - \mathrm{e}^{sL}U(t_n)) \cdot (U(t_n+s) - \mathrm{e}^{sL}U(t_n)) \end{aligned} \tag{2.17}$$

where

$$R_F(s) = \int_0^1 \int_0^1 \theta F''[(1-\sigma)\mathrm{e}^{sL}U(t_n) + \sigma(1-\theta)\mathrm{e}^{sL}U(t_n) + \theta U(t_n+s)]\,\mathrm{d}\sigma\,\mathrm{d}\theta.$$

Then, substituting (2.6) into (2.17), we have

$$F(U(t_n+s)) = F\big(\mathrm{e}^{sL}U(t_n)\big) + F'\big(\mathrm{e}^{sL}U(t_n)\big)\int_0^s \mathrm{e}^{(s-\sigma)L}F(U(t_n+\sigma))\,\mathrm{d}\sigma + \widetilde{R}_3(s), \tag{2.18}$$

where

$$\widetilde{R}_3(s) = R_F(s)\int_0^s \mathrm{e}^{(s-\sigma)L}F(U(t_n+\sigma))\,\mathrm{d}\sigma \cdot \int_0^s \mathrm{e}^{(s-\sigma)L}F(U(t_n+\sigma))\,\mathrm{d}\sigma.$$

Since $F(U) = (F_1(U), F_2(U))^\top$ is vector-valued, with $F_1(U) = 0$ and $F_2(U) = f(u)$, it follows that $F''(U)$ is tensor-valued and satisfying $F''_{ijk}(U) = \partial_{U_k}\partial_{U_j}F_i(U)$, where $U_1 = u$ and $U_2 = v$. In particular, $F''_{211}(U) = f''(u)$ and $F''_{ijk}(U) = 0$ for $(i,j,k) \neq (2,1,1)$. Therefore, for $W = (w_1, w_2)^\top$ and $W^* = (w_1^*, w_2^*)^\top$,

$$\|R_F(s)W \cdot W^*\|_1 \le \|f''(u)w_1w_1^*\|_{L^2} \lesssim \|w_1\|_{L^4}\|w_1^*\|_{L^4} \lesssim \|W\|_1\|W^*\|_1,$$

which implies the following estimate:

$$\begin{aligned} \|\widetilde{R}_3(s)\|_1 &\lesssim \left\| \int_0^s \mathrm{e}^{(s-\sigma)L}F(U(t_n+\sigma))\,\mathrm{d}\sigma \right\|_1^2 \\ &\lesssim \left| \int_0^s \|F(U(t_n+\sigma))\|_1 \mathrm{d}\sigma \right|^2 \\ &\lesssim \left| \int_0^s \|f(u(t_n+\sigma))\|_{L^2} \mathrm{d}\sigma \right|^2 \\ &\lesssim \tau^2\Big(1 + \max_{\sigma\in[0,s]} \|u(t_n+\sigma)\|_{L^2}^2\Big) \\ &\lesssim \tau^2\Big(1 + \max_{\sigma\in[0,\tau]} \|U(t_n+\sigma)\|_0\Big). \end{aligned} \tag{2.19}$$

By substituting (2.18) into (2.7), we obtain

$$\begin{aligned} U(t_{n+1}) &= \mathrm{e}^{\tau L}U(t_n) + \int_0^\tau \mathrm{e}^{(\tau-s)L}F(U(t_n+s))\,\mathrm{d}s \\ &= \mathrm{e}^{\tau L}U(t_n) + \int_0^\tau \mathrm{e}^{(\tau-s)L}F\big(\mathrm{e}^{sL}U(t_n)\big)\,\mathrm{d}s \\ &\quad + \int_0^\tau \mathrm{e}^{(\tau-s)L}\left[F'\big(\mathrm{e}^{sL}U(t_n)\big)\int_0^s \mathrm{e}^{(s-\sigma)L}F(U(t_n+\sigma))\,\mathrm{d}\sigma\right]\mathrm{d}s + R_3(t_n) \\ &=: \mathrm{e}^{\tau L}U(t_n) + I_1(t_n) + I_2(t_n) + R_3(t_n), \end{aligned} \tag{2.20}$$

with a remainder

$$R_3(t_n) = \int_0^\tau \mathrm{e}^{(\tau-s)L} \widetilde{R}_3(s)\,\mathrm{d}s.$$

The estimate in (2.19) implies the following result:

$$\|R_3(t_n)\|_1 \lesssim \tau^3 \Big(1 + \max_{t\in[t_n,t_{n+1}]} \|U(t)\|_0^2\Big). \tag{2.21}$$

The two terms $I_1(t_n)$ and $I_2(t_n)$ will be approximated by computable schemes as follows.

Part 1: Approximation to $I_1(t_n)$.

The key ingredient that significantly improves the accuracy of the numerical method is the discovery of a cancellation structure which allows us to compute $I_1(t_n)$ exactly.

We write $I_1(t_n) = \int_0^\tau \mathrm{e}^{\tau L} G(t_n+s)\,\mathrm{d}s$, with $G(t_n+s) = \mathrm{e}^{-sL} F\big(\mathrm{e}^{sL} U(t_n)\big)$, and substitute the Newton–Leibniz formula

$$G(t_n+s) = G(t_n) + \int_0^s G'(t_n+\sigma)\,\mathrm{d}\sigma \tag{2.22}$$

into the expression of $I_1(t_n)$. Then we obtain

$$\begin{aligned}
I_1(t_n) &= \int_0^\tau \mathrm{e}^{\tau L} G(t_n+s)\,\mathrm{d}s \\
&= \int_0^\tau \mathrm{e}^{\tau L} G(t_n)\,\mathrm{d}s + \int_0^\tau \mathrm{e}^{\tau L} \int_0^s G'(t_n+\sigma)\,\mathrm{d}\sigma\,\mathrm{d}s \\
&= \int_0^\tau \mathrm{e}^{\tau L} G(t_n)\,\mathrm{d}s + \int_0^\tau \mathrm{e}^{\tau L} G'(t_n+\sigma)(\tau-\sigma)\,\mathrm{d}\sigma \\
&= \int_0^\tau \mathrm{e}^{\tau L} G(t_n)\,\mathrm{d}s + \int_0^\tau \mathrm{e}^{(\tau-2s)L}(\tau-s)\mathrm{e}^{2sL} G'(t_n+s)\,\mathrm{d}s \\
&= \int_0^\tau \mathrm{e}^{\tau L} G(t_n)\,\mathrm{d}s + \int_0^\tau \mathrm{e}^{(\tau-2s)L}(\tau-s) G'(t_n)\,\mathrm{d}s \\
&\quad + \int_0^\tau \mathrm{e}^{(\tau-2s)L}(\tau-s) \int_0^s \frac{\mathrm{d}}{\mathrm{d}\sigma}\big[\mathrm{e}^{2\sigma L} G'(t_n+\sigma)\big]\,\mathrm{d}\sigma\,\mathrm{d}s \\
&= \tau \mathrm{e}^{\tau L} F(U(t_n)) + (2L)^{-1}\big[\tau \mathrm{e}^{\tau L} - (2L)^{-1}\big(\mathrm{e}^{\tau L} - \mathrm{e}^{-\tau L}\big)\big] \begin{pmatrix} -f(u(t_n)) \\ f'(u(t_n))\partial_t u(t_n) \end{pmatrix} \\
&\quad + R_*(t_n),
\end{aligned} \tag{2.23}$$

where we have used the expression of $G'(t_n+s)$ in (2.13), and the remainder $R_*(t_n)$ is defined by

$$R_*(t_n) = \int_0^\tau \mathrm{e}^{(\tau-2s)L}(\tau-s) \int_0^s \frac{\mathrm{d}}{\mathrm{d}\sigma}\big[\mathrm{e}^{2\sigma L} G'(t_n+\sigma)\big]\,\mathrm{d}\sigma\,\mathrm{d}s. \tag{2.24}$$

By differentiating $\mathrm{e}^{2sL} G'(t_n+s)$ and using the expression of $G'(t_n+s)$ in (2.13), we also obtain

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}s}\big[\mathrm{e}^{2sL} G'(t_n+s)\big] &= \frac{\mathrm{d}}{\mathrm{d}s}\left[\mathrm{e}^{sL} \begin{pmatrix} -f(\tilde{u}(t_n+s)) \\ f'(\tilde{u}(t_n+s))\tilde{v}(t_n+s) \end{pmatrix}\right] \\
&= \left(\frac{\mathrm{d}}{\mathrm{d}s}\mathrm{e}^{sL}\right) \begin{pmatrix} -f(\tilde{u}(t_n+s)) \\ f'(\tilde{u}(t_n+s))\tilde{v}(t_n+s) \end{pmatrix} + \mathrm{e}^{sL} \frac{\mathrm{d}}{\mathrm{d}s} \begin{pmatrix} -f(\tilde{u}(t_n+s)) \\ f'(\tilde{u}(t_n+s))\tilde{v}(t_n+s) \end{pmatrix} \\
&= \mathrm{e}^{sL} \begin{pmatrix} 0 & 1 \\ \Delta & 0 \end{pmatrix} \begin{pmatrix} -f(\tilde{u}(t_n+s)) \\ f'(\tilde{u}(t_n+s))\tilde{v}(t_n+s) \end{pmatrix}
\end{aligned}$$

$$+ \mathrm{e}^{sL} \begin{pmatrix} -f'(\tilde{u}(t_n+s)) & 0 \\ f''(\tilde{u}(t_n+s))\tilde{v}(t_n+s) & f'(\tilde{u}(t_n+s)) \end{pmatrix} \left[\begin{pmatrix} 0 & 1 \\ \Delta & 0 \end{pmatrix} \begin{pmatrix} \tilde{u}(t_n+s) \\ \tilde{v}(t_n+s) \end{pmatrix} \right], \tag{2.25}$$

where we have used the following properties in the derivation of the last equality:

$$\begin{aligned} &\frac{\mathrm{d}}{\mathrm{d}s} \begin{pmatrix} g_1(\tilde{u}(t_n+s), \tilde{v}(t_n+s)) \\ g_2(\tilde{u}(t_n+s), \tilde{v}(t_n+s)) \end{pmatrix} \\ &\quad = \begin{pmatrix} \partial_{\tilde{u}} g_1(\tilde{u}(t_n+s), \tilde{v}(t_n+s)) & \partial_{\tilde{v}} g_1(\tilde{u}(t_n+s), \tilde{v}(t_n+s)) \\ \partial_{\tilde{u}} g_2(\tilde{u}(t_n+s), \tilde{v}(t_n+s)) & \partial_{\tilde{v}} g_2(\tilde{u}(t_n+s), \tilde{v}(t_n+s)) \end{pmatrix} \frac{\mathrm{d}}{\mathrm{d}s} \begin{pmatrix} \tilde{u}(t_n+s) \\ \tilde{v}(t_n+s) \end{pmatrix} \end{aligned}$$

and

$$\frac{\mathrm{d}}{\mathrm{d}s} \begin{pmatrix} \tilde{u}(t_n+s) \\ \tilde{v}(t_n+s) \end{pmatrix} = \frac{\mathrm{d}}{\mathrm{d}s} \left[\mathrm{e}^{sL} \begin{pmatrix} u(t_n) \\ v(t_n) \end{pmatrix} \right] = L\mathrm{e}^{sL} \begin{pmatrix} u(t_n) \\ v(t_n) \end{pmatrix} = L \begin{pmatrix} \tilde{u}(t_n+s) \\ \tilde{v}(t_n+s) \end{pmatrix}.$$

By summing up the two parts on the right-hand side of (2.25) and noting that the second-order partial derivatives are all cancelled, we obtain the following identity:

$$\frac{\mathrm{d}}{\mathrm{d}s} \left[\mathrm{e}^{2sL} G'(t_n+s) \right] = \mathrm{e}^{sL} \left(\begin{array}{c} 0 \\ f''(\tilde{u}(t_n+s)) \Big(|\tilde{v}(t_n+s)|^2 - |\nabla \tilde{u}(t_n+s)|^2 \Big) \end{array} \right). \tag{2.26}$$

This cancellation structure in the semlinear Klein–Gordon equation has not been discovered before for a general nonlinearity $f(u)$. It allows us to compute $I_1(t_n)$ without requiring the second-order partial derivatives and therefore improves the accuracy of the numerical approximation for low-regularity solutions. As a result, the remainder can be estimated as follows:

$$\begin{aligned} \|R_*(t_n)\|_1 &\lesssim \tau^3 \max_{s\in[0,\tau]} \left(\|\nabla \tilde{u}(t_n+s)\|_{L^4}^2 + \|\tilde{v}(t_n+s)\|_{L^4}^2 \right) \\ &\lesssim \tau^3 \max_{s\in[0,\tau]} \Big(\|\tilde{u}(t_n+s)\|_{H^{1+\frac{d}{4}}}^2 + \|\tilde{v}(t_n+s)\|_{H^{\frac{d}{4}}}^2 \Big) \\ &\lesssim \tau^3 \|U(t_n)\|_{1+\frac{d}{4}}^2. \end{aligned} \tag{2.27}$$

In the case $d = 1$, the following result holds:

$$\begin{aligned} \|R_*(t_n)\|_{\frac{1}{2}-\epsilon} &\lesssim \tau^3 \max_{s\in[0,\tau]} \Big(\Big\| |\nabla \tilde{u}(t_n+s)|^2 \Big\|_{H^{-\frac{1}{2}-\epsilon}} + \Big\| |\tilde{v}(t_n+s)|^2 \Big\|_{H^{-\frac{1}{2}-\epsilon}} \Big) \\ &\lesssim \tau^3 \max_{s\in[0,\tau]} \Big(\Big\| |\nabla \tilde{u}(t_n+s)|^2 \Big\|_{L^1} + \Big\| |\tilde{v}(t_n+s)|^2 \Big\|_{L^1} \Big) \quad (\text{as } L^1 \hookrightarrow H^{-\frac{1}{2}-\epsilon} \text{ in 1D}) \\ &\lesssim \tau^3 \max_{s\in[0,\tau]} \Big(\|\nabla \tilde{u}(t_n+s)\|_{L^2}^2 + \|\tilde{v}(t_n+s)\|_{L^2}^2 \Big) \\ &\lesssim \tau^3 \|U(t_n)\|_1^2. \end{aligned} \tag{2.28}$$

By the definition of $R_*(t_n)$ in (2.23) and the triangle inequality, we also obtain

$$\begin{aligned} \|R_*(t_n)\|_2 &\lesssim \left\| \int_0^\tau \mathrm{e}^{\tau L} G(t_n+s)\, \mathrm{d}s \right\|_2 \\ &\quad + \left\| \tau \mathrm{e}^{\tau L} F(U(t_n)) + (2L)^{-1} \left[\tau \mathrm{e}^{\tau L} - (2L)^{-1} \big(\mathrm{e}^{\tau L} - \mathrm{e}^{-\tau L} \big) \right] \begin{pmatrix} -f(u(t_n)) \\ f'(u(t_n)) \partial_t u(t_n) \end{pmatrix} \right\|_2 \\ &\lesssim \tau \|U(t_n)\|_1. \end{aligned} \tag{2.29}$$

Therefore, the Sobolev interpolation inequality implies that

$$\begin{aligned} \|R_*(t_n)\|_1 &\lesssim \|R_*(t_n)\|_{\frac{1}{2}-\epsilon}^{\frac{1}{3/2+\epsilon}} \|R_*(t_n)\|_2^{\frac{1/2+\epsilon}{3/2+\epsilon}} \lesssim \tau^{\frac{7/2+\epsilon}{3/2+\epsilon}} \big(\|U(t_n)\|_1 + \|U(t_n)\|_1^2 \big), \\ \|R_*(t_n)\|_{\frac{1}{2}+\epsilon} &\lesssim \|R_*(t_n)\|_{\frac{1}{2}-\epsilon}^{\frac{3/2-\epsilon}{3/2+\epsilon}} \|R_*(t_n)\|_2^{\frac{2\epsilon}{3/2+\epsilon}} \lesssim \tau^{\frac{9/2-\epsilon}{3/2+\epsilon}} \big(\|U(t_n)\|_1 + \|U(t_n)\|_1^2 \big). \end{aligned} \tag{2.30}$$

Part 2: Approximation to $I_2(t)$

By approximating $U(t_n+\sigma)$ with $\mathrm{e}^{\sigma L}U(t_n)$ in the expression of $I_2(t_n)$ in (2.20), we have

$$\begin{aligned} I_2(t_n) &= \int_0^\tau \mathrm{e}^{(\tau-s)L}\left[F'\big(\mathrm{e}^{sL}U(t_n)\big)\int_0^s \mathrm{e}^{(s-\sigma)L}F(U(t_n+\sigma))\,\mathrm{d}\sigma\right]\mathrm{d}s \\ &= \int_0^\tau \mathrm{e}^{(\tau-s)L}\left[F'\big(\mathrm{e}^{sL}U(t_n)\big)\int_0^s \mathrm{e}^{(s-\sigma)L}F\big(\mathrm{e}^{\sigma L}U(t_n)\big)\,\mathrm{d}\sigma\right]\mathrm{d}s + R_{41}(t_n) \\ &= \int_0^\tau \mathrm{e}^{(\tau-s)L}\big[F'\big(\mathrm{e}^{sL}U(t_n)\big)s\mathrm{e}^{sL}F(U(t_n))\big]\,\mathrm{d}s + R_{41}(t_n) + R_{42}(t_n) \\ &= \int_0^\tau s\mathrm{e}^{\tau L}\big[F'(U(t_n))F(U(t_n))\big]\,\mathrm{d}s + R_{41}(t_n) + R_{42}(t_n) + R_{43}(t_n) \\ &= R_{41}(t_n) + R_{42}(t_n) + R_{43}(t_n), \end{aligned} \tag{2.31}$$

where the last equality uses the property

$$F'(U(t_n))F(U(t_n)) = \begin{pmatrix} 0 & 0 \\ f'(u) & 0 \end{pmatrix}\begin{pmatrix} 0 \\ f(u) \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix},$$

and the remainders $R_{4j}(t_n)$, $j=1,2,3$, are defined by

$$R_{41}(t_n) = \int_0^\tau \mathrm{e}^{(\tau-s)L}\left[F'\big(\mathrm{e}^{sL}U(t_n)\big)\int_0^s \mathrm{e}^{(s-\sigma)L}[F(U(t_n+\sigma)) - F\big(\mathrm{e}^{\sigma L}U(t_n)\big)]\mathrm{d}\sigma\right]\mathrm{d}s, \tag{2.32}$$

$$R_{42}(t_n) = \int_0^\tau \mathrm{e}^{(\tau-s)L}\left[F'\big(\mathrm{e}^{sL}U(t_n)\big)\int_0^s \Big(\mathrm{e}^{(s-\sigma)L}F\big(\mathrm{e}^{\sigma L}U(t_n)\big) - \mathrm{e}^{sL}F(U(t_n))\Big)\,\mathrm{d}\sigma\right]\mathrm{d}s, \tag{2.33}$$

$$R_{43}(t_n) = \int_0^\tau s\mathrm{e}^{\tau L}\Big(\mathrm{e}^{-sL}\big[F'\big(\mathrm{e}^{sL}U(t_n)\big)\mathrm{e}^{sL}F(U(t_n))\big] - F'(U(t_n))F(U(t_n))\Big)\,\mathrm{d}s. \tag{2.34}$$

The three remainders $R_{41}(t_n)$, $R_{42}(t_n)$ and $R_{43}(t_n)$ are estimated as follows.

Firstly,

$$\begin{aligned} \|R_{41}(t_n)\|_1 &\lesssim \int_0^\tau \left\|F'\big(\mathrm{e}^{sL}U(t_n)\big)\int_0^s \mathrm{e}^{(s-\sigma)L}\big[F(U(t_n+\sigma)) - F\big(\mathrm{e}^{\sigma L}U(t_n)\big)\big]\mathrm{d}\sigma\right\|_1 \mathrm{d}s \\ &\lesssim \int_0^\tau \left\|\int_0^s \mathrm{e}^{(s-\sigma)L}\big[F(U(t_n+\sigma)) - F\big(\mathrm{e}^{\sigma L}U(t_n)\big)\big]\mathrm{d}\sigma\right\|_0 \mathrm{d}s \\ &\lesssim \tau^2 \max_{\sigma\in[0,\tau]}\big\|U(t_n+\sigma)) - \mathrm{e}^{\sigma L}U(t_n)\big\|_0. \end{aligned} \tag{2.35}$$

By using (2.6) we obtain that

$$\big\|U(t_n+s)) - (\mathrm{e}^{sL}U(t_n))\big\|_0 \lesssim s \max_{\sigma\in[0,s]}\|U(t_n+\sigma)\|_0. \tag{2.36}$$

Then, substituting this result into the estimate of $\|R_{41}(t_n)\|_1$, we obtain

$$\|R_{41}(t_n)\|_1 \lesssim \tau^3 \max_{t\in[t_n,t_{n+1}]}\|U(t)\|_0. \tag{2.37}$$

Secondly, substituting the identity

$$\mathrm{e}^{(s-\sigma)L}F\big(\mathrm{e}^{\sigma L}U(t_n)\big) - \mathrm{e}^{sL}F(U(t_n)) = \mathrm{e}^{sL}\int_0^\sigma \frac{\mathrm{d}}{\mathrm{d}\rho}\mathrm{e}^{-\rho L}F\big(\mathrm{e}^{\rho L}U(t_n)\big)\,\mathrm{d}\rho$$

into the expression of $R_{42}(t_n)$ yields

$$R_{42}(t_n) = \int_0^\tau \mathrm{e}^{(\tau-s)L}\Big[F'\big(\mathrm{e}^{sL}U(t_n)\big)\int_0^s \mathrm{e}^{sL}\int_0^\sigma \frac{\mathrm{d}}{\mathrm{d}\rho}\mathrm{e}^{-\rho L}F\big(\mathrm{e}^{\rho L}U(t_n)\big)\,\mathrm{d}\rho\,\mathrm{d}\sigma\Big]\,\mathrm{d}s. \tag{2.38}$$

From this expression we immediately obtain

$$\begin{aligned}\|R_{42}(t_n)\|_1 &\lesssim \int_0^\tau \Big\|F'\big(\mathrm{e}^{sL}U(t_n)\big)\int_0^s \mathrm{e}^{sL}\int_0^\sigma \frac{\mathrm{d}}{\mathrm{d}\rho}\mathrm{e}^{-\rho L}F\big(\mathrm{e}^{\rho L}U(t_n)\big)\,\mathrm{d}\rho\,\mathrm{d}\sigma\Big\|_1\,\mathrm{d}s\\
&\lesssim \int_0^\tau \Big\|\int_0^s \mathrm{e}^{sL}\int_0^\sigma \frac{\mathrm{d}}{\mathrm{d}\rho}\mathrm{e}^{-\rho L}F\big(\mathrm{e}^{\rho L}U(t_n)\big)\,\mathrm{d}\rho\,\mathrm{d}\sigma\Big\|_0\,\mathrm{d}s\\
&\lesssim \int_0^\tau\int_0^s\int_0^\sigma \Big\|\frac{\mathrm{d}}{\mathrm{d}\rho}\mathrm{e}^{-\rho L}F\big(\mathrm{e}^{\rho L}U(t_n)\big)\Big\|_0\,\mathrm{d}\rho\,\mathrm{d}\sigma\,\mathrm{d}s\\
&\lesssim \tau^3\|U(t_n)\|_1,\end{aligned} \tag{2.39}$$

where we have used (2.14) in the last inequality.

Thirdly, we have

$$\begin{aligned}\|R_{43}(t_n)\|_1 &= \Big\|\int_0^\tau s\mathrm{e}^{\tau L}\int_0^s \frac{\mathrm{d}}{\mathrm{d}\sigma}\mathrm{e}^{-\sigma L}\big[F'\big(\mathrm{e}^{\sigma L}U(t_n)\big)\mathrm{e}^{\sigma L}F(U(t_n))\big]\,\mathrm{d}\sigma\,\mathrm{d}s\Big\|_1\\
&\lesssim \int_0^\tau s\int_0^s \Big\|\frac{\mathrm{d}}{\mathrm{d}\sigma}\mathrm{e}^{-\sigma L}\big[F'\big(\mathrm{e}^{\sigma L}U(t_n)\big)\mathrm{e}^{\sigma L}F(U(t_n))\big]\Big\|_1\,\mathrm{d}\sigma\,\mathrm{d}s\\
&\lesssim \tau^3\max_{\sigma\in[0,\tau]}\Big\|\frac{\mathrm{d}}{\mathrm{d}\sigma}\mathrm{e}^{-\sigma L}\big[F'\big(\mathrm{e}^{\sigma L}U(t_n)\big)\mathrm{e}^{\sigma L}F(U(t_n))\big]\Big\|_1.\end{aligned} \tag{2.40}$$

Let

$$\begin{pmatrix}\tilde p(t_n+\sigma)\\ \tilde q(t_n+\sigma)\end{pmatrix} = \mathrm{e}^{\sigma L}F(U(t_n)) = \mathrm{e}^{\sigma L}\begin{pmatrix}0\\ f(u(t_n))\end{pmatrix}$$

which satisfies the following estimate according to the basic estimates in (2.4):

$$\|\tilde p(t_n+\sigma)\|_{H^k(\Omega)} + \|\tilde q(t_n+\sigma)\|_{H^{k-1}(\Omega)} \lesssim \|f(u(t_n))\|_{H^{k-1}(\Omega)} \quad \text{for } k=1,2. \tag{2.41}$$

Then

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}\sigma}F'\big(\mathrm{e}^{\sigma L}U(t_n)\big)\mathrm{e}^{\sigma L}F(U(t_n)) &= \frac{\mathrm{d}}{\mathrm{d}\sigma}\left[\begin{pmatrix}0 & 0\\ f'(\tilde u(t_n+\sigma)) & 0\end{pmatrix}\begin{pmatrix}\tilde p(t_n+\sigma)\\ \tilde q(t_n+\sigma)\end{pmatrix}\right]\\
&= \frac{\mathrm{d}}{\mathrm{d}\sigma}\begin{pmatrix}0\\ f'(\tilde u(t_n+\sigma))\tilde p(t_n+\sigma)\end{pmatrix}\\
&= \begin{pmatrix}0 & 0\\ f''(\tilde u(t_n+\sigma))\tilde p(t_n+\sigma) & 0\end{pmatrix}\left[\begin{pmatrix}0 & 1\\ \Delta & 0\end{pmatrix}\begin{pmatrix}\tilde u(t_n+\sigma)\\ \tilde v(t_n+\sigma)\end{pmatrix}\right]\\
&\quad + \begin{pmatrix}0 & 0\\ f'(\tilde u(t_n+\sigma)) & 0\end{pmatrix}\left[\begin{pmatrix}0 & 1\\ \Delta & 0\end{pmatrix}\begin{pmatrix}\tilde p(t_n+\sigma)\\ \tilde q(t_n+\sigma)\end{pmatrix}\right]\\
&= \begin{pmatrix}0\\ f''(\tilde u(t_n+\sigma))\tilde p(t_n+\sigma)\tilde v(t_n+\sigma) + f'(\tilde u(t_n+\sigma))\tilde q(t_n+\sigma)\end{pmatrix},\end{aligned} \tag{2.42}$$

and therefore

$$\frac{\mathrm{d}}{\mathrm{d}\sigma}\mathrm{e}^{-\sigma L}\big[F'\big(\mathrm{e}^{\sigma L}U(t_n)\big)\mathrm{e}^{\sigma L}F(U(t_n))\big]$$

$$
\begin{aligned}
&= -\mathrm{e}^{-\sigma L} L F'\big(\mathrm{e}^{\sigma L}U(t_n)\big)\mathrm{e}^{\sigma L}F(U(t_n)) + \mathrm{e}^{-\sigma L}\frac{\mathrm{d}}{\mathrm{d}\sigma}F'\big(\mathrm{e}^{\sigma L}U(t_n)\big)\mathrm{e}^{\sigma L}F(U(t_n)) \\
&= \mathrm{e}^{-\sigma L}\begin{pmatrix} -f'(\tilde{u}(t_n+\sigma))\tilde{p}(t_n+\sigma) \\ f''(\tilde{u}(t_n+\sigma))\tilde{p}(t_n+\sigma)\tilde{v}(t_n+\sigma) + f'(\tilde{u}(t_n+\sigma))\tilde{q}(t_n+\sigma) \end{pmatrix}. \qquad (2.43)
\end{aligned}
$$

This implies that

$$
\begin{aligned}
&\left\| \frac{\mathrm{d}}{\mathrm{d}\sigma}\mathrm{e}^{-\sigma L}\big[F'\big(\mathrm{e}^{\sigma L}U(t_n)\big)\mathrm{e}^{\sigma L}F(U(t_n))\big] \right\|_1 \\
&\quad \lesssim \|f'(\tilde{u}(t_n+\sigma))\tilde{p}(t_n+\sigma)\|_{H^1(\Omega)} \\
&\qquad + \big\|f''(\tilde{u}(t_n+\sigma))\tilde{p}(t_n+\sigma)\tilde{v}(t_n+\sigma) + f'(\tilde{u}(t_n+\sigma))\tilde{q}(t_n+\sigma)\big\|_{L^2(\Omega)} \\
&\quad \lesssim \|\tilde{p}(t_n+\sigma)\|_{H^1(\Omega)} + \|\tilde{p}(t_n+\sigma)\|_{L^\infty(\Omega)}\|\tilde{u}(t_n+\sigma)\|_{H^1(\Omega)} \\
&\qquad + \|\tilde{p}(t_n+\sigma)\|_{L^\infty(\Omega)}\|\tilde{v}(t_n+\sigma)\|_{L^2(\Omega)} + \|\tilde{q}(t_n+\sigma)\|_{L^2(\Omega)} \\
&\quad \lesssim \|\tilde{p}(t_n+\sigma)\|_{H^{\frac{3}{2}+\epsilon}(\Omega)}(\|\tilde{u}(t_n+\sigma)\|_{H^1(\Omega)} + \|\tilde{v}(t_n+\sigma)\|_{L^2(\Omega)}) \\
&\qquad + \|\tilde{p}(t_n+\sigma)\|_{H^1(\Omega)} + \|\tilde{q}(t_n+\sigma)\|_{L^2(\Omega)} \\
&\quad \lesssim \|f(u(t_n))\|_{H^{\frac{1}{2}+\epsilon}(\Omega)}(\|\tilde{u}(t_n+\sigma)\|_{H^1(\Omega)} + \|\tilde{v}(t_n+\sigma)\|_{L^2(\Omega)}) \\
&\qquad + \|\tilde{p}(t_n+\sigma)\|_{H^1(\Omega)} + \|\tilde{q}(t_n+\sigma)\|_{L^2(\Omega)} \\
&\quad \lesssim \|U(t_n)\|_1 + \|U(t_n)\|_1^2 + \|U(t_n)\|_0. \qquad (2.44)
\end{aligned}
$$

By substituting this result into (2.40), we obtain

$$
\|R_{43}(t_n)\|_1 \lesssim \tau^3(\|U(t_n)\|_1 + \|U(t_n)\|_1^2 + \|U(t_n)\|_0). \qquad (2.45)
$$

Therefore, from (2.31) we obtain

$$
\begin{aligned}
\|I_2(t_n)\|_1 &\lesssim \|R_{41}(t_n)\|_1 + \|R_{42}(t_n)\|_1 + \|R_{43}(t_n)\|_1 \\
&\lesssim \tau^3(\|U(t_n)\|_1 + \|U(t_n)\|_1^2 + \|U(t_n)\|_0). \qquad (2.46)
\end{aligned}
$$

Therefore, substituting expressions (2.23) and (2.31) into (2.20) yields

$$
\begin{aligned}
U(t_{n+1}) &= \mathrm{e}^{\tau L}U(t_n) + \tau\mathrm{e}^{\tau L}F(U(t_n)) + (2L)^{-1}\big[\tau\mathrm{e}^{\tau L} - (2L)^{-1}\big(\mathrm{e}^{\tau L} - \mathrm{e}^{-\tau L}\big)\big]H(U(t_n)) \\
&\quad + I_2(t_n) + R_*(t_n) + R_3(t_n), \qquad (2.47)
\end{aligned}
$$

where

$$
H(U(t_n)) := \begin{pmatrix} -f(u(t_n)) \\ f'(u(t_n))\partial_t u(t_n) \end{pmatrix}.
$$

By dropping the remainders $R_*(t_n)$ and $R_3(t_n)$, we obtain the following numerical method:

$$
U^{n+1} = \mathrm{e}^{\tau L}U^n + \tau\mathrm{e}^{\tau L}F(U^n) + (2L)^{-1}\big[\tau\mathrm{e}^{\tau L} - (2L)^{-1}\big(\mathrm{e}^{\tau L} - \mathrm{e}^{-\tau L}\big)\big]H(U^n), \qquad (2.48)
$$

which can also be written as (1.3).

In view of (1.3), the new method we constructed here turns out to be a correction of the Lie splitting method without requiring second-order partial derivatives of the solution, *i.e.*, it improves the accuracy of the Lie splitting method under low-regularity conditions.

3. The spatial discretization

Let $\Omega = [0,1]^d$. It is known that any function $V \in H_0^1(\Omega) \times L^2(\Omega)$ can be expanded into the Fourier sine series, *i.e.*,

$$V = \sum_{n_1,\cdots,n_d=1}^{\infty} V_{n_1,\cdots,n_d} \sin(n_1\pi x_1)\cdots\sin(n_d\pi x_d). \tag{3.1}$$

Let

$$S_N = \left\{ \sum_{n_1,\cdots,n_d=1}^{N} V_{n_1,\cdots,n_d} \sin(n_1\pi x_1)\cdots\sin(n_d\pi x_d) : V_{n_1,\cdots,n_d} \in \mathbb{R}^2 \right\}.$$

We denote by I_N and Π_N the trigonometric interpolation and L^2-orthogonal projection operators onto S_N, respectively, *i.e.*, $I_N V$ is the unique function in S_N satisfying the relation $(I_N V)(x) = V(x)$ for $x \in D^d$, with

$$D = \left\{ \frac{2n}{2N+1} : n = 1,\cdots,N \right\},$$

and

$$(W - \Pi_N W, V) = 0 \quad \forall V \in S_N,\ W \in L^2(\Omega).$$

We consider the following fully discrete spectral method for the second-order low-regularity integrator in (2.48):

$$U_N^{n+1} = \mathrm{e}^{\tau L} U_N^n + \frac{\tau}{2}\mathrm{e}^{\tau L} I_N F(U_N^n) + (2L)^{-1}\big[\tau \mathrm{e}^{\tau L} - (2L)^{-1}\big(\mathrm{e}^{\tau L} - \mathrm{e}^{-\tau L}\big)\big] I_N H(U_N^n). \tag{3.2}$$

For given U_N^n, the trigonometric interpolations $I_N F(U_N^n)$ and $I_N H(U_N^n)$ can be computed with FFT.

Let $E_N^n = \Pi_N U(t_n) - U_N^n$ be the error of the numerical solution. Since the exact solution satisfies

$$\begin{aligned}\Pi_N U(t_{n+1}) = {} & \mathrm{e}^{\tau L}\Pi_N U(t_n) + \frac{\tau}{2}\mathrm{e}^{\tau L}\Pi_N F(U(t_n)) \\ & + (2L)^{-1}\big[\tau \mathrm{e}^{\tau L} - (2L)^{-1}\big(\mathrm{e}^{\tau L} - \mathrm{e}^{-\tau L}\big)\big]\Pi_N H(U(t_n)) \\ & + \Pi_N[I_2(t_n) + R_*(t_n) + R_3(t_n)],\end{aligned} \tag{3.3}$$

the difference between (3.3) and (3.2) yields the following error equation:

$$\begin{aligned}E_N^{n+1} = {} & \mathrm{e}^{\tau L} E_N^n + \frac{\tau}{2}\mathrm{e}^{\tau L}\Pi_N\big(F(U(t_n)) - F(U_N^n)\big) \\ & + (2L)^{-1}\big[\tau \mathrm{e}^{\tau L} - (2L)^{-1}\big(\mathrm{e}^{\tau L} - \mathrm{e}^{-\tau L}\big)\big]\Pi_N\big(H(U(t_n) - H(U_N^n)\big) \\ & + \Pi_N I_2(t_n) + \Pi_N R_*(t_n) + \Pi_N R_3(t_n) + R_5(t_n) + R_6(t_n),\end{aligned} \tag{3.4}$$

with

$$\begin{aligned}R_5(t_n) &= \frac{\tau}{2}\mathrm{e}^{\tau L}(\Pi_N - I_N)F(U_N^n), \\ R_6(t_n) &= (2L)^{-1}\big[\tau \mathrm{e}^{\tau L} - (2L)^{-1}\big(\mathrm{e}^{\tau L} - \mathrm{e}^{-\tau L}\big)\big](\Pi_N - I_N)H(U_N^n).\end{aligned} \tag{3.5}$$

The following result shows that for a solution bounded in the energy space $H_0^1(\Omega) \times L^2(\Omega)$ the proposed numerical method can have second-order convergence in time and first-order convergence in space in the same energy space.

Theorem 3.1. *For $d = 1,2,3$ and $U \in L^\infty(0,T; H^{1+\frac{d}{4}}(\Omega) \cap H_0^1(\Omega) \times H^{\frac{d}{4}}(\Omega))$, the numerical solution given by (3.2), with initial value $U_N^0 = \Pi_N U(0)$, has the following error bound:*

$$\max_{0 \le n \le T/\tau} \|E_N^n\|_1 \lesssim \tau^2 + N^{-1-\frac{d}{4}}. \tag{3.6}$$

Proof. If $U \in L^\infty(0,T;H^{1+\frac{d}{4}}(\Omega)\cap H_0^1(\Omega)\times H^{\frac{d}{4}}(\Omega))$ then (2.21) and (2.46) imply that the remainders $\Pi_N I_2(t_n)$ and $\Pi_N R_3(t_n)$ satisfy the following estimates:

$$\|\Pi_N I_2(t_n)\|_1 + \|\Pi_N R_*(t_n)\|_1 + \|\Pi_N R_3(t_n)\|_1 \lesssim \tau^3 \quad \text{in the case } d=1,2,3. \tag{3.7}$$

The remainders $R_5(t_n)$ and $R_6(t_n)$ can be estimated by using mathematical induction on n: assuming that

$$\|U_N^n\|_1 \le \|\Pi_N U(t_n)\|_1 + 1 \tag{3.8}$$

we shall prove the following results:

$$\|U_N^{n+1}\|_1 \le \|\Pi_N U(t_{n+1})\|_1 + 1 \quad \text{and} \quad \|E_N^n\|_1 \lesssim \tau^2 + N^{-1-\frac{d}{4}}. \tag{3.9}$$

Under assumption (3.8) we have

$$\begin{aligned}
\|R_5(t_n)\|_1 &\lesssim \tau\|(\Pi_N - I_N)F(U_N^n)\|_1\\
&\lesssim \tau\|(\Pi_N - I_N)f(u_N^n)\|_{L^2}\\
&\lesssim \tau N^{-2}\|f(u_N^n)\|_{H^2}\\
&\lesssim \tau N^{-2}\|f'(u_N^n)\nabla^2 u_N^n + f''(u_N^n)\nabla u_N^n\otimes\nabla u_N^n\|_{L^2}\\
&\lesssim \tau N^{-2}(\|u_N^n\|_{H^2} + \|\nabla u_N^n\|_{L^4}^2)
\end{aligned}$$

$$\begin{aligned}
\|R_6(t_n)\|_1 &= \big\|(2L)^{-1}\big[\tau \mathrm{e}^{\tau L} - (2L)^{-1}\big(\mathrm{e}^{\tau L} - \mathrm{e}^{-\tau L}\big)\big](\Pi_N - I_N)H(U_N^n)\big\|_1\\
&\lesssim \big\|\big[\tau \mathrm{e}^{\tau L} - (2L)^{-1}\big(\mathrm{e}^{\tau L} - \mathrm{e}^{-\tau L}\big)\big](\Pi_N - I_N)H(U_N^n)\big\|_0\\
&\lesssim \tau\big\|(\Pi_N - I_N)H(U_N^n)\big\|_0\\
&\lesssim \tau N^{-2}(\|f(u_N^n)\|_{H^2} + \|f'(u_N^n)v_N^n\|_{H^1})\\
&\lesssim \tau N^{-2}\big(\big\|f'(u_N^n)\nabla^2 u_N^n + f''(u_N^n)\nabla u_N^n\otimes\nabla u_N^n\big\|_{L^2}\big)\\
&\quad + \tau N^{-2}(\|f''(u_N^n)v_N^n\nabla u_N^n + f'(u_N^n)\nabla v_N^n\|_{L^2})\\
&\lesssim \tau N^{-2}\big(\|u_N^n\|_{H^2} + \|\nabla u_N^n\|_{L^4}^2\big) + \tau N^{-2}(\|v_N^n\|_{L^4}\|\nabla u_N^n\|_{L^4} + \|\nabla v_N^n\|_{L^2}).
\end{aligned}$$

In the case $d=1,2,3$, the Sobolev interpolation inequality $\|\nabla u_N^n\|_{L^4} \le \|u_N^n\|_{H^{1+\frac{d}{4}}}$ implies that

$$\begin{aligned}
\|R_5(t_n)\|_1 &\lesssim \tau N^{-2}\Big(\|u_N^n\|_{H^2} + \|u_N^n\|_{H^{1+\frac{d}{4}}}^2\Big)\\
&\lesssim \tau N^{-1-\frac{d}{4}}\Big(\|u_N^n\|_{H^{1+\frac{d}{4}}} + \|u_N^n\|_{H^1}^2\Big),
\end{aligned} \tag{3.10}$$

$$\begin{aligned}
\|R_6(t_n)\|_1 &\lesssim \tau N^{-2}\Big(\|u_N^n\|_{H^2} + \|v_N^n\|_{H^1} + \|u_N^n\|_{H^{1+\frac{d}{4}}}^2 + \|v_N^n\|_{H^{\frac{d}{4}}}^2\Big)\\
&\lesssim \tau N^{-1-\frac{d}{4}}\Big(\|u_N^n\|_{H^{1+\frac{d}{4}}} + \|v_N^n\|_{H^{\frac{d}{4}}} + \|u_N^n\|_{H^{1+\frac{d}{4}}}^2 + \|v_N^n\|_{H^{\frac{d}{4}}}^2\Big).
\end{aligned} \tag{3.11}$$

By using these estimates and taking the energy norm $|\cdot|_1$ on both sides of (3.4), we obtain

$$\big|E_N^{n+1}\big|_1 \le (1+C\tau)|E_N^n|_1 + C\tau\Big(\tau^2 + N^{-1-\frac{d}{4}}\Big). \tag{3.12}$$

Then, using Gronwall's inequality and the equivalence of norms $|\cdot|_1 \sim \|\cdot\|_1$ on the energy space $H_0^1(\Omega)\times L^2(\Omega)$, we obtain the following error bound:

$$\big\|E_N^{n+1}\big\|_1 \lesssim \tau^2 + N^{-1-\frac{d}{4}}. \tag{3.13}$$

There exist some positive constants τ_0 and N_0 such that for $\tau \le \tau_0$ and $N \ge N_0$ we obtain

$$\big\|E_N^{n+1}\big\|_1 \le 1. \tag{3.14}$$

This proves (3.9) (with an additional triangle inequality). ☐

Remark 3.2. By passing to the limit $N \to \infty$ in Theorem 3.1, one can obtain the semi-discretization results in Theorem 1.1.

Remark 3.3. In the case $d = 1$, the remainder $R_*(t_n)$ can be estimated by using (2.30), which yields the following result:

$$\max_{0\le n\le T/\tau} \|E_N^n\|_1 \lesssim \tau^{\frac{4}{3}-\epsilon} + N^{-1} \quad \text{(for any fixed } \epsilon > 0), \tag{3.15}$$

$$\max_{0\le n\le T/\tau} \|E_N^n\|_{\frac{1}{2}+\epsilon} \lesssim \tau^{2-\epsilon} + N^{-1} \quad \text{(for any fixed } \epsilon > 0). \tag{3.16}$$

These results hold under the weaker regularity condition $U \in C([0,T]; H_0^1(\Omega) \times L^2(\Omega))$, *i.e.*, the numerical solution has higher-order convergence in the energy space. Since $H^{\frac{1}{2}+\epsilon}(\Omega) \hookrightarrow L^\infty(\Omega)$, it follows that that the numerical solution u_N^n has almost second-order convergence in $L^\infty(\Omega)$.

Remark 3.4. For any given initial value $(u^0, v^0) \in H^{1+\frac{d}{4}}(\Omega) \cap H_0^1(\Omega) \times H^{\frac{d}{4}}(\Omega)$, Theorem 3.1 states that the error of the numerical solution is as follows:

$$\|\Pi_N u(t_n) - u_N^n\|_{H^1} + \|\Pi_N v(t_n) - v_N^n\|_{L^2} \lesssim \tau^2 + N^{-1-\frac{d}{4}},$$

which is a superconvergence result that much better than the regularity of the solution in both time and space. In general, for any fixed t, the projection error in space satisfies

$$\|\Pi_N u(t) - u(t)\|_{H^1} + \|\Pi_N v(t) - v(t)\|_{L^2} \lesssim N^{-\frac{d}{4}}.$$

4. Numerical experiments

In this section we present numerical experiments to support the theoretical analysis and to illustrate the performance of our new method in (1.3) on the semilinear Klein–Gordon equation (1.1) with $f(u) = \sin(u)$ in a one-, two-, and three-dimensional domain $\Omega = [0,1]^d$, $d = 1, 2, 3$. For obtaining a sufficiently stiff system of differential equations while keeping the experiments' execution time reasonably low, we chose to use $N_x = 2^{12}$ terms of a Fourier space discretization in the x dimension and, $N_y = N_z = 2^3$ terms in the y and z dimensions, when Ω is two- and three-dimensional. As for the initial state of the differential equation, we generate, as described in Section 5.1 of [26], random initial data u^0 and u_t^0 from the space $H^\theta(\Omega)$ such that $\|u^0\|_{H^1} = 1$ and $\|u_t^0\|_{L^2} = 1$. In particular, we are interested in comparing the smooth case ($\theta \to \infty$) with the low-regularity case ($\theta = 1$).

Our new method is tested in comparison with several well-established numerical techniques for the semilinear Klein–Gordon equation. To define them, it is useful to introduce the operator $\Sigma = \sqrt{-\Delta}$, which satisfies that $\Delta = -\Sigma^2$. This is because the exponential of our linear operator can be easily expressed as

$$\exp(L) = \exp\left(t\begin{pmatrix} 0 & 1 \\ \Delta & 0 \end{pmatrix}\right) = \exp\left(t\begin{pmatrix} 0 & 1 \\ -\Sigma^2 & 0 \end{pmatrix}\right) = \begin{pmatrix} \cos(t\Sigma) & t\,\mathrm{sinc}(t\Sigma) \\ -\Sigma\sin(t\Sigma) & \cos(t\Sigma) \end{pmatrix}.$$

This expression is worth using only in case the operator Δ can be discretized in space by means of a diagonal matrix or if the resulting discretization matrix's size is particularly modest. In fact, in the other cases, computing the matrix square root is generally unfeasible. The above-mentioned numerical techniques are:

- The second-order low-regularity exponential-type scheme from [31], that we refer to as `rs21` that we apply to the reformulation of (1.1) into the first order equation (1.2) through the transformation $w = u - \mathrm{i}(-\Delta)^{-\frac{1}{2}}\partial_t u$. This method computes approximations w^{n+1} to $w(t_{n+1})$ at discrete times $t_{n+1} = t_0 + (n+1)\tau$ with the time step size τ as
$$w^{n+1} = \exp\left(\tau\sqrt{-\Delta}\right)\left(w^n - \tau\sqrt{-\Delta}^{-1}F(w^n)\right) - \tau\sqrt{-\Delta}^{-1}E(w^n)$$

where

$$F(w^n) = \sin\left(\frac{w^n}{2}\right)\left(\varphi_1(-2\tau\sqrt{-\Delta}) - 2\varphi_2(-2\tau\sqrt{-\Delta})\right)\overline{\cos\left(\frac{w^n}{2}\right)}$$
$$+ \cos\left(\frac{w^n}{2}\right)\left(\varphi_1(-2\tau\sqrt{-\Delta}) - 2\varphi_2(-2\tau\sqrt{-\Delta})\right)\overline{\sin\left(\frac{w^n}{2}\right)}$$
$$+ \sin\left(\frac{w^n}{2}\right)\varphi_2(-2\tau\sqrt{-\Delta})\exp(2\tau\sqrt{-\Delta})\cos\left(\exp(-2\tau\sqrt{-\Delta})\frac{\overline{w^n}}{2}\right)$$
$$+ \cos\left(\frac{w^n}{2}\right)\varphi_2(-2\tau\sqrt{-\Delta})\exp(2\tau\sqrt{-\Delta})\sin\left(\exp(-2\tau\sqrt{-\Delta})\frac{\overline{w^n}}{2}\right)$$

and

$$E(w^n) = \sin\left(\exp(\tau\sqrt{-\Delta})w^n\right)\varphi_2(-2\tau\sqrt{-\Delta})\cos\left(\exp(\tau\sqrt{-\Delta})\overline{w^n}\right)$$
$$+ \cos\left(\exp(\tau\sqrt{-\Delta})w^n\right)\varphi_2(-2\tau\sqrt{-\Delta})\sin\left(\exp(\tau\sqrt{-\Delta})\overline{w^n}\right).$$

– The recent second-order IMEX method for semilinear second-order wave equations from [17], that we refer to as `hl21`. This method computes approximations u^{n+1}, v^{n+1} to $u(t_{n+1})$, $u_t(t_{n+1})$ at discrete times $t_{n+1} = t_0 + (n+1)\tau$ with the time step size τ as

$$v^{n+\frac{1}{2}} = \left(1 - \frac{\tau^2}{4}\Delta\right)^{-1}\left(v^n + \frac{\tau}{2}\sin(u^n) + \frac{\tau}{2}\Delta u^n\right),$$
$$u^{n+1} = u^n + \tau v^{n+\frac{1}{2}},$$
$$v^{n+1} = 2v^{n+\frac{1}{2}} - v^n + \frac{\tau}{2}\left(\sin(u^{n+1}) - \sin(u^n)\right).$$

– Another natural choice for measuring the performances of our scheme is the class of second-order trigonometric integrators expressly designed for the discretization in time of the spatially discrete nonlinear Klein–Gordon equation with periodic boundary conditions. This class of trigonometric integrators computes approximations u^{n+1}, v^{n+1} to $u(t_{n+1})$, $u_t(t_{n+1})$ at discrete times $t_{n+1} = t_0 + (n+1)\tau$ with the time stepsize τ as

$$\begin{pmatrix} u^{n+1} \\ v^{n+1} \end{pmatrix} = \exp\left(\tau\begin{pmatrix} 0 & 1 \\ \Delta & 0 \end{pmatrix}\right)\begin{pmatrix} u^n \\ v^n \end{pmatrix} + \frac{\tau}{2}\begin{pmatrix} \tau\Psi\sin(\Psi u^n) \\ \Psi_0\sin(\Psi u^n) + \Psi_1\sin(\Psi u^n) \end{pmatrix}.$$

The matrices Φ, Ψ, Ψ_0, and Ψ_1 are filters defined by

$$\Phi = \phi(\tau\Sigma), \quad \Psi = \psi(\tau\Sigma), \quad \Psi_0 = \psi_0(\tau\Sigma), \quad \Psi_1 = \psi_1(\tau\Sigma)$$

with filter functions ϕ, ψ, ψ_0, and ψ_1 that satisfy $\phi(0) = \psi(0) = \psi_0(0) = \psi_1(0) = 1$. The choice of such filters uniquely characterizes a method. For even filter functions, the method is symmetric if and only if

$$\psi(x) = \operatorname{sinc}(x)\psi_1(x), \quad \psi_0(x) = \cos(x)\psi_1(x), \tag{4.1}$$

and it is symplectic if and only if $\psi(x) = \operatorname{sinc}(x)\phi(x)$. Popular choices of the filter functions are

(B) The one with $\psi(x) = \operatorname{sinc}(x), \phi(x) = 1$, ψ_0 and ψ_1 as in (4.1). This is the impulse method by Deuflhard [9].

(C) The one with $\psi(x) = \operatorname{sinc}^2(x), \phi(x) = \operatorname{sinc}(x)$, ψ_0 and ψ_1 as in (4.1). This is the mollified impulse method by García-Archilla *et al.* [10].

(E) The one with $\psi(x) = \operatorname{sinc}^2(x), \phi(x) = 1$, ψ_0 and ψ_1 as in (4.1). This is the trigonometric exponential-type integrator by Hairer and Lubich [14].

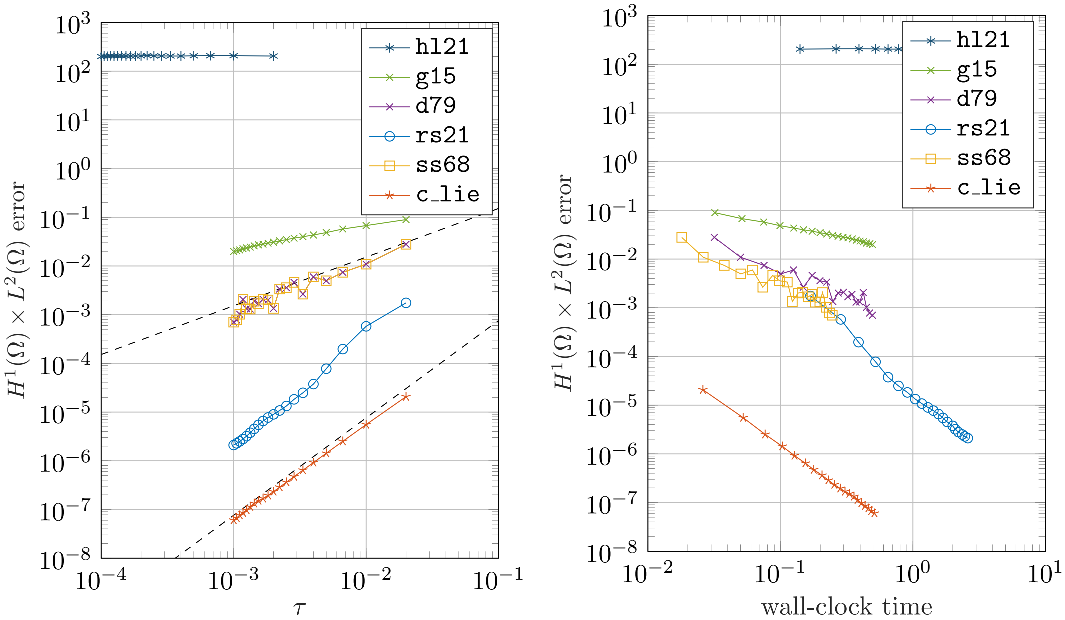

FIGURE 1. Errors of the numerical solutions with one-dimensional $H^1(\Omega) \times L^2(\Omega)$ initial data. The dashed lines indicate orders 1 and 2, respectively.

(G) The one with $\psi(x) = \operatorname{sinc}^3(x), \phi(x) = \operatorname{sinc}(x)$, ψ_0 and ψ_1 as in (4.1). This is the trigonometric exponential-type integrator by Grimm and Hochbruck [13].

($\tilde{B}$) The one with $\psi(x) = \chi_{[-\pi,\pi]}(x)\operatorname{sinc}(x), \phi(x) = \chi_{[-\pi,\pi]}(x)$ ψ_0 and ψ_1 as in (4.1). This is the method introduced by Gauckler [11].

For a precise overview and for more information on this class of trigonometric methods we refer the reader to [11]. In our tests it turned out that the methods B and $\tilde{B}$ are neatly superior to all the other options, therefore we will only include these two into the data presentation, referring to them as, respectively, `d79` and `g15`.

– The second order classical Strang splitting scheme from [32], that we refer to as `ss68`. This method computes approximations u^{n+1}, v^{n+1} to $u(t_{n+1})$, $u_t(t_{n+1})$ at discrete times $t_{n+1} = t_0 + (n+1)\tau$ with the time step size τ as

$$\begin{pmatrix} u^{n+\frac12} \\ v^{n+\frac12} \end{pmatrix} = \exp\left(\frac{\tau}{2}\begin{pmatrix} 0 & 1 \\ \Delta & 0 \end{pmatrix}\right)\begin{pmatrix} u^n \\ v^n \end{pmatrix},$$

$$\begin{pmatrix} u^{n+1} \\ v^{n+1} \end{pmatrix} = \exp\left(\frac{\tau}{2}\begin{pmatrix} 0 & 1 \\ \Delta & 0 \end{pmatrix}\right)\begin{pmatrix} u^{n+\frac12} \\ v^{n+\frac12} + \tau \sin\left(u^{n+\frac12}\right) \end{pmatrix}.$$

The $H^1(\Omega) \times L^2(\Omega)$ relative errors of the numerical solutions given by the above-mentioned methods and our new method – the corrected Lie method (which we refer to as `c_lie`) – are presented in Figures 1–6 for nonsmooth $H^1(\Omega) \times L^2(\Omega)$ initial data and smooth initial data, respectively. The numerical results indicate that the new method proposed in this article has second-order convergence for the nonsmooth $H^1(\Omega) \times L^2(\Omega)$ initial data, while all other second-order methods are practically first-order convergent in the nonsmooth case. Finally, all methods have second-order convergence for sufficiently smooth initial data.

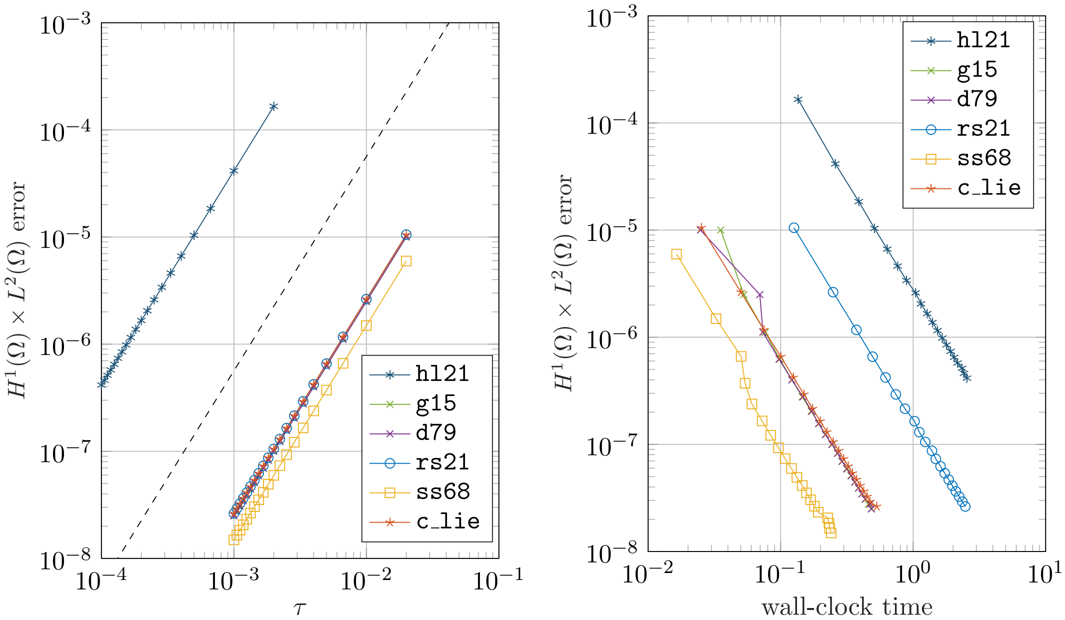

FIGURE 2. Errors of the numerical solutions with one-dimensional smooth initial data. The dashed line indicates order 2.

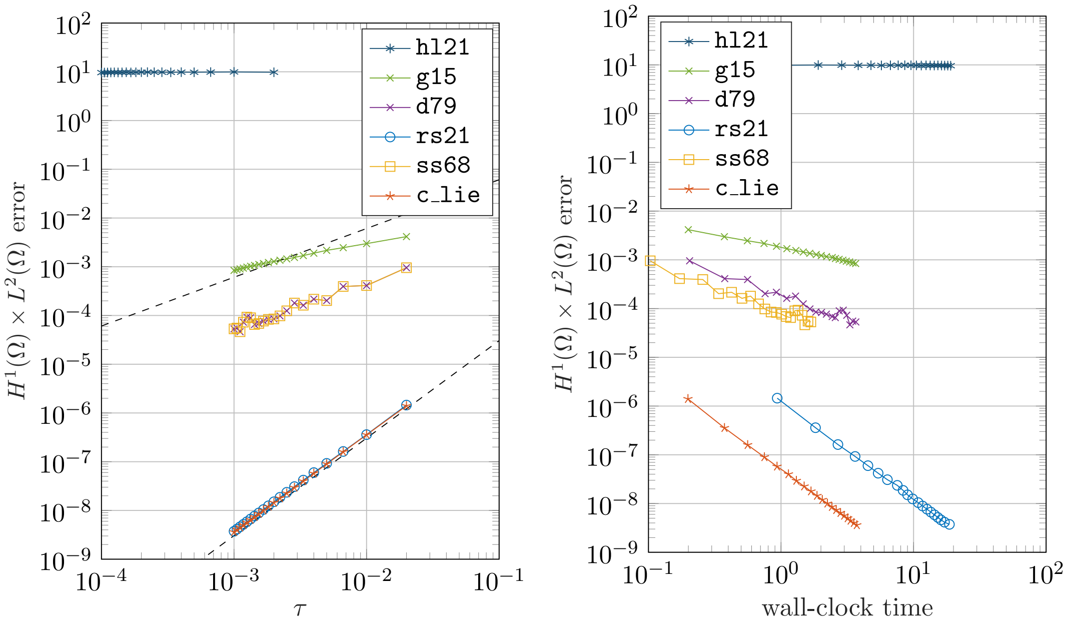

FIGURE 3. Errors of the numerical solutions with two-dimensional $H^1(\Omega) \times L^2(\Omega)$ initial data. The dashed lines indicate orders 1 and 2, respectively.

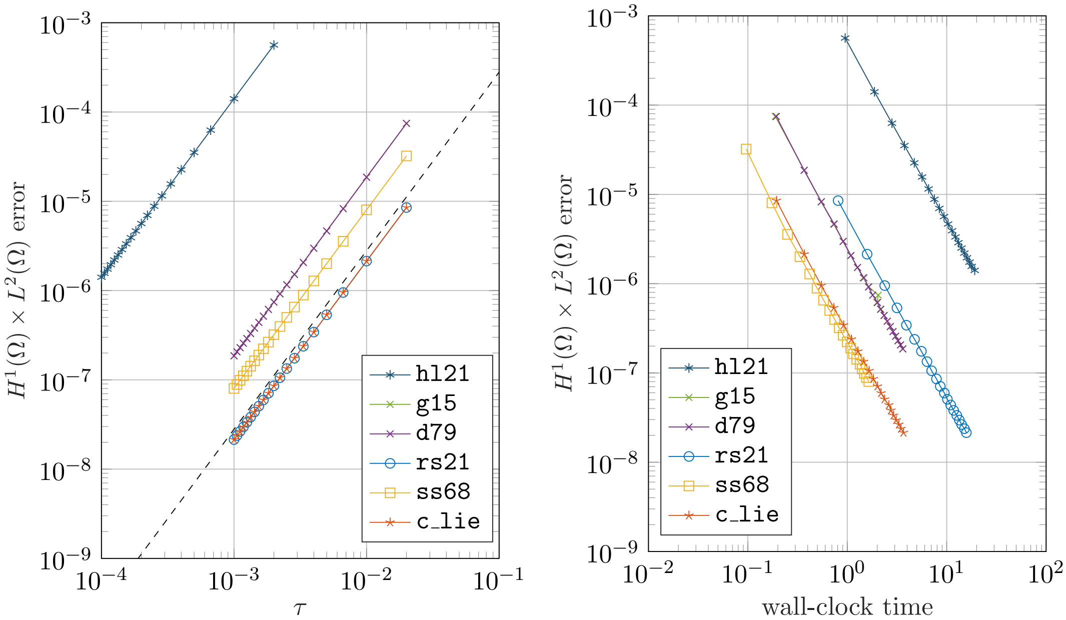

FIGURE 4. Errors of the numerical solutions with two-dimensional smooth initial data. The dashed line indicates order 2.

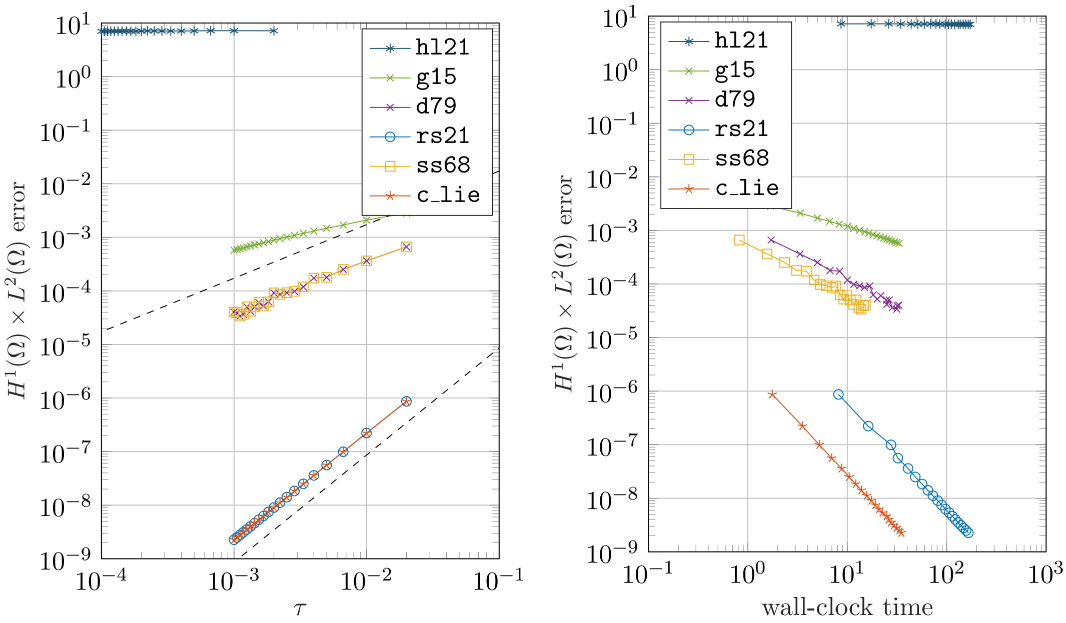

FIGURE 5. Errors of the numerical solutions with three-dimensional $H^1(\Omega) \times L^2(\Omega)$ initial data. The dashed lines indicate orders 1 and 2, respectively.

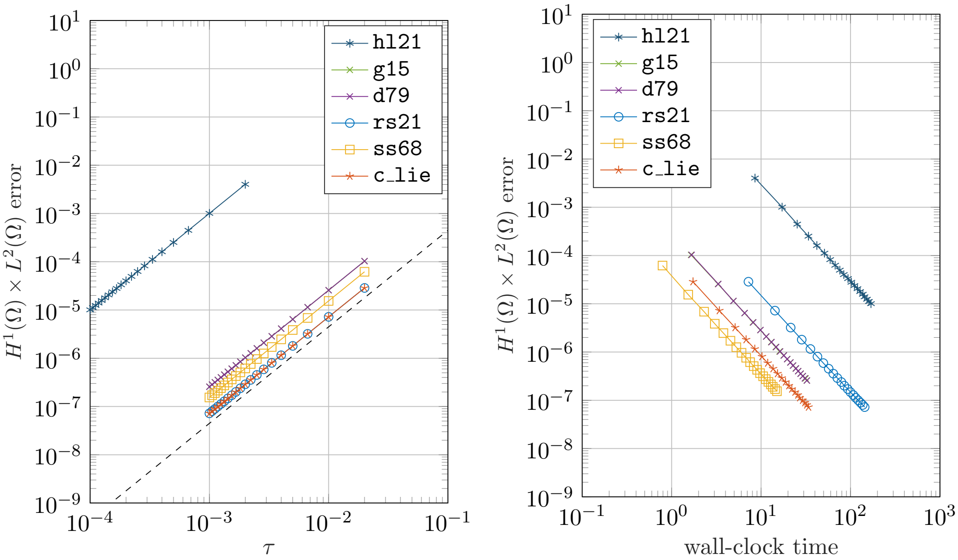

FIGURE 6. Errors of the numerical solutions with three-dimensional smooth initial data. The dashed line indicates order 2.

Acknowledgements. The work of Buyang Li is partially supported by the Hong Kong Research Grants Council (General Research Fund, project no. 15300519) and an internal grant at The Hong Kong Polytechnic University (Project ID: P0031035, Work programme: ZZKQ). Franco Zivcovich and Katharina Schratz have received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (grant agreement No. 850941).

REFERENCES

[1] W. Bao and L. Yang, Efficient and accurate numerical methods for the Klein–Gordon–Schrödinger equations. *J. Comput. Phys.* **225** (2007) 1863–1893.

[2] W. Bao, Y. Feng and C. Su, Uniform error bounds of time-splitting spectral methods for the long-time dynamics of the nonlinear Klein–Gordon equation with weak nonlinearity. *Math. Comp.* **91** (2022) 811–842.

[3] A. Barone, F. Esposito and C.J. Magee, Theory and applications of the sine-gordon equation. *La Rivista del Nuovo Cimento* **1** (1971) 227–267.

[4] Y. Bruned and K. Schratz, Resonance based schemes for dispersive equations via decorated trees, in Forum of Mathematics, Pi. Vol. 10. Cambridge University Press (2022) E2.

[5] S. Buchholz, B. Dörich and M. Hochbruck, On averaged exponential integrators for semilinear Klein–Gordon equations with solutions of low-regularity. *SN Part. Differ. Equ. Appl.* **2** (2021) 2662–2963.

[6] W. Cao, D. Li and Z. Zhang, Unconditionally optimal convergence of an energy-conserving and linearly implicit scheme for nonlinear Klein–Gordon equations. *Sci. China Math.* **65** (2021) 1731–1748.

[7] C. Chen, J. Hong, C. Sim and K. Sonwu, Energy and quadratic invariants preserving (EQUIP) multi-symplectic methods for Hamiltonian Klein–Gordon equations. *J. Comput. Phys.* **418** (2020) 10959.

[8] D. Cohen, E. Hairer and C. Lubich, Conservation of energy, momentum and actions in numerical discretizations of non-linear wave equations. *Numer. Math.* **110** (2008) 113–143.

[9] P. Deuflhard, A study of extrapolation methods based on multistep schemes without parasitic solutions. *Z. Angew. Math. Phys.* **30** (1979) 177–189.

[10] B. García-Archilla, J.M. Sanz-Serna and R.D. Skeel, Long-time-step methods for oscillatory differential equations. *SIAM J. Sci. Comput.* **20** (1998) 930–963.

[11] L. Gauckler, Error analysis of trigonometric integrators for semilinear Klein–Gordon equations. *SIAM J. Numer. Anal.* **53** (2015) 1082–1106.

[12] R. Glowinski and A. Quaini, On the numerical solution to a nonlinear wave equation associated with the first Painlevé equation: an operator-splitting approach, in Partial Differential Equations: Theory, Control and Approximation. Springer, Dordrecht (2014) 243–264.

[13] V. Grimm and M. Hochbruck, Error analysis of exponential integrators for oscillatory second-order differential equations. *J. Phys. A* **39** (2006) 5495–5507.
[14] E. Hairer and C. Lubich, Long-time energy conservation of numerical methods for oscillatory differential equations. *SIAM J. Numer. Anal.* **38** (2000) 414–441.
[15] E. Hairer, C. Lubich and G. Wanner, Geometric Numerical Integration. Structure-Preserving Algorithms for Ordinary Differential Equations, 2nd edition. Springer (2006).
[16] E. Hansen and A. Ostermann, High-order splitting schemes for semilinear evolution equations. *BIT Numer. Math.* **56** (2016) 1303–1316.
[17] M. Hochbruck and J. Leibold, An implicit-explicit time discretization scheme for second-order semilinear Klein–Gordon equations with application to dynamic boundary conditions. *Numer. Math.* **147** (2021) 869–899.
[18] M. Hochbruck and C. Lubich, A Gautschi-type method for oscillatory second-order differential equations. *Numer. Math.* **83** (1999) 403–426.
[19] M. Hofmanová and K. Schratz, An exponential-type integrator for the KdV equation. *Numer. Math.* **136** (2017) 1117–1137.
[20] W. Layton, Y. Li and C. Trenchea, Recent developments in IMEX methods with time filters for systems of evolution equations. *J. Comput. Appl. Math.* **299** (2016) 50–67.
[21] D. Li and W. Sun, Linearly implicit and high-order energy-conserving schemes for nonlinear Klein–Gordon equations. *J. Sci. Comput.* **83** (2020) 65.
[22] J. Li and M.R. Visbal, High-order compact schemes for nonlinear dispersive waves. *J. Sci. Comput.* **26** (2006) 1–23.
[23] Y. Li, Y. Wu and F. Yao, Convergence of an embedded exponential-type low-regularity integrators for the KdV equation without loss of regularity. *Ann. Appl. Math.* **37** (2021) 1–21.
[24] B. Li, S. Ma and K. Schratz, A semi-implicit low-regularity integrator for Navier–Stokes equations. *SIAM J. Numer. Anal.* **60** (2022) 2273–2292.
[25] D. Murai and T. Koto, Stability and convergence of staggered Runge–Kutta schemes for semilinear Klein–Gordon equations. *J. Comput. Appl. Math.* **235** (2011) 4251–4264.
[26] A. Ostermann and K. Schratz, Low regularity exponential-type integrators for semilinear Schrödinger equations. *Found. Comput. Math.* **18** (2018) 731–755.
[27] A. Ostermann, F. Rousset and K. Schratz, Fourier integrator for periodic NLS: low regularity estimates via discrete Bourgain spaces. *J. Eur. Math. Soc.* (2022). DOI: 10.4171/jems/1275.
[28] R. Qi and X. Wang, Error estimates of finite element method for semilinear stochastic strongly damped Klein–Gordon equation. *IMA J. Numer. Anal.* **39** (2019) 1594–1626.
[29] A. Quaini and R. Glowinski, Splitting methods for some nonlinear wave problems, in Splitting Methods in Communication, Imaging, Science, and Engineering. *Scientific Computation Series.* Springer, Cham (2016) 643–676.
[30] Z. Rong and C. Xu, Numerical approximation of acoustic waves by spectral element methods. *Appl. Numer. Math.* **58** (2008) 999–1016.
[31] F. Rousset and K. Schratz, A general framework of low-regularity integrators. *SIAM J. Numer. Anal.* **59** (2021) 1735–1768.
[32] G. Strang, On the construction and comparison of difference schemes. *SIAM J. Numer. Anal.* **5** (1968) 506–517.
[33] B. Wang and X. Wu, The formulation and analysis of energy-preserving schemes for solving high-dimensional nonlinear Klein–Gordon equations. *IMA J. Numer. ANal.* **39** (2019) 2016–2044.
[34] B. Wang and X. Wu, Global error bounds of one-stage extended RKN integrators for semilinear Klein–Gordon equations. *Numer. Algorithm* **81** (2019) 1203–1218.
[35] Y. Wang and X. Zhao, A symmetric low-regularity integrator for nonlinear Klein–Gordon equation. *Math. Comp.* **91** (2022) 2215–2245.
[36] Y. Wu and X. Zhao, Optimal convergence of a first order low-regularity integrator for the KdV equation. *IMA J. Numer. Anal.* **42** (2022) 3499–3528.
[37] Y. Wu and X. Zhao, Embedded exponential-type low-regularity integrators for KdV equation under rough data. *BIT Numer. Math.* **62** (2022) 1049–1090.