IMA Journal of Numerical Analysis (2018) **00**, 1–29
doi:10.1093/imanum/dry047

The formulation and analysis of energy-preserving schemes for solving high-dimensional nonlinear Klein–Gordon equations

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[Received on 5 December 2017; revised on 17 March 2018]

In this paper we focus on the analysis of energy-preserving schemes for solving high-dimensional nonlinear Klein–Gordon equations. A novel energy-preserving scheme is developed based on the discrete gradient method and the Duhamel principle. The local error, global convergence and nonlinear stability of the new scheme are analysed in detail. Numerical experiments are implemented to compare with existing numerical methods in the literature, and the numerical results show the remarkable efficiency of the new energy-preserving scheme presented in this paper.

Keywords: high-dimensional nonlinear Klein–Gordon equations; energy-preserving schemes; discrete gradient methods; nonlinear stability; convergence analysis.

1. Introduction

It is well known that the nonlinear Klein–Gordon equation is one of the important models in quantum mechanics and mathematical physics. Energy conservation is a key feature of the Klein–Gordon equation. Hence, the subject of this paper is to formulate and analyse energy-preserving schemes for the high-dimensional nonlinear Klein–Gordon equation

$$\begin{cases} \frac{\partial u}{\partial t} = v, & u(x,0) = g_1(x), \\ \frac{\partial v}{\partial t} = \omega^2 \Delta u - G'(u), & v(x,0) = g_2(x), \end{cases} \tag{1.1}$$

where

$$\Delta = \sum_{j=1}^{d} \frac{\partial^2}{\partial x_j^2},$$

ω is a real parameter and the real-valued function $u(x,t)$ is defined in $(x,t) \in \Omega \times [0,T]$ with $\Omega := (0,X_1) \times \cdots \times (0,X_d) \subset \mathbb{R}^d$. Further, $G(u)$ is a smooth potential energy function with $G(u) \geqslant 0$. In this

work we consider periodic boundary conditions

$$u(x,t)|_{\partial\boldsymbol{\Omega}\cap\{x_j=0\}} = u(x,t)|_{\partial\boldsymbol{\Omega}\cap\{x_j=X_j\}}, \quad j=1,2,\ldots,d. \tag{1.2}$$

The Hamiltonian of system (1.1) is

$$\mathscr{H}[u,v](t) = \int_{\Omega}\left[\tfrac{1}{2}|v(x,t)|^2 + \tfrac{1}{2}\omega^2|\nabla u(x,t)|^2 + G\big(u(x,t)\big)\right]\mathrm{d}x \tag{1.3}$$

with $\mathrm{d}x = \mathrm{d}x_1\mathrm{d}x_2\ldots\mathrm{d}x_d$.

As is well known (1.1) can be rewritten as the following infinite-dimensional Hamiltonian system:

$$\mathbf{z}_t = J\frac{\delta\mathscr{H}}{\delta\mathbf{z}}, \tag{1.4}$$

where

$$J = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}, \quad \mathbf{z} = \begin{pmatrix} u \\ v \end{pmatrix},$$

and

$$\frac{\delta\mathscr{H}}{\delta\mathbf{z}} = \Big(\frac{\delta\mathscr{H}}{\delta u}, \frac{\delta\mathscr{H}}{\delta v}\Big)^{\mathsf{T}}$$

is the functional derivative of $\mathscr{H}$.

The Klein–Gordon equation frequently arises in various fields of scientific applications such as solid state physics, nonlinear optics, quantum field theory and relativistic quantum mechanics. It is used to model many different phenomena, including the propagation of dislocations in crystals and the behaviour of elementary particles. Several numerical methods have been developed to solve Klein–Gordon equations (see, e.g., Li & Vu-Quoc, 1995; Duncan, 1997; Shakeri & Dehghan, 2008; Dehghan & Shokri, 2009; Lakestani & Dehghan, 2010; Bao & Dong, 2012; Liu & Wu, 2017a). In recent decades structure-preserving algorithms have been receiving much attention and they have been shown to be useful when studying the long-time behaviour of dynamical systems. Various structure-preserving algorithms have been designed to preserve as much as possible the physical/geometric properties of the systems under consideration. For the work related to this topic we refer the reader to Sanz-Serna (1992), Hairer & Lubich (2000), Hochbruck & Ostermann (2010), Wu *et al.* (2012), Wang *et al.* (2016), Wang *et al.* (2017a), Wang *et al.* (2017b), Wang *et al.* (2017c), Wang *et al.* (2017d), Mei & Wu (2017) and references therein. For a good theoretical foundation of structure-preserving algorithms for ordinary differential equations (ODEs) we refer the reader to Hairer *et al.* (2006). Surveys of structure-preserving algorithms for oscillatory differential equations are referred to in Wu *et al.* (2015a), Wu *et al.* (2013b), Wu & Wang (2018). By extending ideas and tools related to structure-preserving algorithms of ODEs, various numerical schemes have been proposed and investigated for specific or general classes of partial differential equations (PDEs). Among typical categories of them are multi-symplectic methods, semidiscretisations by means of the method of lines and energy-preserving schemes.

By assigning a distinct symplectic operator for each unbounded space direction and time, the multi-symplectic structure for a class of PDEs generalises the classical symplectic structure of Hamiltonian ODEs. Multi-symplectic integrators precisely conserve a discrete space–time symplectic structure of Hamiltonian PDEs and we refer to Bridges (1997), Bridges & Reich (2006), Feng & Qin (2006), Frank *et al.* (2006), Shi *et al.* (2012), Hu *et al.* (2013) and Li & Wu (2015) for related work. With

regard to the method of lines the spatial derivatives are usually approximated by finite differences or by discrete Fourier transform and the resulting system is then integrated in time by a suitable ODE integrator. This approach has become one of the central topics for much research in PDEs, and we refer the reader to Schiesser (1991), Bratsos (2007), Hesthaven *et al.* (2007), Liu *et al.* (2014) and Wu *et al.* (2016) for examples on this subject.

Research into energy-preserving schemes for PDEs has a long history, which dates back to an old paper of Courant *et al.* (1928) where a discrete energy conservation law for the 5-point finite difference approximation was derived. In Li & Vu-Quoc (1995) a historical survey of energy-preserving methods for PDEs and their applications is given. Some recent relevant work can be found in Matsuo (2007), Cohen *et al.* (2008), Matsuo & Yamaguchi (2009), Ringler *et al.* (2010), Celledoni *et al.* (2012), Li & Wu (2015) and Mei *et al.* (2017). Energy conservation methods have also been the subject of many investigations of ODEs during recent years. Various different effective energy-preserving methods have been proposed and investigated, such as discrete gradient (DG) methods (see, e.g., McLachlan *et al.*, 1999; McLachlan & Quispel, 2014; Li & Wu, 2016), time finite elements (see, e.g., Betsch & Steinmann, 2000a,b), the average vector field (AVF) method (see, e.g., Quispel & McLaren, 2008; Celledoni *et al.*, 2009; Celledoni *et al.*, 2014), Hamiltonian boundary value methods (HBVMs) (see, e.g., Brugnano *et al.*, 2014; Brugnano *et al.*, 2015b) and the adapted average vector field (AAVF) method (see, e.g., Wang & Wu, 2012; Wu *et al.*, 2013a). All the energy-preserving methods mentioned above were originally designed for ODEs and have also been considered in a PDE setting. In Dahlby & Owren (2010) the authors discussed numerical methods for PDEs that are based on the DG method. A systematic introduction to finite element methods for efficient numerical solution of PDEs is referred to Ŝolin (2006). The AVF method for discretising Hamiltonian PDEs was studied in Celledoni *et al.* (2012), and HBVMs related to the numerical solution of the semilinear wave equation were researched in Brugnano *et al.* (2015a). The authors in Liu & Wu (2016) analysed the AAVF method for one-dimensional Hamiltonian wave equations.

It is well known that an important aspect in the numerical simulation of Hamiltonian systems is the approximate conservation of the total energy over long times. The DG method is a useful tool to construct energy-preserving schemes and various DG methods for ODEs were researched in Gonzalez (1996), McLachlan *et al.* (1999) and McLachlan & Quispel (2014). DG methods have also been applied to PDEs in the form of the AVF method in Celledoni *et al.* (2012) and in a somewhat more general setting, the discrete variational derivative method in Dahlby & Owren (2010) and Liu *et al.* (2017). On the other hand, the authors in Wu *et al.* (2015b) established a novel operator-variation-of-constants formula for wave equations on the basis of which, many efficient numerical methods have been designed (see, e.g., Liu & Wu, 2016; Wu *et al.*, 2016; Liu *et al.*, 2017; Liu & Wu, 2017a,b). With this premise this paper focuses on the formulation and analyses of energy-preserving schemes for high-dimensional nonlinear Klein–Gordon equations, based on the DG method and the Duhamel principle. We will formulate the energy-preserving scheme and analyse its errors, nonlinear stability, convergence and implementation issues. Numerical simulations will be presented to show the remarkable superiority of the new scheme in comparison with well-known energy-preserving methods in the scientific literature.

2. Formulation of energy-preserving schemes

In order to derive energy-preserving schemes for high-dimensional nonlinear Klein–Gordon equations we first formulate equation (1.1) as an abstract Hamiltonian system of ODEs on an infinite-dimensional Hilbert space $L^2(\Omega)$.

Define the linear differential operator $\mathscr{A}$ by

$$(\mathscr{A}u)(x,t) = -\omega^2 \Delta u(x,t). \tag{2.1}$$

For the periodic boundary condition (1.2) the domain of this operator is

$$\begin{aligned} D(\mathscr{A}) =& \{u \in H^2(\boldsymbol{\Omega}) : u(x,t)|_{\partial\boldsymbol{\Omega}\cap\{x_j=0\}} = u(x,t)|_{\partial\boldsymbol{\Omega}\cap\{x_j=X_j\}}, \\ & \nabla u(x,t)|_{\partial\boldsymbol{\Omega}\cap\{x_j=0\}} = \nabla u(x,t)|_{\partial\boldsymbol{\Omega}\cap\{x_j=X_j\}}, \quad j=1,2,\ldots,d\}. \end{aligned} \tag{2.2}$$

On the basis of self-adjoint operator theories we introduce the following semigroup generated by $\mathscr{A}$:

$$\phi_j(\mathscr{A}) := \sum_{k=0}^{\infty} \frac{(-1)^k \mathscr{A}^k}{(2k+j)!}, \quad j = 0,1,2,\ldots. \tag{2.3}$$

It is noted that the definitions and properties of these functions for different boundary conditions have been researched in Liu & Wu (2017b). Here we summarise the following two propositions that are needed in this paper.

Proposition 2.1 (See Liu & Wu, 2017b). All the operator-argument functions ϕ_j for $j \in \mathbb{N}$ are symmetric operators with respect to the inner product of the space $L^2(\boldsymbol{\Omega})$,

$$(p,q) = \int_{\boldsymbol{\Omega}} p(x)\overline{q(x)}\,\mathrm{d}x. \tag{2.4}$$

The norm of the function in $L^2(\boldsymbol{\Omega})$ can be characterised in the frequency space by

$$\|q\|^2 = (q,q) = \int_{\boldsymbol{\Omega}} |q(x)|^2\,\mathrm{d}x.$$

Proposition 2.2 (See Liu & Wu, 2017b). All the operator-argument functions defined by (2.3) are bounded as

$$\|\phi_j(t\mathscr{A})\|_* \leqslant \gamma_j, \qquad j \in \mathbb{N}, \qquad t \geqslant 0, \tag{2.5}$$

where $\|\cdot\|_*$ is the Sobolev norm and γ_j are the bounds of the functions $\phi_j(x)$ with $x \geqslant 0$. It follows from (2.5) that

$$\|\phi_j(t\mathscr{A})\|_* \leqslant 1, \quad j = 0,1, \qquad \|\phi_2(t\mathscr{A})\|_* \leqslant \tfrac{1}{2}.$$

Obviously, the operator $\mathscr{A}$ defined by (2.1) is a positive semidefinite operator, i.e.,

$$\Big(\mathscr{A}u(x,t), u(x,t)\Big) = \int_{\boldsymbol{\Omega}} \mathscr{A}u(x,t)\cdot u(x,t)\,\mathrm{d}x = \omega^2 \int_{\boldsymbol{\Omega}} |\nabla u(x,t)|^2\,\mathrm{d}x \geqslant 0, \quad \forall\, u(x,t) \in D(\mathscr{A}). \tag{2.6}$$

Therefore, the exact energy (1.3) can be presented in the form

$$\mathscr{H}[u,v](t) \equiv \tfrac{1}{2}\Big(v(x,t), v(x,t)\Big) + \tfrac{1}{2}\Big(\mathscr{A}u(x,t), u(x,t)\Big) + \int_{\boldsymbol{\Omega}} G\big(u(x,t)\big)\,\mathrm{d}x = \mathscr{H}[u,v](0). \tag{2.7}$$

By defining $u(t)$ as the function that maps x to $u(x,t)$,

$$u(t) = [x \mapsto u(x,t)],$$

we formulate the original system (1.1) as

$$\begin{cases} u'(t) = v(t), & u(0) = g_1(x), \\ v'(t) = -\mathscr{A}u(t) - G'(u(t)), & v(0) = g_2(x). \end{cases} \tag{2.8}$$

We then have the following Duhamel principle for the nonlinear Klein–Gordon equation (1.1):

$$\begin{cases} u(t) = \phi_0\big(t^2\mathscr{A}\big)u(0) + t\phi_1\big(t^2\mathscr{A}\big)v(0) - \displaystyle\int_0^t (t-\zeta)\phi_1\big((t-\zeta)^2\mathscr{A}\big)G'\big(u(\zeta)\big)\,\mathrm{d}\zeta, \\ v(t) = -t\mathscr{A}\phi_1\big(t^2\mathscr{A}\big)u(0) + \phi_0\big(t^2\mathscr{A}\big)v(0) - \displaystyle\int_0^t \phi_0\big((t-\zeta)^2\mathscr{A}\big)G'\big(u(\zeta)\big)\,\mathrm{d}\zeta, \end{cases} \tag{2.9}$$

for all $t \in [0,T]$.

It follows from (2.9) that

$$\begin{cases} u(t_{n+1}) = \phi_0\big(\mathscr{V}\big)u(t_n) + h\phi_1\big(\mathscr{V}\big)v(t_n) - h^2\displaystyle\int_0^1 (1-\zeta)\phi_1\big((1-\zeta)^2\mathscr{V}\big)G'\big(u(t_n+h\zeta)\big)\,\mathrm{d}\zeta, \\ v(t_{n+1}) = -h\mathscr{A}\phi_1\big(\mathcal{V}\big)u(t_n) + \phi_0\big(\mathscr{V}\big)v(t_n) - h\displaystyle\int_0^1 \phi_0\big((1-\zeta)^2\mathscr{V}\big)G'\big(u(t_n+h\zeta)\big)\,\mathrm{d}\zeta, \end{cases} \tag{2.10}$$

where h is the time-step size, $t_n = nh$ and $\mathscr{V} = h^2\mathscr{A}$.

We recall the definition of a DG and define the following DG of function $G(u)$:

$$\begin{cases} \overline{\nabla}G(u,\hat{u}) \cdot \big(\hat{u} - u\big) = G(\hat{u}) - G(u), \\ \overline{\nabla}G(u,u) = G'(u). \end{cases} \tag{2.11}$$

Replacing $G'\big(u(t_n+h\zeta)\big)$ with $\overline{\nabla}G(u_n,u_{n+1})$ the integrals appearing in (2.10) can be approximated by

$$\begin{aligned} &\int_0^1 (1-\zeta)\phi_1\big((1-\zeta)^2\mathscr{V}\big)G'\big(u(t_n+h\zeta)\big)\,\mathrm{d}\zeta \\ &\quad\approx \int_0^1 (1-\zeta)\phi_1\big((1-\zeta)^2\mathscr{V}\big)\,\mathrm{d}\zeta\,\overline{\nabla}G(u_n,u_{n+1}) = \phi_2\big(\mathscr{V}\big)\overline{\nabla}G(u_n,u_{n+1}), \\ &\int_0^1 \phi_0\big((1-\zeta)^2\mathscr{V}\big)G'\big(u(t_n+h\zeta)\big)\,\mathrm{d}\zeta \approx \int_0^1 \phi_0\big((1-\zeta)^2\mathscr{V}\big)\,\mathrm{d}\zeta\,\overline{\nabla}G(u_n,u_{n+1}) = \phi_1\big(\mathscr{V}\big)\overline{\nabla}G(u_n,u_{n+1}), \end{aligned}$$

where the following results given in Liu & Wu (2016) have been used:

$$\int_0^1 (1-\zeta)\phi_1\big((1-\zeta)^2\mathscr{V}\big)\,\mathrm{d}\zeta = \phi_2(\mathscr{V}), \qquad \int_0^1 \phi_0\big((1-\zeta)^2\mathscr{V}\big)\,\mathrm{d}\zeta = \phi_1(\mathscr{V}).$$

The above analysis yields a continuous function $u_n := u_n(x) \approx u(x,t_n)$ and we present the following numerical scheme for the high-dimensional nonlinear Klein–Gordon equation (2.8).

DEFINITION 2.3 The DG scheme for solving the high-dimensional nonlinear Klein–Gordon equation (2.8) is defined as

$$\begin{cases} u_{n+1} = \phi_0(\mathscr{V})u_n + h\phi_1(\mathscr{V})v_n - h^2\phi_2(\mathscr{V})\overline{\nabla}G(u_n, u_{n+1}), \\ v_{n+1} = -h\mathscr{A}\phi_1(\mathscr{V})u_n + \phi_0(\mathscr{V})v_n - h\phi_1(\mathscr{V})\overline{\nabla}G(u_n, u_{n+1}), \end{cases} \tag{2.12}$$

which is referred to as the KGDG scheme, where $\overline{\nabla}G(u_n, u_{n+1})$ is determined by (2.11).

REMARK 2.4 It is noted that this KGDG scheme is based on the functions ϕ_j for $j = 0, 1, 2$. There are some other numerical integrators for Klein–Gordon equations, which are also formulated by the ϕ_j functions (see, e.g., Liu *et al.*, 2017; Liu & Wu, 2017a). Although these methods share the same ϕ_j functions they are derived for different purposes. The schemes given in Liu *et al.* (2017) and Liu & Wu (2017a) are formulated to be of any high order and our KGDG scheme is devoted to preserving the continuous energy (1.3) exactly.

THEOREM 2.5 The KGDG scheme (2.12) exactly preserves the Hamiltonian (2.7), i.e.,

$$\mathscr{H}[u_{n+1}, v_{n+1}] = \mathscr{H}[u_n, v_n], \quad n = 0, 1, \ldots. \tag{2.13}$$

Proof. Inserting (2.12) into (2.7) and calculating carefully with Proposition 2.1 we have

$$\begin{aligned} \mathscr{H}[u_{n+1}, v_{n+1}] = {} & \tfrac{1}{2}\Big(\big(\phi_0^2(\mathscr{V}) + \mathscr{V}\phi_1^2(\mathscr{V})\big)v_n, v_n\Big) + \tfrac{1}{2}\Big(\mathscr{A}\big(\phi_0^2(\mathscr{V}) + \mathscr{V}\phi_1^2(\mathscr{V})\big)u_n, u_n\Big) \\ & + \Big(\mathscr{V}\big(\phi_1^2(\mathscr{V}) - \phi_0(\mathscr{V})\phi_2(\mathscr{V})\big)u_n, \overline{\nabla}G(u_n, u_{n+1})\Big) \\ & - \Big(h\big(\phi_0(\mathscr{V})\phi_1(\mathscr{V}) + \mathscr{V}\phi_1(\mathscr{V})\phi_2(\mathscr{V})\big)v_n, \overline{\nabla}G(u_n, u_{n+1})\Big) \\ & + \tfrac{1}{2}\Big(h^2\big(\phi_1^2(\mathscr{V}) + \mathscr{V}\phi_2^2(\mathscr{V})\big)\overline{\nabla}G(u_n, u_{n+1}), \overline{\nabla}G(u_n, u_{n+1})\Big) + \int_{\boldsymbol{\Omega}} G\big(u_{n+1}\big)\,\mathrm{d}x. \end{aligned} \tag{2.14}$$

On the basis of the following results on the operator-argument functions (see Liu & Wu, 2017b),

$$\begin{cases} \phi_0^2(\mathscr{V}) + \mathscr{V}\phi_1^2(\mathscr{V}) = I, \\ \phi_1^2(\mathscr{V}) - \phi_0(\mathscr{V})\phi_2(\mathscr{V}) = \phi_2(\mathscr{V}), \\ \phi_0(\mathscr{V})\phi_1(\mathscr{V}) + \mathscr{V}\phi_1(\mathscr{V})\phi_2(\mathscr{V}) = \phi_1(\mathscr{V}), \\ \frac{1}{2}\big(\phi_1^2(\mathscr{V}) + \mathscr{V}\phi_2^2(\mathscr{V})\big) = \phi_2(\mathscr{V}), \end{cases}$$

(2.14) can be simplified as

$$\begin{aligned} \mathscr{H}[u_{n+1}, v_{n+1}] = {} & \tfrac{1}{2}(v_n, v_n) + \tfrac{1}{2}(\mathscr{A}u_n, u_n) + \Big(\mathscr{V}\phi_2(\mathscr{V})u_n, \overline{\nabla}G(u_n, u_{n+1})\Big) \\ & - \Big(h\phi_1(\mathscr{V})v_n, \overline{\nabla}G(u_n, u_{n+1})\Big) + \Big(h^2\phi_2(\mathscr{V})\overline{\nabla}G(u_n, u_{n+1}), \overline{\nabla}G(u_n, u_{n+1})\Big) \\ & + \int_{\boldsymbol{\Omega}} G\big(u_{n+1}\big)\,\mathrm{d}x. \end{aligned} \tag{2.15}$$

In the case of $u_{n+1}-u_n=0$ the first equation of (2.12) yields

$$\begin{aligned}0=u_{n+1}-u_n&=\Big(\phi_0\big(\mathscr{V}\big)-I\Big)u_n+h\phi_1\big(\mathscr{V}\big)v_n-h^2\phi_2\big(\mathscr{V}\big)\overline{\nabla}G(u_n,u_{n+1})\\&=-\mathscr{V}\phi_2(\mathscr{V})u_n+h\phi_1\big(\mathscr{V}\big)v_n-h^2\phi_2\big(\mathscr{V}\big)\overline{\nabla}G(u_n,u_{n+1}),\end{aligned}$$

where we have used the following result given in Liu & Wu (2017b):

$$\phi_0(\mathscr{V})-I=-\mathscr{V}\phi_2(\mathscr{V}).$$

According to $\overline{\nabla}G(u_n,u_n)=\nabla G(u_n)$, (2.15) becomes

$$\begin{aligned}\mathscr{H}[u_{n+1},v_{n+1}]&=\mathscr{H}[u_n,v_{n+1}]\\&=\tfrac{1}{2}(v_n,v_n)+\tfrac{1}{2}(\mathscr{A}u_n,u_n)+\Big(\mathscr{V}\phi_2(\mathscr{V})u_n,G'(u_n)\Big)\\&\quad-\Big(h\phi_1(\mathscr{V})v_n,G'(u_n)\Big)+\Big(h^2\phi_2(\mathscr{V})G'(u_n),G'(u_n)\Big)+\int_{\boldsymbol{\Omega}}G\big(u_n\big)\,\mathrm{d}x\\&=\tfrac{1}{2}(v_n,v_n)+\tfrac{1}{2}(\mathscr{A}u_n,u_n)+\int_{\boldsymbol{\Omega}}G\big(u_n\big)\,\mathrm{d}x\\&\quad+\Big(\mathscr{V}\phi_2(\mathscr{V})u_n-h\phi_1(\mathscr{V})v_n+h^2\phi_2(\mathscr{V})G'(u_n),\nabla G(u_n)\Big)\\&=\mathscr{H}[u_n,v_n]+\Big(0,G'(u_n)\Big)=\mathscr{H}[u_n,v_n].\end{aligned}$$

If $u_{n+1}-u_n\neq 0$ then

$$G\big(u_{n+1}\big)-G\big(u_n\big)=\overline{\nabla}G(u_n,u_{n+1})\cdot\big(u_{n+1}-u_n\big),$$

and we arrive at

$$\begin{aligned}\int_{\boldsymbol{\Omega}}G\big(u_{n+1}\big)\,\mathrm{d}x&=\int_{\boldsymbol{\Omega}}G\big(u_n\big)\,\mathrm{d}x+\int_{\boldsymbol{\Omega}}\Big(G\big(u_{n+1}\big)-G\big(u_n\big)\Big)\,\mathrm{d}x\\&=\int_{\boldsymbol{\Omega}}G\big(u_n\big)\,\mathrm{d}x+\Big(\big(u_{n+1}-u_n\big)I,\overline{\nabla}G(u_n,u_{n+1})\Big).\end{aligned}\tag{2.16}$$

It follows from the first equation of (2.12) that

$$u_{n+1}-u_n=-\mathscr{V}\phi_2(\mathscr{V})u_n+h\phi_1\big(\mathscr{V}\big)v_n-h^2\phi_2\big(\mathscr{V}\big)\overline{\nabla}G(u_n,u_{n+1}).$$

Equation (2.16) then can accordingly be rewritten as

$$\begin{aligned}\int_{\boldsymbol{\Omega}}G\big(u_{n+1}\big)\,\mathrm{d}x&=\int_{\boldsymbol{\Omega}}G\big(u_n\big)\,\mathrm{d}x-\Big(\mathscr{V}\phi_2(\mathscr{V})u_n,\overline{\nabla}G(u_n,u_{n+1})\Big)\\&\quad+\Big(h\phi_1\big(\mathscr{V}\big)v_n,\overline{\nabla}G(u_n,u_{n+1})\Big)-\Big(h^2\phi_2\big(\mathscr{V}\big)\overline{\nabla}G(u_n,u_{n+1}),\overline{\nabla}G(u_n,u_{n+1})\Big).\end{aligned}\tag{2.17}$$

Inserting (2.17) into (2.15) yields

$$\begin{aligned}\mathscr{H}[u_{n+1},v_{n+1}] =& \tfrac{1}{2}(v_n,v_n)+\tfrac{1}{2}(\mathscr{A}u_n,u_n)+\Big(\mathscr{V}\phi_2(\mathscr{V})u_n,\overline{\nabla}G(u_n,u_{n+1})\Big)-\Big(h\phi_1(\mathscr{V})v_n,\overline{\nabla}G(u_n,u_{n+1})\Big)\\ &+\Big(h^2\phi_2(\mathscr{V})\overline{\nabla}G(u_n,u_{n+1}),\overline{\nabla}G(u_n,u_{n+1})\Big)+\int_{\Omega}G(u_n)\,\mathrm{d}x-\Big(\mathscr{V}\phi_2(\mathscr{V})u_n,\overline{\nabla}G(u_n,u_{n+1})\Big)\\ &+\Big(h\phi_1(\mathscr{V})v_n,\overline{\nabla}G(u_n,u_{n+1})\Big)-\Big(h^2\phi_2(\mathscr{V})\overline{\nabla}G(u_n,u_{n+1}),\overline{\nabla}G(u_n,u_{n+1})\Big)\\ =&\tfrac{1}{2}(v_n,v_n)+\tfrac{1}{2}(\mathscr{A}u_n,u_n)+\int_{\Omega}G(u_n)\,\mathrm{d}x=\mathscr{H}[u_n,v_n].\end{aligned}$$

This proof is complete. □

Remark 2.6 There are many possible choices of DGs for a function; see Hairer *et al.* (2006) and McLachlan *et al.* (1999) for example. Among typical DGs is the well-known AVF method defined by

$$\overline{\nabla}_{\mathrm{AVF}}G(u_n,u_{n+1})=\int_0^1 G'\big((1-\tau)u_n+\tau u_{n+1}\big)\,\mathrm{d}\tau.$$

Under this special choice the KGDG scheme (2.12) reduces to the AAVF method, which has been researched in Liu & Wu (2016, 2017b) for nonlinear wave equations. Moreover, when $\omega=0$, the energy-preserving scheme (2.12) reduces to the AVF method for the semidiscretised Hamiltonian PDEs studied in Celledoni *et al.* (2012). In other words, the KGDG scheme (2.12) is an essential extension of AAVF and AVF methods from Hamiltonian ODEs to Hamiltonian PDEs. Furthermore, it is noted that the analyses of errors, nonlinear stability and convergence of AAVF and AVF methods for PDEs have not been considered so far. Therefore, a primary mission of this work is to analyse the errors, nonlinear stability and convergence of KGDG methods for high-dimensional nonlinear Klein–Gordon equations, which puts the present work in a more general setting.

Remark 2.7 It is noted that an extended DG method for Hamiltonian ODEs was researched in Liu *et al.* (2013) and applied to conservative (dissipative) nonlinear wave PDEs in Liu *et al.* (2017). However, this method was presented in a scheme for ODEs and applied only to semidiscrete PDEs; i.e., spatial derivatives are discretised in advance. Therefore, it cannot preserve the continuous energy of the PDEs exactly. Moreover, the errors, nonlinear stability and convergence of this method were not analysed in Liu *et al.* (2017). It is remarked that our scheme (2.12) reduces to the extended DG method when applied to second-order oscillatory ODEs considered in Liu *et al.* (2013). Furthermore, our method for nonlinear Klein–Gordon equations is based on the operator-variation-of-constants formula and depends on the differential operator $\mathscr{V}$. This means that our scheme does not require the PDEs to be discretised in space and avoids the semidiscretisation of the spatial derivative. Moreover, our scheme can preserve the continuous energy of the PDEs exactly. Scheme (2.12) is more suitable and competitive since different efficient ways to approximate the operator in the literature can be chosen in a flexible approach, according to different situations and requirements.

Theorem 2.8 The KGDG scheme (2.12) is symmetric with respect to the time variable.

Proof. It follows immediately from exchanging $u_{n+1}\leftrightarrow u_n$, $v_{n+1}\leftrightarrow v_n$ and replacing h by $-h$ in (2.12). □

3. Error analysis

In this section we analyse the local error bounds of the energy-preserving scheme (2.12) under the following assumption.

ASSUMPTION 3.1 It is assumed that $f(u) = -G'(u) : D(\mathscr{A}) \to \mathbb{R}$ is sufficiently often Fréchet differentiable in a strip along the exact solution and is sufficiently smooth with respect to time. Moreover, there exists a real number k such that

$$\|f(w_1) - f(w_2)\| \leqslant k\|w_1 - w_2\|$$

for all $w_1, w_1 \in L^2(\Omega)$.

THEOREM 3.2 Assume that the Klein–Gordon equation (1.1) possesses uniformly bounded and sufficiently smooth solutions with respect to time and $f(u)$ satisfies Assumption 3.1. Suppose that $f_t'' \in L^\infty(0,T;L^2(\Omega))$. Under the local assumptions of $u_n = u(t_n)$, $v_n = v(t_n)$, if the sufficiently small time-step size h satisfies $0 < h \leqslant \sqrt{\frac{2}{k}}$ then the local error bounds of (2.12) are given as

$$\|u(t_{n+1}) - u_{n+1}\| \leqslant Ch^3 \quad \text{and} \quad \|v(t_{n+1}) - v_{n+1}\| \leqslant Ch^3. \tag{3.1}$$

Proof. Inserting the exact solution of (2.8) into the approximation (2.12) we obtain

$$\begin{cases} u(t_{n+1}) = \phi_0(\mathscr{V})u(t_n) + h\phi_1(\mathscr{V})v(t_n) - h^2\phi_2(\mathscr{V})\overline{\nabla}G\big(u(t_n), u(t_{n+1})\big) + \delta_{n+1}, \\ v(t_{n+1}) = -h\mathscr{A}\phi_1(\mathscr{V})u(t_n) + \phi_0(\mathscr{V})v(t_n) - h\phi_1(\mathscr{V})\overline{\nabla}G\big(u(t_n), u(t_{n+1})\big) + \delta'_{n+1}, \end{cases} \tag{3.2}$$

where δ_{n+1} and δ'_{n+1} express the discrepancies. It follows from (3.2) and (2.10) that

$$\begin{cases} \delta_{n+1} = h^2\displaystyle\int_0^1 (1-\zeta)\phi_1\big((1-\zeta)^2\mathscr{V}\big)f\big(u(t_n + h\zeta)\big)\,\mathrm{d}\zeta + h^2\phi_2(\mathscr{V})\overline{\nabla}G\big(u(t_n), u(t_{n+1})\big), \\ \delta'_{n+1} = h\displaystyle\int_0^1 \phi_0\big((1-\zeta)^2\mathscr{V}\big)f\big(u(t_n + h\zeta)\big)\,\mathrm{d}\zeta + h\phi_1(\mathscr{V})\overline{\nabla}G\big(u(t_n), u(t_{n+1})\big). \end{cases} \tag{3.3}$$

Expressing f and G of formula (3.3) by the Taylor series expansion at $u(t_n)$ yields

$$\delta_{n+1} = h^2\phi_2(\mathscr{V})f\big(u(t_n)\big) + \mathcal{O}\big(h^3\big) - h^2\phi_2(\mathscr{V})f\big(u(t_n)\big) + \mathcal{O}\big(h^3\big) = \mathcal{O}\big(h^3\big),$$

and

$$\begin{aligned} \delta'_{n+1} =& h\phi_1(\mathscr{V})f\big(u(t_n)\big) + h^2\phi_2(\mathscr{V})\frac{\partial f\big(u(t)\big)}{\partial t}|_{t=t_n} + \mathcal{O}\big(h^3\big) \\ & - h\phi_1(\mathscr{V})f\big(u(t_n)\big) - \tfrac{1}{2}h\phi_1(\mathscr{V})f'\big(u(t_n)\big)\big(u(t_{n+1}) - u(t_n)\big) + \mathcal{O}\big(h^3\big) \\ =& h^2\phi_2(\mathscr{V})\frac{\partial f\big(u(t)\big)}{\partial t}|_{t=t_n} - \tfrac{1}{2}h\phi_1(\mathscr{V})f'\big(u(t_n)\big)\big(u(t_{n+1}) - u(t_n)\big) + \mathcal{O}\big(h^3\big) \\ =& h^2\phi_2(\mathscr{V})\frac{\partial f\big(u(t)\big)}{\partial t}|_{t=t_n} - \tfrac{1}{2}h\phi_1(\mathscr{V})f'\big(u(t_n)\big)\left(h\frac{\partial u(t)}{\partial t}|_{t=t_n} + \mathcal{O}\big(h^2\big)\right) + \mathcal{O}\big(h^3\big) \\ =& h^2\left(\phi_2(\mathscr{V}) - \tfrac{1}{2}\phi_1(\mathscr{V})\right)\frac{\partial f\big(u(t)\big)}{\partial t}|_{t=t_n} + \mathcal{O}\big(h^3\big) = \mathcal{O}\big(h^3\big). \end{aligned}$$

We set

$$e_n^u = u(t_n) - u_n, \qquad e_n^v = v(t_n) - v_n.$$

Subtracting (2.12) from (3.2) yields

$$\begin{cases} e_{n+1}^u = h^2\phi_2(\mathscr{V})\overline{\nabla}G(u_n, u_{n+1}) - h^2\phi_2(\mathscr{V})\overline{\nabla}G\big(u(t_n), u(t_{n+1})\big) + \delta_{n+1}, \\ e_{n+1}^v = h\phi_1(\mathscr{V})\overline{\nabla}G(u_n, u_{n+1}) - h\phi_1(\mathscr{V})\overline{\nabla}G\big(u(t_n), u(t_{n+1})\big) + \delta'_{n+1}, \end{cases}$$

which gives

$$\begin{aligned} \big\|e_{n+1}^u\big\| &\leqslant h^2\|\phi_2(\mathscr{V})\|\tfrac{1}{2}k\big\|e_{n+1}^u\big\| + \big\|\delta_{n+1}\big\| \leqslant \tfrac{1}{4}h^2k\big\|e_{n+1}^u\big\| + \|\delta_{n+1}\|, \\ \big\|e_{n+1}^v\big\| &\leqslant h\|\phi_1(\mathscr{V})\|\tfrac{1}{2}k\big\|e_{n+1}^u\big\| + \big\|\delta'_{n+1}\big\| \leqslant \tfrac{1}{2}hk\big\|e_{n+1}^u\big\| + \big\|\delta'_{n+1}\big\|. \end{aligned} \tag{3.4}$$

If the time-step size h satisfies $h \leqslant \sqrt{\frac{2}{k}}$ then the first inequality in (3.4) implies

$$\big\|e_{n+1}^u\big\| \leqslant 2\big\|\delta_{n+1}\big\| \leqslant Ch^3.$$

Furthermore, from this result and the second inequality in (3.4) we obtain $\|e_{n+1}^v\| \leqslant Ch^3$. We thus obtain the desired result. □

4. Analysis of the nonlinear stability

This section is devoted to the study of the nonlinear stability of our energy-preserving scheme (2.12). To this end we consider the following perturbed problem of (2.8):

$$\begin{cases} \tilde{u}'(t) = \tilde{v}(t), & \tilde{u}(0) = g_1(x) + \tilde{g}_1(x), \\ \tilde{v}'(t) = -\mathscr{A}\tilde{u}(t) - G'(\tilde{u}(t)), & \tilde{v}(0) = g_2(x) + \tilde{g}_2(x), \end{cases} \tag{4.1}$$

where $\tilde{g}_1(x), \tilde{g}_2(x)$ are perturbation functions. Let

$$\hat{u}(t) = \tilde{u}(t) - u(t), \qquad \hat{v}(t) = \tilde{v}(t) - v(t).$$

Subtracting (2.8) from (4.1) leads to

$$\begin{cases} \hat{u}'(t) = \hat{v}(t), & \hat{u}(0) = \tilde{g}_1(x), \\ \hat{v}'(t) = -\mathscr{A}\hat{u}(t) - G'(\tilde{u}(t)) + G'(u(t)), & \hat{v}(0) = \tilde{g}_2(x). \end{cases} \tag{4.2}$$

Applying the approximation (2.12) to (2.8) and (4.1), respectively, we obtain two numerical schemes, which give an approximation of (4.2) as

$$\begin{cases} \hat{u}_{n+1} = \phi_0(\mathscr{V})\hat{u}_n + h\phi_1(\mathscr{V})\hat{v}_n + h^2\phi_2(\mathscr{V})\tilde{\mathscr{I}}, \\ \hat{v}_{n+1} = -h\mathscr{A}\phi_1(\mathscr{V})\hat{u}_n + \phi_0(\mathscr{V})\hat{v}_n + h\phi_1(\mathscr{V})\tilde{\mathscr{I}}, \end{cases} \tag{4.3}$$

where

$$\tilde{\mathscr{I}} = \overline{\nabla} G(u_n, u_{n+1}) - \overline{\nabla} G(\tilde{u}_n, \tilde{u}_{n+1}). \tag{4.4}$$

Until now we have mostly considered the situation where the PDE is discretised in time while remaining continuous in space. In order to obtain practical numerical schemes it remains to deal with the differential operator $\mathscr{A}$ in an appropriate way. Arguably, one straightforward approach to dealing with the space derivatives is simply to discretise them in the Hamiltonian. In this situation the operator $\mathscr{A}$ is approximated by a suitable differential matrix. For ODEs it is common to devise relatively general frameworks for structure preservation. Therefore, we usually approximate the operator $\mathscr{A}$ by a symmetric and positive semidefinite differential matrix, in such a way that we can derive corresponding Hamiltonian ODEs and obtain reasonable and rigorous nonlinear stability and convergence analysis. Fortunately, there are many publications that have proposed various effective ways to deal with the spatial derivatives (see, e.g., Hesthaven *et al.*, 2007; Bank *et al.*, 2008; Shen *et al.*, 2011), and the symmetric and positive semidefinite differential matrix is easily found. Through the space discretisation of a Hamiltonian PDE one may obtain a system of Hamiltonian ODEs to which a geometric numerical integrator may be applied.

The following result states the nonlinear stability of our energy-preserving approximation (2.12) when the operator $\mathscr{A}$ is approximated by a suitable differential matrix.

THEOREM 4.1 It is assumed that the conditions of Theorem 3.2 are true and that the operator $\mathscr{A}$ is approximated by a symmetric and positive semidefinite differential matrix A. Then if the time-step size h satisfies $0 < h \leqslant \sqrt{\frac{2}{k}}$ we have the following nonlinear stability results:

$$\begin{aligned} \|\hat{u}_n\| &\leqslant \exp\big(\hat{C}T\big)\left(\|\tilde{g}_1\| + \sqrt{\|\sqrt{A}\tilde{g}_1\|^2 + \|\tilde{g}_2\|^2}\right), \\ \|\hat{v}_n\| &\leqslant \exp\big(\hat{C}T\big)\left(\|\tilde{g}_1\| + \sqrt{\|\sqrt{A}\tilde{g}_1\|^2 + \|\tilde{g}_2\|^2}\right), \end{aligned} \tag{4.5}$$

where $k > 0$ is a Lipchitz constant, and $\hat{C}$ and $\sqrt{A}$ are defined in the proof.

Proof. Under the condition given in this theorem the matrix A can be expressed as

$$A = P^{\intercal} D^2 P = \sqrt{A}^2,$$

where P is an orthogonal matrix, D is a positive semidefinite diagonal matrix and $\sqrt{A} = P^{\intercal} D P$. Thus, (4.3) becomes

$$\begin{cases} \hat{u}_{n+1} = \phi_0\big(K\big)\hat{u}_n + h\phi_1\big(K\big)\hat{v}_n + h^2\phi_2\big(K\big)\tilde{\mathscr{I}}, \\ \hat{v}_{n+1} = -hA\phi_1\big(K\big)\hat{u}_n + \phi_0\big(K\big)\hat{v}_n + h\phi_1\big(K\big)\tilde{\mathscr{I}} \end{cases} \tag{4.6}$$

with $K = h^2 A$. It follows from the first formula of (4.6) that

$$\|\hat{u}_{n+1}\| \leqslant \|\hat{u}_n\| + h\|\hat{v}_n\| + \tfrac{1}{2}h^2\|\tilde{\mathscr{I}}\|. \tag{4.7}$$

Rewriting (4.6) in the matrix–vector form

$$\begin{pmatrix}\sqrt{A}\hat{u}_{n+1}\\ \hat{v}_{n+1}\end{pmatrix}=\begin{pmatrix}\phi_0(K) & h\sqrt{A}\phi_1(K)\\ -h\sqrt{A}\phi_1(K) & \phi_0(K)\end{pmatrix}\begin{pmatrix}\sqrt{A}\hat{u}_n\\ \hat{v}_n\end{pmatrix}+h\begin{pmatrix}h\sqrt{A}\phi_2(K) & \\ & \phi_1(K)\end{pmatrix}\begin{pmatrix}\tilde{\mathscr{I}}\\ \tilde{\mathscr{I}}\end{pmatrix},$$

we arrive at

$$\sqrt{\|\sqrt{A}\hat{u}_{n+1}\|^2+\|\hat{v}_{n+1}\|^2}\leqslant\sqrt{\|\sqrt{A}\hat{u}_n\|^2+\|\hat{v}_n\|^2}+h\tilde{\alpha}\|\tilde{\mathscr{I}}\|.$$

Here $\tilde{\alpha}$ is the uniformly bound of $\begin{pmatrix}h\sqrt{A}\phi_2(K) & \\ & \phi_1(K)\end{pmatrix}$ and we used the fact (see Liu & Wu, 2017a) that

$$\left\|\begin{pmatrix}\phi_0(K) & h\sqrt{A}\phi_1(K)\\ -h\sqrt{A}\phi_1(K) & \phi_0(K)\end{pmatrix}\right\|=1.$$

Summing the above results yields

$$\begin{aligned}\|\hat{u}_{n+1}\|+&\sqrt{\|\sqrt{A}\hat{u}_{n+1}\|^2+\|\hat{v}_{n+1}\|^2}\\ &\leqslant\|\hat{u}_n\|+\sqrt{\|\sqrt{A}\hat{u}_n\|^2+\|\hat{v}_n\|^2}+h\|\hat{v}_n\|+h\left(\tilde{\alpha}+\frac{h}{2}\right)\|\tilde{\mathscr{I}}\|.\end{aligned}\tag{4.8}$$

With reference to definition (4.4) of $\tilde{\mathscr{I}}$ the following result is obtained:

$$\|\tilde{\mathscr{I}}\|\leqslant k\int_0^1\left\|\left((1-\tau)\hat{u}_n+\tau\hat{u}_{n+1}\right)\right\|\mathrm{d}\tau\leqslant\tfrac{1}{2}k\left(\|\hat{u}_n\|+\|\hat{u}_{n+1}\|\right).\tag{4.9}$$

Inserting (4.9) into (4.7) yields

$$\|\hat{u}_{n+1}\|\leqslant\|\hat{u}_n\|+h\|\hat{v}_n\|+\tfrac{1}{4}h^2k\left(\|\hat{u}_n\|+\|\hat{u}_{n+1}\|\right),$$

so that we obtain

$$\left(1-\tfrac{1}{4}h^2k\right)\|\hat{u}_{n+1}\|\leqslant\left(1+\tfrac{1}{4}h^2k\right)\|\hat{u}_n\|+h\|\hat{v}_n\|.$$

If h satisfies $h\leqslant\sqrt{\frac{2}{k}}$ then we get

$$\|\hat{u}_{n+1}\|\leqslant3\|\hat{u}_n\|+2h\|\hat{v}_n\|.$$

Combining this result with (4.8) and (4.9) gives

$$\begin{aligned}
&\|\hat{u}_{n+1}\| + \sqrt{\|\sqrt{A}\hat{u}_{n+1}\|^2 + \|\hat{v}_{n+1}\|^2} \\
&\quad\leqslant \|\hat{u}_n\| + \sqrt{\|\sqrt{A}\hat{u}_n\|^2 + \|\hat{v}_n\|^2} + h\|\hat{v}_n\| + \frac{h}{2}\left(\tilde{\alpha} + \frac{h}{2}\right)k\big(\|\hat{u}_n\| + 3\|\hat{u}_n\| + 2h\|\hat{v}_n\|\big) \\
&\quad\leqslant \|\hat{u}_n\| + \sqrt{\|\sqrt{A}\hat{u}_n\|^2 + \|\hat{v}_n\|^2} + \left(h + h^2\left(\tilde{\alpha} + \frac{h}{2}\right)k\right)\|\hat{v}_n\| + 2h\left(\tilde{\alpha} + \frac{h}{2}\right)k\|\hat{u}_n\| \\
&\quad\leqslant \|\hat{u}_n\| + \sqrt{\|\sqrt{A}\hat{u}_n\|^2 + \|\hat{v}_n\|^2} + h\hat{C}\Big(\|\hat{u}_n\| + \sqrt{\|\sqrt{A}\hat{u}_n\|^2 + \|\hat{v}_n\|^2}\Big),
\end{aligned}$$

where $\hat{C} = \max\big(1 + \tilde{\alpha}kh + \frac{kh^2}{2}, 2\tilde{\alpha}k + \frac{kh}{2}\big)$. The following result follows immediately by induction:

$$\begin{aligned}
\|\hat{u}_{n+1}\| + \sqrt{\|\sqrt{A}\hat{u}_{n+1}\|^2 + \|\hat{v}_{n+1}\|^2} &\leqslant \big(1 + h\hat{C}\big)^n\left(\|\hat{u}_0\| + \sqrt{\|\sqrt{A}\hat{u}_0\|^2 + \|\hat{v}_0\|^2}\right) \\
&\leqslant \exp\big(\hat{C}T\big)\left(\|\tilde{g}_1\| + \sqrt{\|\sqrt{A}\tilde{g}_1\|^2 + \|\tilde{g}_2\|^2}\right),
\end{aligned}$$

which proves this theorem. □

5. Convergence

In this section we pay attention to the convergence of the fully discrete approximation. By some suitable spatial discretisation strategies we discretise the original continuous system (2.8) as

$$\begin{cases} U'(t) = V(t), & U(0) = g_1(x), \\ V'(t) = -AU(t) - \nabla\widetilde{G}(U(t)) + \hat{\delta}(\Delta x), & V(0) = g_2(x), \end{cases} \tag{5.1}$$

where A is a symmetric and positive semidefinite differential matrix, Δx is the spatial-step size in the space discretisation, and U and V are assumed to be vectors belonging to R^M and $\widetilde{G}(U) = \sum_{j=1}^{M} G(U_j)$. It is noted that $\hat{\delta}(\Delta x)$ is the truncation error brought by approximating the spatial differential operator $\mathscr{A}$ through a matrix A.

Applying the numerical approximation (2.12) to (5.1) and ignoring $\hat{\delta}(\Delta x)$ we obtain

$$\begin{cases} U_{n+1} = \phi_0\big(K\big)U_n + h\phi_1\big(K\big)V_n - h^2\phi_2\big(K\big)\overline{\nabla}\widetilde{G}(U_n, U_{n+1}), \\ V_{n+1} = -hA\phi_1\big(K\big)U_n + \phi_0\big(K\big)V_n - h\phi_1\big(K\big)\overline{\nabla}\widetilde{G}(U_n, U_{n+1}). \end{cases} \tag{5.2}$$

The following result states the convergence of (5.2).

THEOREM 5.1 Under the conditions of Theorem 4.1 there exists a constant C such that

$$\begin{cases} \|U(t_n) - U_n\| \leqslant CT\exp(\hat{C}T)\big(h^2 + \|\hat{\delta}(\Delta x)\|\big), \\ \|V(t_n) - V_n\| \leqslant CT\exp(\hat{C}T)\big(h^2 + \|\hat{\delta}(\Delta x)\|\big), \end{cases} \tag{5.3}$$

where C is a constant independent of n, h and Δx.

Proof. Inserting the exact solution of (5.1) into the numerical approximation (2.12) yields

$$\begin{cases} U(t_{n+1}) = \phi_0(K)U(t_n) + h\phi_1(K)V(t_n) + h^2\phi_2(K)\displaystyle\int_0^1 f\big((1-\tau)U(t_n) + \tau U(t_{n+1})\big)\,\mathrm{d}\tau + \hat{\delta}_{n+1}, \\ V(t_{n+1}) = -hA\phi_1(K)U(t_n) + \phi_0(K)V(t_n) + h\phi_1(K)\displaystyle\int_0^1 f\big((1-\tau)U(t_n) + \tau U(t_{n+1})\big)\,\mathrm{d}\tau + \hat{\delta}'_{n+1}, \end{cases} \tag{5.4}$$

where $\hat{\delta}_{n+1}$ and $\hat{\delta}'_{n+1}$ are the discrepancies. According to these formulae and the operator-variation-of-constants formula (2.9) of (5.1) we have

$$\begin{cases} \hat{\delta}_{n+1} = h^2\displaystyle\int_0^1 (1-\zeta)\phi_1\big((1-\zeta)^2K\big)f\big(U(t_n+h\zeta)\big)\,\mathrm{d}\zeta + h^2\phi_2(K)\overline{\nabla}\widetilde{G}(U_n, U_{n+1}) \\ \qquad\quad + h^2\displaystyle\int_0^1 (1-z)\phi_1\big((1-z)^2K\big)\hat{\delta}(\Delta x)\,\mathrm{d}z, \\ \hat{\delta}'_{n+1} = h\displaystyle\int_0^1 \phi_0\big((1-\zeta)^2K\big)f\big(U(t_n+h\zeta)\big)\,\mathrm{d}\zeta + h\phi_1(K)\overline{\nabla}\widetilde{G}(U_n, U_{n+1}) \\ \qquad\quad + h\displaystyle\int_0^1 \phi_0\big((1-z)^2K\big)\hat{\delta}(\Delta x)\,\mathrm{d}z. \end{cases} \tag{5.5}$$

By repeating the same steps as Section 3 the following discrepancies are obtained:

$$\begin{aligned} \left\|\hat{\delta}_{n+1}\right\| &\leqslant C_1h^3 + h^2\left\|\int_0^1 (1-z)\phi_1\big((1-z)^2K\big)\hat{\delta}(\Delta x)\,\mathrm{d}z\right\|, \\ \left\|\hat{\delta}'_{n+1}\right\| &\leqslant C_2h^3 + h\left\|\int_0^1 \phi_0\big((1-z)^2K\big)\hat{\delta}(\Delta x)\,\mathrm{d}z\right\|. \end{aligned}$$

Consequently, we obtain

$$\|\hat{\delta}_{n+1}\| \leqslant C_1h^3 + \tfrac{1}{2}h^2\|\hat{\delta}(\Delta x)\|, \quad \left\|\hat{\delta}'_{n+1}\right\| \leqslant C_2h^3 + h\|\hat{\delta}(\Delta x)\|. \tag{5.6}$$

Denote

$$e_n^U = U(t_n) - U_n, \qquad e_n^V = V(t_n) - V_n.$$

The following system then easily follows by subtracting (5.2) from (5.4):

$$\begin{cases} e_{n+1}^U = \phi_0(K)e_n^U + h\phi_1(K)e_n^V + h^2\phi_2(K)\hat{\mathscr{I}} + \hat{\delta}_{n+1}, \\ e_{n+1}^V = -hA\phi_1(K)e_n^U + \phi_0(K)e_n^V + h\phi_1(K)\hat{\mathscr{I}} + \hat{\delta}'_{n+1}, \end{cases} \tag{5.7}$$

where

$$\hat{\mathscr{I}} = \overline{\nabla}\widetilde{G}(U_n, U_{n+1}) - \overline{\nabla}\widetilde{G}\big(U(t_n), U(t_{n+1})\big) \tag{5.8}$$

with the initial conditions $e_0^U = \mathbf{0}$ and $e_0^V = \mathbf{0}$. We rewrite (5.7) as

$$\begin{pmatrix} \sqrt{A}e_{n+1}^U \\ e_{n+1}^V \end{pmatrix} = \begin{pmatrix} \phi_0(K) & h\sqrt{A}\phi_1(K) \\ -h\sqrt{A}\phi_1(K) & \phi_0(K) \end{pmatrix} \begin{pmatrix} \sqrt{A}e_n^U \\ e_n^V \end{pmatrix} + h \begin{pmatrix} h\sqrt{A}\phi_2(K) & \\ & \phi_1(K) \end{pmatrix} \begin{pmatrix} \hat{\mathscr{I}} \\ \hat{\mathscr{I}} \end{pmatrix} + \begin{pmatrix} \sqrt{A}\hat{\delta}_{n+1} \\ \hat{\delta}'_{n+1} \end{pmatrix},$$

which yields

$$\sqrt{\left\|\sqrt{A}e_{n+1}^U\right\|^2 + \left\|e_{n+1}^V\right\|^2} \leqslant \sqrt{\left\|\sqrt{A}e_n^U\right\|^2 + \left\|e_n^V\right\|^2} + h\tilde{\alpha}\|\hat{\mathscr{I}}\| + \sqrt{\left\|\sqrt{A}\hat{\delta}_{n+1}\right\|^2 + \left\|\hat{\delta}'_{n+1}\right\|^2}.$$

Taking into account (5.8) gives

$$\|\hat{\mathscr{I}}\| \leqslant k\int_0^1 \left\|(1-\tau)e_n^U + \tau e_{n+1}^U\right\| \mathrm{d}\tau \leqslant \tfrac{1}{2}k\big(\left\|e_n^U\right\| + \left\|e_{n+1}^U\right\|\big).$$

It then follows from the first formula of (5.7) that

$$\begin{aligned} \left\|e_{n+1}^U\right\| &\leqslant \left\|e_n^U\right\| + h\left\|e_n^V\right\| + \tfrac{1}{2}h^2\left\|\hat{\mathscr{I}}\right\| + \left\|\hat{\delta}_{n+1}\right\| \\ &\leqslant \left\|e_n^U\right\| + h\left\|e_n^V\right\| + \tfrac{1}{4}h^2k\big(\left\|e_n^U\right\| + \left\|e_{n+1}^U\right\|\big) + \left\|\hat{\delta}_{n+1}\right\|. \end{aligned}$$

Using the condition $h \leqslant \sqrt{\frac{2}{k}}$ we arrive at

$$\left\|e_{n+1}^U\right\| \leqslant 3\left\|e_n^U\right\| + 2h\left\|e_n^V\right\| + 2\left\|\hat{\delta}_{n+1}\right\|$$

and

$$\left\|\hat{\mathscr{I}}\right\| \leqslant k\big(2\left\|e_n^U\right\| + h\left\|e_n^V\right\| + \left\|\hat{\delta}_{n+1}\right\|\big).$$

Now summing the above results yields

$$\begin{aligned} &\left\|e_{n+1}^U\right\| + \sqrt{\left\|\sqrt{A}e_{n+1}^U\right\|^2 + \left\|e_{n+1}^V\right\|^2} \leqslant \left\|e_n^U\right\| + \sqrt{\left\|\sqrt{A}e_n^U\right\|^2 + \left\|e_n^V\right\|^2} \\ &\quad + h\left\|e_n^V\right\| + h\left(\tilde{\alpha} + \tfrac{1}{2}h\right)\left\|\hat{\mathscr{I}}\right\| + \left\|\hat{\delta}_{n+1}\right\| + \sqrt{\left\|\sqrt{A}\hat{\delta}_{n+1}\right\|^2 + \left\|\hat{\delta}'_{n+1}\right\|^2} \\ &\leqslant \left\|e_n^U\right\| + \sqrt{\left\|\sqrt{A}e_n^U\right\|^2 + \left\|e_n^V\right\|^2} + \sqrt{\left\|\sqrt{A}\hat{\delta}_{n+1}\right\|^2 + \left\|\hat{\delta}'_{n+1}\right\|^2} \\ &\quad + h\left\|e_n^V\right\| + h\left(\tilde{\alpha} + \tfrac{1}{2}h\right)k\big(2\left\|e_n^U\right\| + h\left\|e_n^V\right\| + \left\|\hat{\delta}_{n+1}\right\|\big) + \left\|\hat{\delta}_{n+1}\right\| \\ &\leqslant \big(1 + h\hat{C}\big)\left(\left\|e_n^U\right\| + \sqrt{\left\|\sqrt{A}e_n^U\right\|^2 + \left\|e_n^V\right\|^2}\right) \\ &\quad + \sqrt{\left\|\sqrt{A}\hat{\delta}_{n+1}\right\|^2 + \left\|\hat{\delta}'_{n+1}\right\|^2} + \left(1 + h\left(\tilde{\alpha} + \tfrac{1}{2}h\right)k\right)\left\|\hat{\delta}_{n+1}\right\|. \end{aligned}$$

On noticing the truncation errors (5.6) there exists a constant C such that

$$\sqrt{\left\|\sqrt{A}\hat{\delta}_{n+1}\right\|^2+\left\|\hat{\delta}'_{n+1}\right\|^2}+\left(1+h\left(\tilde{\alpha}+\tfrac{1}{2}h\right)k\right)\left\|\hat{\delta}_{n+1}\right\|\leqslant Ch\big(h^2+\|\hat{\delta}(\Delta x)\|\big).$$

The following result is straightforward by applying the Gronwall inequality:

$$\begin{aligned}&\left\|e^U_{n+1}\right\|+\sqrt{\left\|\sqrt{A}e^U_{n+1}\right\|^2+\left\|e^V_{n+1}\right\|^2}\\&\qquad\leqslant\exp(nh\hat{C})\Big(\left\|e^U_0\right\|+\sqrt{\left\|\sqrt{A}e^U_0\right\|^2+\left\|e^V_0\right\|^2}+Cnh\big(h^2+\|\hat{\delta}(\Delta x)\|\big)\Big),\end{aligned}$$

which confirms this theorem. □

6. Practical implementations of the KGDG scheme

This section concerns the practical implementations of the energy-preserving KGDG scheme (2.12). It is clear that (2.12) itself falls well short of being a practical scheme unless the $\overline{\nabla}G(u_n,u_{n+1})$ can be approximated. Fortunately, because of the special structure of the function $G'(u)$ appearing in the Klein–Gordon equation (1.1) the $\overline{\nabla}G(u_n,u_{n+1})$ can be computed as

$$\begin{cases}\overline{\nabla}G(u_n,u_{n+1})=\dfrac{1}{(u_{n+1}-u_n)}G\left(u_{n+1}\right)-G\big(u_n\big) & \text{when } u_{n+1}-u_n\neq 0,\\ \overline{\nabla}G(u_n,u_n)=G'(u_n) & \text{when } u_{n+1}-u_n=0.\end{cases}\tag{6.1}$$

Consequently, we are now in a position to present the following practical energy-preserving scheme for the high-dimensional nonlinear Klein–Gordon equation, which is still called a KGDG scheme.

THEOREM 6.1 A practical KGDG scheme for the high-dimensional nonlinear Klein–Gordon equation (1.1) is defined by

$$\begin{cases}u_{n+1}=\phi_0\big(\mathscr{V}\big)u_n+h\phi_1\big(\mathscr{V}\big)v_n-h^2\phi_2\big(\mathscr{V}\big)\dfrac{1}{u_{n+1}-u_n}\Big(G\left(u_{n+1}\right)-G\big(u_n\big)\Big),\\ v_{n+1}=-h\mathscr{A}\phi_1\big(\mathscr{V}\big)u_n+\phi_0\big(\mathscr{V}\big)v_n-h\phi_1\big(\mathscr{V}\big)\dfrac{1}{u_{n+1}-u_n}\Big(G\left(u_{n+1}\right)-G\big(u_n\big)\Big).\end{cases}\tag{6.2}$$

If $u_{n+1}-u_n=0$, the corresponding scheme is given by

$$\begin{cases}u_{n+1}=\phi_0\big(\mathscr{V}\big)u_n+h\phi_1\big(\mathscr{V}\big)v_n-h^2\phi_2\big(\mathscr{V}\big)G'\big(u_n\big),\\ v_{n+1}=-h\mathscr{A}\phi_1\big(\mathscr{V}\big)u_n+\phi_0\big(\mathscr{V}\big)v_n-h\phi_1\big(\mathscr{V}\big)G'\big(u_n\big).\end{cases}$$

The above analysis considered the situation where the PDE is discretised in time while remaining continuous in space. In practical computations one usually discretises the spatial derivative first, for instance, by finite difference methods or spectral methods. This means that the operator $\mathscr{A}$ is replaced by a suitable differential matrix A. This also implies that the high-dimensional nonlinear Klein–Gordon equation (1.1) is approximated by the following system of ODEs:

$$\begin{cases}q'(t)=p(t), & q(0)=g_1(x),\\ p'(t)=-Aq(t)-\nabla\widetilde{G}(q(t)), & p(0)=g_2(x),\end{cases}\tag{6.3}$$

where $q(t), p(t)$ are assumed to be $q(t), p(t) \in R^M$ and

$$\widetilde{G}\big(q(t)\big) = \sum_{j=1}^{M} G\big(q_j(t)\big).$$

This Hamiltonian system has a corresponding energy conservation law, which can be characterised by

$$\tilde{H}(q,p) = \frac{\Delta x}{2} p^{\mathsf{T}} p + \frac{\Delta x}{2} q^{\mathsf{T}} A q + \Delta x \widetilde{G}\big(q(t)\big) = \cdots = \tilde{H}(q(0), p(0)), \tag{6.4}$$

where the norm $\|\cdot\|$ is the standard vector 2-norm, and Δx is the spatial-step size. In fact, this energy can be regarded as an approximate energy (a semidiscrete energy) of the original nonlinear Klein–Gordon equation (1.1). As stated above we have the following practical energy-preserving scheme for the nonlinear Klein–Gordon equation (1.1), which is called a semidiscrete KGDG (SKGDG) scheme.

Definition 6.2 An energy-preserving SKGDG scheme for (6.3) is defined by

$$\begin{cases} q_{n+1} = \phi_0\big(K\big) q_n + h\phi_1\big(K\big) p_n - h^2 \phi_2\big(K\big) \overline{\nabla}_{\mathrm{S}} G(q_n, q_{n+1}), \\ p_{n+1} = -hA\phi_1\big(K\big) q_n + \phi_0\big(K\big) p_n - h\phi_1\big(K\big) \overline{\nabla}_{\mathrm{S}} G(q_n, q_{n+1}), \end{cases} \tag{6.5}$$

where $K = h^2 A$, $\overline{\nabla}_{\mathrm{S}} G(q_n, q_{n+1})$ is defined as

$$\begin{cases} \overline{\nabla}_{\mathrm{S}} G(q_n, q_{n+1}) = \Big(G\left(q_{n+1}\right) - G\big(q_n\big)\Big) / (q_{n+1} - q_n) & \text{when } q_{n+1} - q_n \neq \mathbf{0}, \\ \overline{\nabla}_{\mathrm{S}} G(q_n, q_n) = \nabla \widetilde{G}(u_n) & \text{when } q_{n+1} - q_n = \mathbf{0}, \end{cases} \tag{6.6}$$

and $\cdot/\cdot$ denotes elementwise division of vectors. It is noted that for a vector $q = (q_1, q_2, \ldots, q_M)^{\mathsf{T}}$, $G(q)$ is defined by

$$G(q) = \Big(G(q_1), G(q_2), \ldots, G(q_M)\Big)^{\mathsf{T}}. \tag{6.7}$$

Theorem 6.3 The SKGDG scheme (6.5) exactly preserves the semidiscrete energy $\tilde{H}$, i.e., we have

$$\tilde{H}(q_{n+1}, p_{n+1}) = \tilde{H}(q_n, p_n), \quad n = 0, 1, \ldots.$$

Proof. (I) : $q_{n+1} - q_n \neq \mathbf{0}$.

In order to prove the conclusion under this condition we first need to show that

$$(q_{n+1} - q_n)^{\mathsf{T}} \overline{\nabla}_{\mathrm{S}} G(q_n, q_{n+1}) = \widetilde{G}\left(q_{n+1}\right) - \widetilde{G}\big(q_n\big).$$

According to (6.5) and (6.7) the following result is obtained:

$$(q_{n+1}-q_n)^{\intercal}\overline{\nabla}_{\mathrm{S}}G(q_n,q_{n+1}) = (q_{n+1}-q_n)^{\intercal}\Big(\big(G(q_{n+1})-G(q_n)\big)/(q_{n+1}-q_n)\Big)$$
$$= \sum_{j=1}^{M}\Big(G(q_{n+1,j})-G(q_{n,j})\Big) = \widetilde{G}\,(q_{n+1})-\widetilde{G}\big(q_n\big), \tag{6.8}$$

where $q_{n,j}$ denotes the jth component of the vector q_n.

Then inserting the SKGDG scheme (6.5) into the semidiscrete energy $\tilde{H}$, (6.4) with some careful calculations yields

$$\tilde{H}(q_{n+1},p_{n+1}) = \frac{\Delta x}{2}p_n^{\intercal}p_n + \frac{\Delta x}{2}q_n^{\intercal}Aq_n + \Delta x\widetilde{G}\big(q_n\big) + \Delta x\Big(\widetilde{G}\,(q_{n+1})-\widetilde{G}\big(q_n\big)\Big)$$
$$+ \Delta x q_n^{\intercal}K\phi_2(K)\overline{\nabla}_{\mathrm{S}}G(q_n,q_{n+1}) - \Delta x h p_n^{\intercal}K\phi_1(K)\overline{\nabla}_{\mathrm{S}}G(q_n,q_{n+1})$$
$$+ \Delta x h^2\overline{\nabla}_{\mathrm{S}}G(q_n,q_{n+1})^{\intercal}\phi_2(K)\overline{\nabla}_{\mathrm{S}}G(q_n,q_{n+1}). \tag{6.9}$$

It follows from the first formula of (6.5) and (6.8) that

$$\widetilde{G}\,(q_{n+1})-\widetilde{G}\big(q_n\big) = (q_{n+1}-q_n)^{\intercal}\overline{\nabla}_{\mathrm{S}}G(q_n,q_{n+1})$$
$$= -q_n^{\intercal}K\phi_2(K)\overline{\nabla}_{\mathrm{S}}G(q_n,q_{n+1}) + hp_n^{\intercal}K\phi_1(K)\overline{\nabla}_{\mathrm{S}}G(q_n,q_{n+1})$$
$$- h^2\overline{\nabla}_{\mathrm{S}}G(q_n,q_{n+1})^{\intercal}\phi_2(K)\overline{\nabla}_{\mathrm{S}}G(q_n,q_{n+1}).$$

Inserting this result into (6.9) we obtain

$$\tilde{H}(q_{n+1},p_{n+1}) = \frac{\Delta x}{2}p_n^{\intercal}p_n + \frac{\Delta x}{2}q_n^{\intercal}Aq_n + \Delta x\widetilde{G}\big(q_n\big) = \tilde{H}(q_n,p_n).$$

(II) : $q_{n+1}-q_n = \mathbf{0}$.

Under this condition the conclusion is easily obtained by considering (6.5) and (6.9). □

Remark 6.4 We remark that schemes (6.2) and (6.5) are presented in a completely closed form because the $\overline{\nabla}G(u_n,u_{n+1})$ is evaluated exactly. This makes the schemes more practical and robust, which can be thought of as an efficient and straightforward approach to implementing our energy-preserving scheme (2.12) for nonlinear Klein–Gordon equations.

Remark 6.5 It should be emphasised that schemes (6.2) and (6.5) for nonlinear Klein–Gordon equations are different from the AVF and AAVF methods for Hamiltonian ODEs since both AVF and AAVF methods are dependent on the evaluation of the integrals appearing in their formulae. Both AVF and AAVF methods as time integration methods for nonlinear Klein–Gordon equations, cannot exactly preserve the energy in practical computation, in general. Moreover, for scheme (6.5) the difference between the continuous energy and the discrete energy is dependent only on the spatial discretisation and is independent of the time integration, since the integral appearing in the formula has been calculated without error, which is different from the case for Hamiltonian ODEs.

REMARK 6.6 In the sense of structure preservation, scheme (6.5) is a genuine energy-preserving formula from both theoretical and computation aspects since it exactly preserves the discrete energy without error. This point is significant for the study of structure-preserving algorithms for differential equations. This is also the main motivation of this study.

REMARK 6.7 One of the important applications of numerical ODEs is to solving PDEs efficiently. The traditional and popular way is to discretise the spatial derivative first. Then numerical methods for ODEs are applied to the underlying semidiscretised ODEs. Sometimes this approach will result in a gap between PDEs and ODEs in terms of numerical analysis issues, in particular, the analysis of global errors, since the true solution of the underlying PDEs, or the true solution of the semidiscretised ODEs may not be available. Fortunately, however, on the basis of the so-called operator-variation-of-constants formula and the matrix-variation-of-constants formula we can get an insight into the true solutions of both the underlying PDEs and the semidiscretised ODEs. Therefore, we are hopeful of obtaining the important numerical analysis of the structure-preserving computation for nonlinear Klein–Gordon equations.

It is noted that scheme (2.12) is implicit and an iterative procedure is required. In what follows we discuss the convergence of fixed-point iteration for (2.12).

THEOREM 6.8 Assume that the DG $\overline{\nabla} G(\cdot, y)$ satisfies the Lipschitz condition for y with the Lipschitz constant L. If the time-step size h satisfies $0 < h \leqslant \tilde{h} \leqslant \sqrt{\frac{2}{L}}$ then the fixed-point iteration for (2.12) is convergent.

Proof. Letting

$$\Psi : \ y \to \phi_0(\mathscr{V})u_n + h\phi_1(\mathscr{V})v_n - h^2\phi_2(\mathscr{V})\overline{\nabla} G(u_n, y)$$

and using Proposition 2.2 we obtain

$$\|\Psi(y_1) - \Psi(y_2)\| \leqslant \tfrac{1}{2}h^2 L\|y_1 - y_2\|,$$

which proves the result by the contraction mapping theorem. □

REMARK 6.9 It is remarked that the convergence of the fixed-point iteration for our method is independent of $\mathscr{A}$. However, the convergence of other methods such as the AVF method and HBVMs depends on $\mathscr{A}$. This allows us to use a large time-step size and a simple iteration method with a small iteration number for our method, which will be demonstrated clearly by the numerical experiments given in the next section.

7. Numerical experiments

In this section we compare our energy-preserving KGDG scheme with the well-known leap frog scheme and two classes of energy-preserving methods, AVF methods and HBVMs, by applying them to nonlinear Klein–Gordon equations.

The solvers chosen for comparison are

- KGDG: the energy-preserving KGDG scheme of order 2 presented in this paper;
- AVF: the energy-preserving AVF method of order 2 stated in Celledoni *et al.* (2012);
- HBVM11: the HBVM(1,1) of order 2 described in Brugnano *et al.* (2014, 2015a);

- LFS: the well-known leap frog scheme;
- HBVM22: the HBVM(2,2) of order 4 given in Brugnano *et al.* (2014, 2015a).

It is noted that the first four methods are all of order 2 while HBVM22 is of order 4. The purpose of choosing the fourth-order method is to show the superiority of our KGDG scheme of order 2 in comparison with higher-order methods. We also remark that KGDG, AVF, HBVM11 and HBVM22 are all implicit and in order to show that our method can perform well even for a simple iteration method with a small iteration number we use standard fixed-point iteration in the practical computations. We set 10^{-15} as the error tolerance and 10 as the maximum number of each iteration for all the problems. It is possible to change to the quasi-Newton or Newton iteration for improved efficiency and in this paper, for brevity, we do not consider this issue further.

7.1 *One-dimensional problems*

We first consider three one-dimensional nonlinear Klein–Gordon equations and approximate the operator $\mathscr{A}$ by Fourier spectral collocation (FSC) (see, Hesthaven *et al.*, 2007; Shen *et al.*, 2011) as

$$\mathscr{A} \approx A = \frac{1}{(\pi/L)^2}\Big(a_{kj}\Big)_{M\times M} \text{ with } a_{kj} = \begin{cases} \frac{(-1)^{k+j}}{2}\sin^{-2}\left(\frac{(k-j)\pi}{M}\right), & k \neq j, \\ \frac{M^2}{12} + \frac{1}{6}, & k = j. \end{cases} \tag{7.1}$$

Problem 7.1 Consider the following sine-Gordon equation (see, e.g., Brugnano *et al.*, 2015a):

$$\frac{\partial^2 u}{\partial t^2} = \frac{\partial^2 u}{\partial x^2} - \sin u, \qquad x \in [-20, 20], \qquad t \in [0, T].$$

In particular, we consider soliton-like solutions, defined by the initial conditions

$$u(x, 0) \equiv 0, \quad u_t(x, 0) = 4/\gamma \operatorname{sech}\Big(x/\gamma\Big), \quad \gamma \geqslant 0.$$

Depending on the value of γ the solution is given by

$$u(x, t) = 4\arctan\big(\psi(t, \gamma)\operatorname{sech}(x/\gamma)\big)$$

with

$$\psi(t, \gamma) = \begin{cases} \sinh\left(\frac{\sqrt{1-\gamma^2}t}{\gamma}\right)/\sqrt{1-\gamma^2}, & 0 < \gamma < 1, \\ t, & \gamma = 1, \\ \sin\left(\frac{\sqrt{\gamma^2-1}t}{\gamma}\right)/\sqrt{\gamma^2-1}, & \gamma > 1. \end{cases}$$

The exact solutions of $\gamma = 0.99, 1$ and 1.01 are shown in Fig. 1. The case $0 < \gamma < 1$ is named kink–antikink and the case $\gamma > 1$ is named breather. The case $\gamma = 1$ is named double pole, which separates the two different types of dynamics.

We discretise the spatial derivative by the FSC method (7.1) with $M = 200$, and then integrate the semidiscrete system with $h = 0.1$ and $T = 1000$. See Fig. 2 (top row) for the errors of the semidiscrete

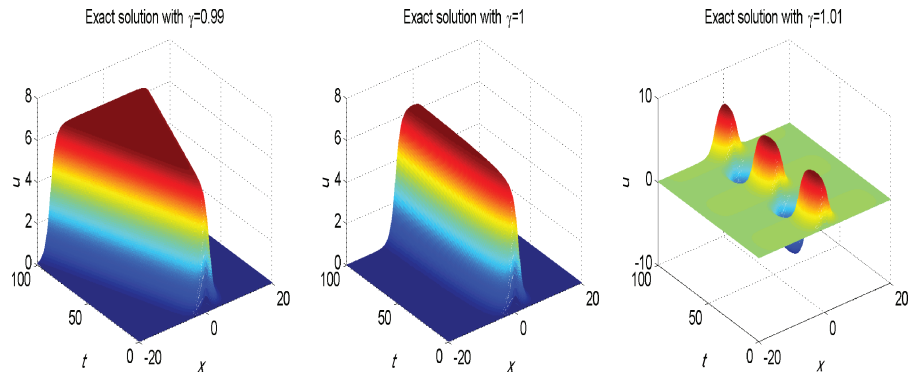

FIG. 1. Exact solutions of Problem 7.1.

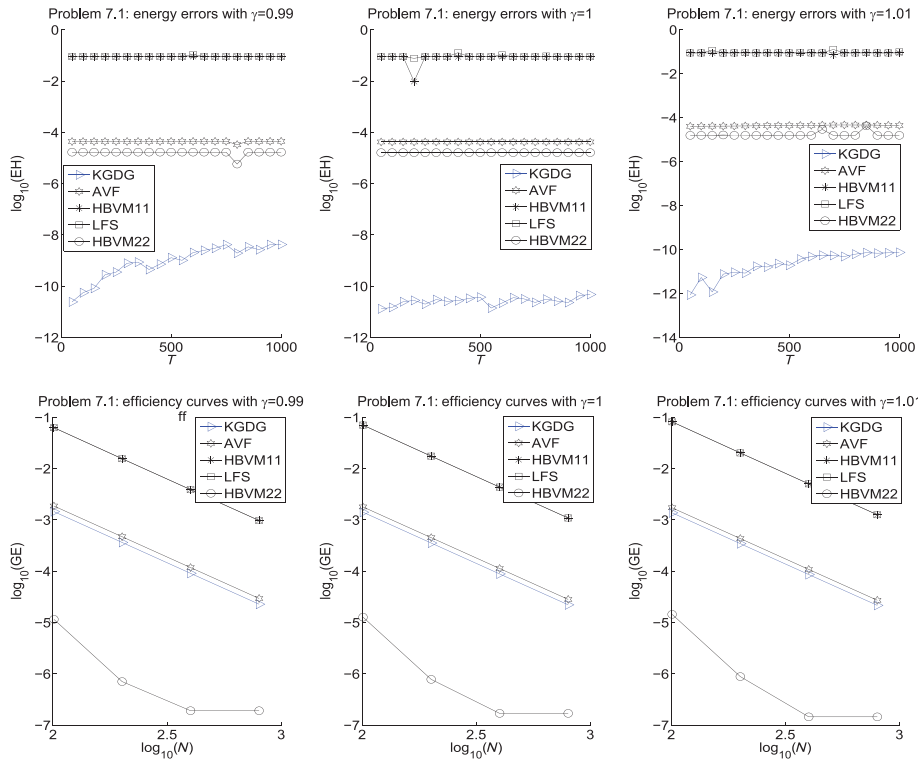

FIG. 2. Energy errors and efficiency curves for Problem 7.1. (We note that 'EH' is referred to the energy errors of the semidiscrete Hamiltonian system and 'GE' denotes the global errors.)

energy conservation for $\gamma = 0.99, 1, 1.01$. It is noted that for the energy errors we use the semidiscrete energy (6.4) at the initial values as the 'exact' energy of this problem and show the energy errors for each numerical method. Similar situations are encountered in the next four problems and we deal with them in a similar way.

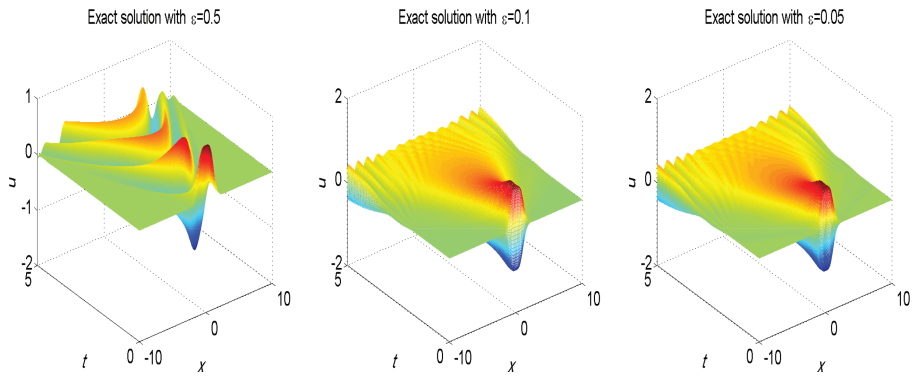

FIG. 3. The 'exact' solutions of Problem 7.2.

Then the problem is solved in $[0, 10]$ with different step sizes $h = 0.1/2^j$ for $j = 0, 1, 2, 3$. The efficiency curves (the global error vs. $N = T/h$) are shown in Fig. 2 (bottom row). It is clear that our KGDG scheme shows remarkable numerical behaviour.

PROBLEM 7.2 We consider the dimensionless relativistic Klein–Gordon equation whose solution is highly oscillating in time (see, e.g., Bao & Dong, 2012),

$$\begin{cases} \varepsilon^2 \frac{\partial^2 u}{\partial t^2} - \frac{\partial^2 u}{\partial x^2} + \frac{1}{\varepsilon^2} u + f(u) = 0, \quad -L \leqslant x \leqslant L, \ \ 0 \leqslant t \leqslant T, \quad u(-L, t) = u(L, t), \\ u(x, 0) = \phi(x), \ \ u_t(x, 0) = \frac{1}{\varepsilon^2} \gamma(x). \end{cases}$$

Here ε is a dimensionless parameter, $\varepsilon > 0$. According to Bao & Dong (2012) the following conditions are chosen:

$$f(u) = 4u^3, \ \ \phi(x) = \frac{2}{\exp(x^2) + \exp(-x^2)}, \ \ \gamma(x) = 0.$$

Let $u(x, t)$ be the 'exact' solution that is obtained numerically by using the fourth-order method HBVM22 with small time step $h = 1/1000$. The results with $\varepsilon = 0.5, 0.1$ and 0.05 are presented in Fig. 3.

We discretise the spatial derivative by the FSC method with $L = 10, M = 100$ for $\varepsilon = 0.5$ and $M = 400$ for $\varepsilon = 0.1$ and 0.05. The problem is solved with $T = 1000, h = 0.05$ for $\varepsilon = 0.5$, $T = 200, h = 0.004$ for $\varepsilon = 0.1$ and $T = 100, h = 0.002$ for $\varepsilon = 0.05$. The errors of the semidiscrete energy conservation are shown in Fig. 4 (top row). We then choose $T = 10$ and $h = 0.04/2^j$ for $j = 0, 1, 2, 3$ with $\varepsilon = 0.2$ and for $j = 2, 3, 4, 5$ with $\varepsilon = 0.1$ and 0.05. The efficiency curves are displayed in Fig. 4 (bottom row). Again, our KGDG scheme shows remarkable numerical behaviour. Moreover, it can be observed from Fig. 4 (bottom row) that for this highly oscillatory system, our KGDG method is allowed to take larger time-step sizes than the other methods.

PROBLEM 7.3 Consider the nonlinear Klein–Gordon equation

$$\begin{cases} \frac{\partial^2 u}{\partial t^2} - a^2 \frac{\partial^2 u}{\partial x^2} = bu^3 - au, \quad -20 \leqslant x \leqslant 20, \ \ 0 \leqslant t \leqslant T, \quad u(-20, t) = u(20, t), \\ u(x, 0) = \sqrt{\frac{2a}{b}} \operatorname{sech}(\lambda x), \ \ u_t(x, 0) = c\lambda \sqrt{\frac{2a}{b}} \operatorname{sech}(\lambda x) \tanh(\lambda x) \end{cases}$$

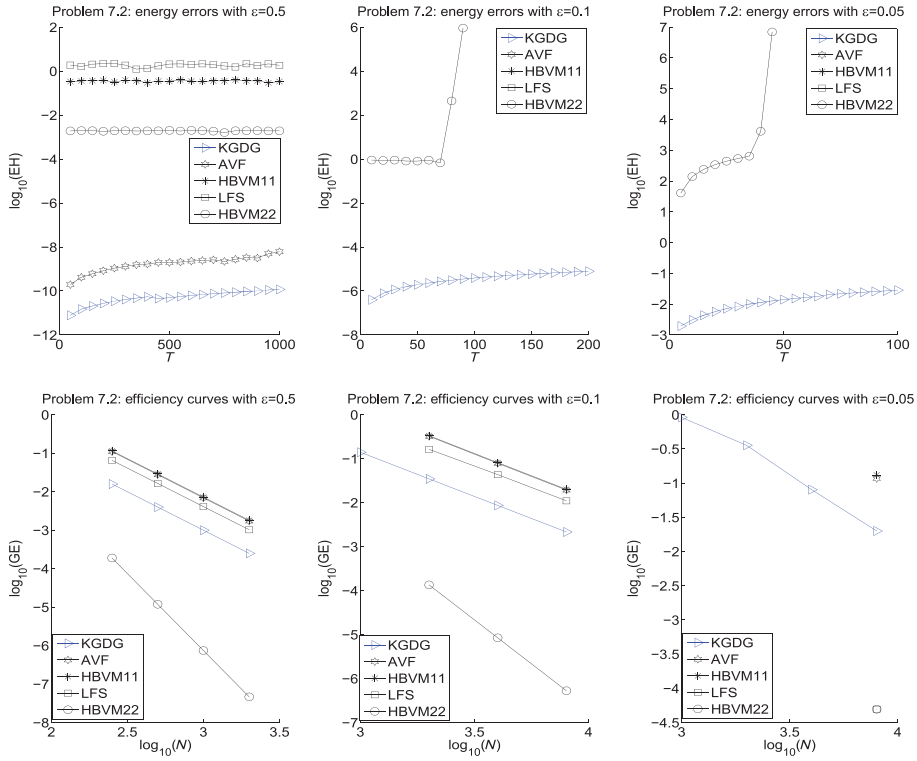

FIG. 4. Energy errors and efficiency curves for Problem 7.2.

with $\lambda = \sqrt{\frac{a}{a^2-c^2}}$ and $a, b, a^2 - c^2 > 0$. The exact solution is given by

$$u(x,t) = \sqrt{\frac{2a}{b}}\operatorname{sech}(\lambda(x - ct))$$

and is shown in Fig. 5 (left). Following Liu *et al.* (2014) the parameters $a = 0.3, b = 1$ and $c = 0.25$ are used. We choose $M = 200$ and integrate the semidiscrete system with $T = 1000$ and $h = 0.2$. The errors of the semidiscrete energy conservation are presented in Fig. 5 (middle). See Fig. 5 (right) for the efficiency curves with $T = 10$ and $h = 0.05/2^j$ for $j = 0, 1, 2, 3$. Our KGDG scheme gives good numerical results.

7.2 *Two-dimensional problems*

In what follows we show the remarkable efficiency of our KGDG scheme for high-dimensional nonlinear Klein–Gordon equations by considering two two-dimensional problems.

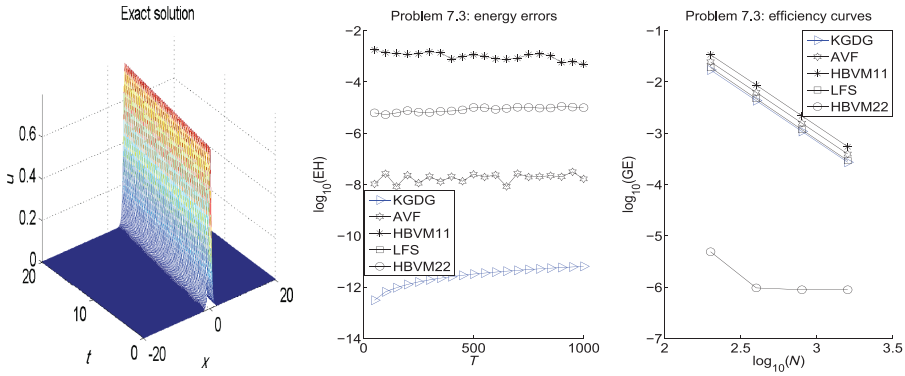

FIG. 5. Exact solutions, energy errors and efficiency curves for Problem 7.3.

PROBLEM 7.4 We consider the following two-dimensional nonlinear wave equation (see, e.g., Celledoni *et al.*, 2012):

$$\frac{\partial^2 u(x,y,t)}{\partial t^2} = \Delta u(x,y,t) - u^3(x,y,t), \quad (x,y) \in [-1,1] \times [-1,1], \ \ t > 0$$

with periodic boundary conditions. The initial conditions are given by

$$u(x,y,0) = \operatorname{sech}(10x)\operatorname{sech}(10y), \ \ u_t(x,y,0) = 0.$$

Following Celledoni *et al.* (2012) we use spectral elements method to semidiscretise the wave equation. The space is discretised with a tensor product Lagrange quadrature formula based on $p+1$ Gauss–Lobatto–Legendre (GLL) quadrature nodes in each space direction. Then it is obtained that (see Celledoni *et al.*, 2012 for more details)

$$\tilde{H}(U) = \frac{1}{2}\sum_{j_1=0}^{p}\sum_{j_2=0}^{p} w_{j_1} w_{j_2} \left(\left(\sum_{k=0}^{p} \mathrm{d}_{j_1,k} u_{k,j_2} \right)^2 + \left(\sum_{m=0}^{p} \mathrm{d}_{j_2,m} u_{j_1,m} \right)^2 + \tfrac{1}{2} u_{j_1,j_2}^4 \right),$$

where $l_k(x)$ is the kth Lagrange basis function based on the GLL quadrature nodes $x_0, \ldots, x_p$ with the corresponding quadrature weights $w_0, \ldots, w_p$, and $\mathrm{d}_{j_1,k} = \frac{\mathrm{d}l_k(x)}{\mathrm{d}x}$. The numerical approximation is given by

$$u_p(x,y,t) = \sum_{k=0}^{p}\sum_{m=0}^{p} u_{k,m}(t) l_k(x) l_m(y)$$

with $u_p(x_{j_1}, y_{j_2}, t) = u_{j_1,j_2}(t)$.

We first show some snapshots of the numerical solutions by KGDG and AVF with a small step size $h = 0.005$, in Fig. 6. Here the spatial derivatives are discretised with six Gauss–Lobatto nodes in each spatial direction and numerical solutions interpolate on an equidistant grid of 26 nodes in each spatial

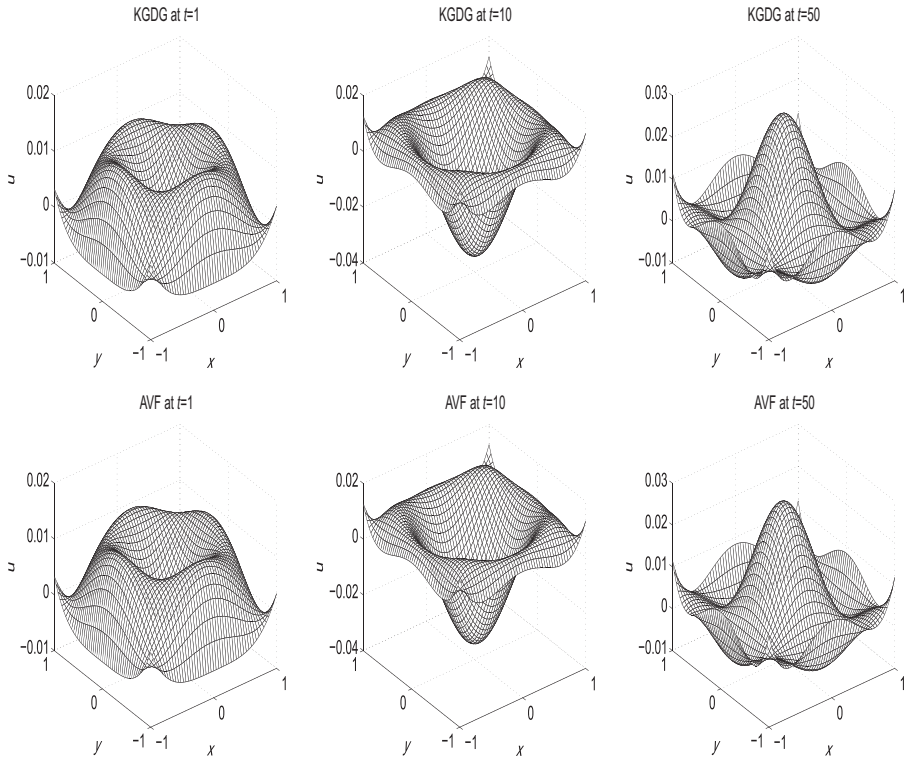

FIG. 6. Snapshots of the solution of Problem 7.4.

direction. Then the system is integrated with $p = 5$, $h = \frac{1}{5}$ and $T = 1000$, and the results of energy conservation are presented in Fig. 7 (left). Finally, we integrate the problem in the interval $[0, 100]$ with $h = \frac{1}{2^i}$ for $i = 0, 1, 2, 3$. The global errors are shown in Fig. 7 (right). Our KGDG scheme is the most efficient among these methods.

PROBLEM 7.5 Consider the following two-dimensional sine-Gordon equation:

$$\begin{cases} u_{tt} - (u_{xx} + u_{yy}) = -\sin u, \ (x, y) \in [-1, 1] \times [-1, 1], \ \ t > 0, \\ u(x, y, 0) = 4 \arctan\left(\exp\left(\frac{4-\sqrt{(x+3)^2+(y+3)^2}}{0.436}\right)\right), \\ u_t(x, y, 0) = \dfrac{4.13}{\cosh\left(\exp\left(\left(4-\sqrt{(x+3)^2+(y+3)^2}\right)/0.436\right)\right)} \end{cases}$$

with periodic boundary conditions.

Similarly to Problem 7.4, we use the spectral element method to semidiscretise the wave equation and the space is discretised with a tensor product Lagrange quadrature formula based on six GLL quadrature nodes in each spatial direction. We first solve the system with $h = \frac{1}{5}$ and $T = 1000$. See Fig. 8 (left) for the results of energy conservation. Then the problem is integrated in $[0, 100]$ with $h = \frac{1}{2^i}$ for

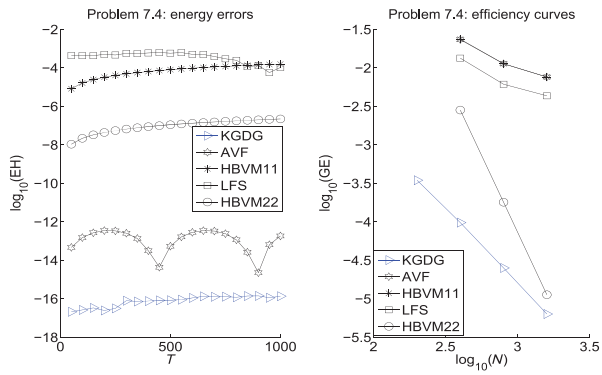

FIG. 7. Energy errors and efficiency curves for Problem 7.4.

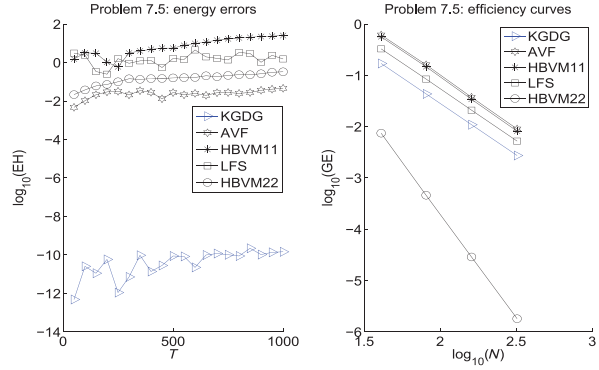

FIG. 8. Energy errors and efficiency curves for Problem 7.5.

$i = 1, 2, 3, 4$. The global errors are presented in Fig. 8 (right). Again, our KGDG scheme is the most efficient among these methods.

8. Conclusions

The concept of energy preservation has far-reaching consequences in the physical sciences. Therefore, many methods for energy preservation have been proposed for ODEs and PDEs. In this paper, using a blend of the DG method and the Duhamel principle, we have presented a systematic and unified way to discretise high-dimensional nonlinear Klein–Gordon equations so that the semidiscrete energy can be preserved precisely. The resulting energy-preserving scheme is analysed in detail for local truncation error, nonlinear stability, convergence and implementations. Furthermore, the remarkable efficiency of the energy-preserving scheme is demonstrated by the numerical experiments in comparison with some existing numerical methods in the literature. This paper also tries to patch the gap between numerical ODEs and PDEs in terms of numerical analysis issues, via the Duhamel principle for nonlinear Klein–Gordon equations. The Duhamel principle transfers the information of solution to the underlying nonlinear Klein–Gordon equation, which is needed for the numerical analysis. Both the nonlinear

stability analysis and convergence analysis are of prime importance in the study of structure-preserving algorithms for Hamiltonian PDEs. This point has been addressed in this paper.

Last but not least, in comparison with symplectic methods, the apparent advantage of energy-preserving methods is that they can preserve the energy of the considered system exactly. Our future exploration will be devoted to the numerical behaviour of energy-preserving methods in other aspects, such as the long-time numerical conservation of momentum and actions of Hamiltonian PDEs. The key technique for the analysis is modulated Fourier expansion and we hope to obtain some interesting results on this topic.

Acknowledgements

The authors are sincerely thankful to two anonymous reviewers for their valuable suggestions, which have helped to improve the presentation of the manuscript significantly. The authors are also grateful to Prof. Christian Lubich for his careful reading of the manuscript and for his helpful comments.

Funding

Alexander von Humboldt Foundation, by the Natural Science Foundation of Shandong Province (Outstanding Youth Foundation) (ZR2017JL003); National Natural Science Foundation of China (11671200).

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