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Finite-difference schemes for nonlinear wave equation that inherit energy conservation property

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Abstract

We propose two general finite-difference schemes that inherit energy conservation property from nonlinear wave equations, such as the nonlinear Klein–Gordon equation (NLKGE). One of proposed schemes is implicit and another is explicit. Many studies exist on FDSs that inherit energy conservation property from NLKGE and we can derive all of their schemes from the proposed general schemes in this paper. The most important feature of our procedure is a rigorous discretization of variational derivatives using summation by parts, which implies that the inherited properties are satisfied exactly. Because of this the derived schemes are expected to be numerically stable and yield solutions converging to PDE solutions. We make new FDSs for Fermi–Pasta–Ulam equation, string vibration equation, Shimoji–Kawai equation (SKE) and Ebihara equation and verify numerically the inheritance of the energy conservation property for NLKGE and SKE.

MSC: 65M06

Keywords: Finite-difference method; Energy conservation; Nonlinear wave equation; Fermi–Pasta–Ulam problem; Nonlinear Klein–Gordon equation

1. Introduction

We consider finite-difference schemes that inherit energy conservation property from nonlinear wave equations.

The study of schemes with conservation property was initiated by Courant et al. [9] in 1928. This so-called "energy method" attracted widespread attention in 1950s, as is documented by Richtmyer and Morton [27, Section 6]. This method was primarily studied to prove stability, existence and uniqueness of solutions of schemes. Namely, the main emphasis was laid on stability rather than conservation property.

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Since 1970s the main interest shifts from stability to conservation property itself. Studies with more emphasis on conservation property itself include Strauss and Vazquez [30], Greenspan [20], Li and Vu-Quoc [25], and Fla [18]. For energy conservation, Strauss and Vazquez [30] discussed schemes for the linear Klein–Gordon equation, Greenspan [20] for initial-value problem $\ddot{x} = f(x)$ and Li and Vu-Quoc [25] for the nonlinear Klein–Gordon equation. Fla [18] showed schemes that inherit energy conservation property and mass conservation property from derivative nonlinear Schrödinger (DNLS) equation. The famous "symplectic method" [28], applicable to Hamilton systems, may be regarded as one application based on this formulation. Looking back at this history, Li and Vu-Quoc describe, in the recent paper [25], the shift of the emphasis and write "*in some areas*, *the ability to preserve some invariant properties of the original differential equation is a criterion to judge the success of a numerical simulation*".

The family of nonlinear wave equations that we consider is

$$\frac{\partial^2 u}{\partial t^2} = -\frac{\delta G}{\delta u}, \tag{1}$$

where $G = G(u, u_x)$ is a function of both u and $u_x = \partial u/\partial x$, and $\delta G/\delta u$ is a variational derivative of function $G(u, u_x)$ for u. Boundary conditions, properties of this family, definition of G, etc. are described in Section 2. The property of the equations to be inherited by finite-difference schemes is $(\mathrm{d}/\mathrm{d}t) \int_0^L \{\frac{1}{2}(u_t)^2 + G(u, u_x)\}\,\mathrm{d}x = 0$ and is called "energy conservation property" in this paper.

The objective of this paper is to introduce two unified framework for finite-difference schemes that inherit the energy conservation property, rather than to analyze numerical properties of the derived individual schemes.

The contents of this paper are as follows. In Section 2, we describe the "target" equations and the characteristic properties precisely. The relationship between the target equations and the inherited properties is shown in the continuous context. In Section 3, definitions and properties of discrete operators are shown. In Section 4, we propose two new general schemes designed to inherit the energy conservation property and prove the inheritance. The proof is the form of the discrete relationship between the target equations and the property in the context of finite-difference calculus. In Section 5, we apply the proposed generic schemes to some PDEs, the Fermi–Pasta–Ulam equation, string vibration equation, the nonlinear Klein–Gordon equation, the Shimoji–Kawai equation and Ebihara equation. We show that all of known completely discrete schemes which inherit the energy conservation property for NLKGE are derived from the proposed generic schemes. The schemes for the Fermi–Pasta–Ulam equation, string vibration equation, the Shimoji–Kawai equation and Ebihara equation are new ones. We show some numerical solutions for the PDEs and that the derived schemes have some good features. In conclusion we summarize the results in this paper.

2. Equations and properties

The purpose of this section is to describe equations and their characteristic properties which we consider. The relationship between the equation and its properties, which is described in this section, is fundamental for this paper.

We consider the following equation in function $u(x,t)$:

$$\frac{\partial^2 u}{\partial t^2} = -\frac{\delta G}{\delta u}, \tag{2}$$

where $x \in \Omega = [0,L]$, $L < \infty$, is the one-dimensional space variable and t is the time variable. Function $G = G(u, u_x)$ is called "energy function" in this paper since $\frac{1}{2}(\partial u/\partial t)^2 + G$ often corresponds to a local free energy function in physical applications. $\delta G/\delta u$ is a variational derivative of the function G for u and is calculated as $\delta G/\delta u = \partial G/\partial u - \mathrm{d}/\mathrm{d}x(\partial G/\partial u_x)$.

We consider a class of boundary conditions which satisfy the following assumption. The assumption is

$$\left[\frac{\partial G}{\partial u_x}\frac{\partial u}{\partial t}\right]_{x=0}^{L} = 0, \tag{3}$$

which is satisfied, e.g., by the Dirichlet b.c. or the natural b.c. or the periodical b.c.

For the solution $u(x,t)$ of (2) under boundary conditions which satisfy assumption (3), time dependency of the integral of the energy function is indicated as follows:

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\int_0^L \left\{\frac{1}{2}(u_t)^2 + G\right\}\mathrm{d}x &= \int_0^L \left\{u_t u_{tt} + \frac{\partial G}{\partial u}u_t + \frac{\partial G}{\partial u_x}u_{xt}\right\}\mathrm{d}x \\
&= \int_0^L \left\{u_t u_{tt} + \frac{\partial G}{\partial u}u_t - u_t\frac{\partial}{\partial x}\frac{\partial G}{\partial u_x}\right\}\mathrm{d}x + \left[\frac{\partial G}{\partial u_x}u_t\right]_{x=0}^{L} \\
&= \int_0^L u_t\left\{u_{tt} + \frac{\delta G}{\delta u}\right\}\mathrm{d}x + \left[\frac{\partial G}{\partial u_x}u_t\right]_{x=0}^{L} \\
&= \left[\frac{\partial G}{\partial u_x}u_t\right]_{x=0}^{L} \\
&= 0.
\end{aligned} \tag{4}$$

We call this property "energy conservation property". Note that Eq. (4) is the most fundamental continuous equation in this paper since it describes the cause and effect relationship between the equations and the property. If the condition

$$\left[\frac{\partial G}{\partial u_x}u_x + \frac{1}{2}(u_t)^2 - G\right]_{x=0}^{L} = 0 \tag{5}$$

is satisfied, the time dependency of integral of $(\partial u/\partial x)(\partial u/\partial t)$ is

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\int_0^L u_t u_x\,\mathrm{d}x &= \int_0^L (u_{xt}u_t + u_x u_{tt})\,\mathrm{d}x \\
&= \int_0^L \left\{\frac{1}{2}\frac{\partial}{\partial x}(u_t)^2 - u_x\frac{\delta G}{\delta u}\right\}\mathrm{d}x \\
&= \int_0^L \left\{-u_x\frac{\partial G}{\partial u} - u_{xx}\frac{\partial G}{\partial u_x}\right\}\mathrm{d}x + \left[\frac{1}{2}(u_t)^2 + \frac{\partial G}{\partial u_x}u_x\right]_{x=0}^{L}
\end{aligned}$$

$$= -\int_0^L \frac{\partial}{\partial x} G \,\mathrm{d}x + \left[\frac{1}{2}(u_t)^2 + \frac{\partial G}{\partial u_x} u_x\right]_{x=0}^{L}$$

$$= \left[\frac{1}{2}(u_t)^2 - G + \frac{\partial G}{\partial u_x} u_x\right]_{x=0}^{L}. \tag{6}$$

We call this property "momentum conservation property". We do not pay more attention to momentum conservation property in this paper.

For example, linear wave equation

$$\frac{\partial^2 u}{\partial t^2} = \frac{\partial^2 u}{\partial x^2}, \tag{7}$$

nonlinear wave equation studied by Fermi et al. [17]

$$\frac{\partial^2 u}{\partial t^2} = \frac{\partial^2 u}{\partial x^2}\left(1 + \varepsilon \frac{\partial u}{\partial x}\right), \tag{8}$$

$$\frac{\partial^2 u}{\partial t^2} = \frac{\partial^2 u}{\partial x^2}\left(1 + \varepsilon \left(\frac{\partial u}{\partial x}\right)^2\right), \tag{9}$$

string vibration equation [8],

$$\frac{\partial^2 u}{\partial t^2} = \frac{\partial}{\partial x}\left(\frac{\partial u/\partial x}{\sqrt{1 + (\partial u/\partial x)^2}}\right), \tag{10}$$

the sine-Gordon equation

$$\frac{\partial^2 u}{\partial t^2} = \frac{\partial^2 u}{\partial x^2} - \sin u, \tag{11}$$

the nonlinear Klein–Gordon equation

$$\frac{\partial^2 u}{\partial t^2} = \frac{\partial^2 u}{\partial x^2} - \phi'(u), \tag{12}$$

where $\phi(u)$ is a function of u, the Shimoji–Kawai equation [29] (SKE)

$$\frac{\partial^2 u}{\partial t^2} = \left(\frac{\partial u}{\partial x}\right)^2 \frac{\partial^2 u}{\partial x^2} \tag{13}$$

and the Ebihara equation [12]

$$\frac{\partial^2 u}{\partial t^2} = x^{\alpha}\frac{\partial^2 u}{\partial x^2} + \alpha x^{\alpha-1}\frac{\partial u}{\partial x} - x^{-\gamma}u^{2p+1}, \tag{14}$$

where $1 \leqslant \alpha \leqslant 2$, $0 \leqslant \gamma$, $p \in \mathbb{N}$ and $\alpha + 2\gamma \leqslant 2p + 1$ are the problems we consider in this paper. Note that the linear wave equation and the sine-Gordon equation are included in the nonlinear Klein–Gordon equation.

In more general case, when G involves u_{xx}, u_{xxx}, etc., for example, vibration equation of a thin beam $\partial^2 u/\partial t^2 = -\partial^4 u/\partial x^4$, properties described in this section is similar.

As described in the introduction, our main interest in this paper is to propose schemes that satisfy discretized derivation process which is similar to (4). To prove this property all operations and calculus, i.e., differential, integral, integral by parts and variational derivative, in Eq. (4) must be discretized consistently. We choose one consistent "set" of discrete operators carefully for this purpose and describe them in Section 3.

3. Discrete symbols

In this section we introduce a consistent set of discrete operators and define the two-point discrete variational derivative and four-point discrete variational derivative. One of the proposed schemes in Section 4 uses two-point discrete variational derivative and another uses four-point discrete variational derivative.

3.1. Symbol definitions

We suppose that the space mesh size and time mesh size are uniform. First, we show a generic rule to define mth degree operator $\mathrm{o}^{\langle m\rangle}$ using two operators o^+ and o^- where o^+ and o^- are commutable:

$$\mathrm{o}^{\langle 0\rangle} \stackrel{\text{def}}{=} 1, \tag{15}$$

$$\mathrm{o}^{\langle 1\rangle} \stackrel{\text{def}}{=} \tfrac{1}{2}(\mathrm{o}^+ + \mathrm{o}^-), \tag{16}$$

$$\mathrm{o}^{\langle 2\rangle} \stackrel{\text{def}}{=} \mathrm{o}^+\mathrm{o}^-, \tag{17}$$

$$\mathrm{o}^{\langle 2m+1\rangle} \stackrel{\text{def}}{=} \mathrm{o}^{\langle 1\rangle}\mathrm{o}^{\langle 2m\rangle}, \quad m \geqslant 1, \tag{18}$$

$$\mathrm{o}^{\langle 2m+2\rangle} \stackrel{\text{def}}{=} \mathrm{o}^{\langle 2\rangle}\mathrm{o}^{\langle 2m\rangle}, \quad m \geqslant 1. \tag{19}$$

This rule is often used to construct mth degree difference operators. Next, we define some basic operators. We define shift operators s^+, s^-, average operators μ^+, μ^-, difference operators δ^+, δ^-,

$$s_j^{\pm} f(j) \stackrel{\text{def}}{=} f(j \pm 1), \tag{20}$$

$$\mu_j^{\pm} \stackrel{\text{def}}{=} \frac{s_j^{\pm} + 1}{2}, \tag{21}$$

$$\delta_j^{\pm} \stackrel{\text{def}}{=} \frac{s_j^{\pm} - 1}{\pm\Delta j}, \tag{22}$$

where $\Delta n \stackrel{\text{def}}{=} \Delta t$ and $\Delta k \stackrel{\text{def}}{=} \Delta x$ in this paper. For convenience, we define a syntax sugar

$$\mathrm{o}_j^{\langle m\pm\rangle} \stackrel{\text{def}}{=} \mu_j^{\pm}\mathrm{o}_j^{\langle m\rangle}. \tag{23}$$

As a discretization of the integral we adopt the summation $\sum''$ that is defined by

$$\sum_{k=0}^{N}{}'' f_k \Delta x \stackrel{\text{def}}{=} \left(\frac{1}{2}f_0 + \sum_{k=1}^{N-1} f_k + \frac{1}{2}f_N\right)\Delta x. \tag{24}$$

The following relationship "summation by parts" that corresponds to integration by parts

$$\sum_{k=0}^{N}{}'' f_k(\delta_k^+ g_k)\Delta x + \sum_{k=0}^{N}{}'' (\delta_k^- f_k) g_k \Delta x = \left[\frac{f_k(s_k^+ g_k) + (s_k^- f_k) g_k}{2}\right]_{k=0}^{N} \tag{25}$$

is satisfied by these definitions.

3.2. Two-point discrete variational derivative

In this subsection we describe definition and properties of the two-point discrete variational derivative which is derived from the definitions in Section 3.1. This derivative is used to define the proposed explicit scheme in Section 4. Hirota [22] mentions a similar notion, the discrete Euler derivative, and obtains them heuristically for some special examples.

First, we assume that a "discrete energy function" $G_\mathrm{d}(U) = (G_\mathrm{d}(U)_k)_{k\in\mathbb{Z}}$, where $U = (U_k)_{k\in\mathbb{Z}}$, which is given as an approximation to $G(u, u_x)$, takes the following form:

$$G_\mathrm{d}(U)_k = \sum_{l=1}^{m} f_l(U_k) g_l^+(\delta_k^+ U_k) g_l^-(\delta_k^- U_k), \quad k \in \mathbb{Z}, \tag{26}$$

where $m \in \mathbb{Z}^+$ and f_l, g_l^+, $g_l^- : \mathbb{R} \to \mathbb{R}$ are differentiable functions. U_k is intended to be an approximation to $u(k\Delta x)$. For such G_d we define the discrete variational derivative $\delta G_\mathrm{d}/\delta(U,V) = ((\delta G_\mathrm{d}/\delta(U,V))_k)_{k\in\mathbb{Z}}$ of G_d for (U,V) as

$$\left(\frac{\delta G_\mathrm{d}}{\delta(U,V)}\right)_k \stackrel{\mathrm{def}}{=} \sum_{l=1}^{m} \{\mathscr{P}_l(U,V)_k - \delta_k^+ \mathscr{Q}_l^-(U,V)_k - \delta_k^- \mathscr{Q}_l^+(U,V)_k\}, \tag{27}$$

where $U = (U_k)_{k\in\mathbb{Z}}, V = (V_k)_{k\in\mathbb{Z}}$ and

$$\mathscr{P}_l(U,V)_k \stackrel{\mathrm{def}}{=} \frac{\mathrm{d} f_l}{\mathrm{d}(U_k, V_k)} \frac{g_l^+(\delta_k^+ U_k) g_l^-(\delta_k^- U_k) + g_l^+(\delta_k^+ V_k) g_l^-(\delta_k^- V_k)}{2}, \tag{28}$$

$$\mathscr{Q}_l^\pm(U,V)_k \stackrel{\mathrm{def}}{=} \frac{f_l(U_k) + f_l(V_k)}{2} \frac{g_l^\mp(\delta_k^\mp U_k) + g_l^\mp(\delta_k^\mp V_k)}{2} \frac{\mathrm{d} g_l^\pm}{\mathrm{d}(\delta_k^\pm U_k, \delta_k^\pm V_k)}, \tag{29}$$

$$\frac{\mathrm{d} f}{\mathrm{d}(a,b)} \stackrel{\mathrm{def}}{=} \begin{cases} \dfrac{f(a) - f(b)}{a - b}: & a \neq b, \\ \dfrac{\mathrm{d} f}{\mathrm{d} a}: & a = b. \end{cases} \tag{30}$$

We note that this definition is well-defined.

The above definition of the discrete variational derivative parallels the definition of $\delta G/\delta u$. First, recall that the variational derivative satisfies (by definition)

$$J[u] - J[v] \cong \int_\Omega \frac{\delta G}{\delta u}(u - v)\,\mathrm{d}x + \left[\frac{\partial G}{\partial u_x}(u - v)\right]_{\partial\Omega}, \tag{31}$$

where

$$J[u] \stackrel{\mathrm{def}}{=} \int_\Omega G(u)\,\mathrm{d}x. \tag{32}$$

Consider a discrete functional $J_d[U]$ defined as

$$J_d[U] = \sum_{k=0}^{N}{}'' G_d(U)_k \Delta x. \tag{33}$$

By the summation by parts (25) applied to difference $J_d[U] - J_d[V]$ we obtain

$$J_d[U] - J_d[V] = \sum_{k=0}^{N}{}'' \frac{\delta G_d}{\delta(U,V)}_k (U_k - V_k)\Delta x + \left[\frac{\partial G_d}{\partial \delta U}(U,V)_k \right]_{k=0}^{N}, \tag{34}$$

where

$$\frac{\partial G_d}{\partial \delta U}(U,V)_k$$
$$\stackrel{\text{def}}{=} \frac{1}{2}\sum_{l=1}^{m}(\mathscr{Q}_l^+(U,V)_k s_k^+(U_k - V_k) + \mathscr{Q}_l^-(U,V)_k s_k^-(U_k - V_k)$$
$$+ (s_k^+ \mathscr{Q}_l^-(U,V)_k + s_k^- \mathscr{Q}_l^+(U,V)_k)(U_k - V_k)). \tag{35}$$

This yields the following equation:

$$J_d[U] - J_d[V] = \sum_{k=0}^{N}{}'' \frac{\delta G_d}{\delta(U,V)_k}(U_k - V_k)\Delta x \tag{36}$$

if $[(\partial G_d/\partial\delta U)(U,V)_k]_{k=0}^{N} = 0$. Eq. (34) may be regarded as a discrete analogue of (31).

Remark 1. In more general case when G involves u_{xx}, u_{xxx}, etc., the discrete variational derivative of G can be treated in a similar manner, which will be reported soon elsewhere.

3.3. Four-point discrete variational derivative

In this subsection we describe definition and properties of the four-point discrete variational derivative which is derived from the definitions in Section 3.1. This derivative is used to define the proposed implicit scheme in Section 4.

First, we assume that a "discrete energy function" $G_d(U,V) = (G_d(U,V)_k)_{k\in\mathbb{Z}}$, where $U = (U_k)_{k\in\mathbb{Z}}$, $V = (V_k)_{k\in\mathbb{Z}}$, which is given as an approximation to $G(u,u_x)$, takes the following form:

$$G_d(U,V)_k = \sum_{l=1}^{m} f_l(U_k,V_k)\; g_l^+(\delta_k^+ U_k, \delta_k^+ V_k)\; g_l^-(\delta_k^- U_k, \delta_k^- V_k), \quad k \in \mathbb{Z}. \tag{37}$$

For such G_d we define the four-point discrete variational derivative $\delta(G_d, \mathrm{loc})/\delta(U,V:W,X) = ((\delta(G_d,\mathrm{loc})/\delta(U,V:W,X))_k)_{k\in\mathbb{Z}}$ of G_d for $(U,V:W,X)$ as

$$\left(\frac{\delta(G_d,\mathrm{loc})}{\delta(U,V:W,X)}\right)_k$$
$$\stackrel{\text{def}}{=} \sum_{l=1}^{m}\{\mathscr{P}_l(U,V:W,X)_k - \delta_k^+ \mathscr{Q}_l^-(U,V:W,X)_k - \delta_k^- \mathscr{Q}_l^+(U,V:W,X)_k\}, \tag{38}$$

where $U=(U_k)_{k\in\mathbb{Z}},\ V=(V_k)_{k\in\mathbb{Z}},\ W=(W_k)_{k\in\mathbb{Z}},\ X=(X_k)_{k\in\mathbb{Z}}$,

$$\mathscr{P}_l(U,V:W,X)_k \stackrel{\text{def}}{=} \frac{\mathrm{d}(f_l,\mathrm{loc})}{\mathrm{d}(U_k,V_k:W_k,X_k)} \times \left(\frac{g_l^+(\delta_k^+U_k,\delta_k^+V_k)g_l^-(\delta_k^-U_k,\delta_k^-V_k)+g_l^+(\delta_k^+W_k,\delta_k^+X_k)g_l^-(\delta_k^-W_k,\delta_k^-X_k)}{2}\right), \tag{39}$$

$$\mathscr{Q}_l^+(UV:W,X)_k \stackrel{\text{def}}{=} \left(\frac{f_l(U_k,V_k)+f_l(W_k,X_k)}{2}\right)\left(\frac{g_l^\mp(\delta_k^\mp U_k,\delta_k^\mp V_k)+g_l^\mp(\delta_k^\mp W_k,\delta_k^\mp X_k)}{2}\right) \times \frac{\mathrm{d}(g_l^\pm,\mathrm{loc})}{\mathrm{d}(\delta_k^\pm U_k,\delta_k^\pm V_k:\delta_k^\pm W_k,\delta_k^\pm X_k)}, \tag{40}$$

$$\frac{\mathrm{d}(f,\mathrm{loc})}{\mathrm{d}(a,b:c,d)} \stackrel{\text{def}}{=} \begin{cases} \dfrac{f(a,b)-f(c,d)}{\mathrm{loc}(a,b)-\mathrm{loc}(c,d)}: & \mathrm{loc}(a,b)\neq\mathrm{loc}(c,d),\\ \left.\dfrac{\mathrm{d}f(x,x)}{\mathrm{d}x}\right|_{x=\mathrm{loc}(a,b)}: & \mathrm{loc}(a,b)=\mathrm{loc}(c,d), \end{cases} \tag{41}$$

and

$$\mathrm{loc}(a,b)\stackrel{\text{def}}{=}\tfrac{1}{2}(a+b). \tag{42}$$

Consider a discrete functional $J_\mathrm{d}[U,V]$ defined as

$$J_\mathrm{d}[U,V]=\sum_{k=0}^{N}{}'' G_\mathrm{d}(U,V)_k\Delta x. \tag{43}$$

By the summation by parts (25) applied to difference $J_\mathrm{d}[U,V]-J_\mathrm{d}[W,X]$ we obtain

$$J_\mathrm{d}[U,V]-J_\mathrm{d}[W,X] = \sum_{k=0}^{N}{}''\left\{\left(\frac{\delta(G_\mathrm{d},\mathrm{loc})}{\delta(U,V:W,X)}\right)_k(\mathrm{loc}(U_k,V_k)-\mathrm{loc}(W_k,X_k))\right\}\Delta x + \left[\frac{\partial(G_\mathrm{d},\mathrm{loc})}{\partial\delta U}(U,V:W,X)_k\right]_{k=0}^{N}, \tag{44}$$

where

$$\frac{\partial G_\mathrm{d}}{\partial\delta U}(U,V:W,X)_k \stackrel{\text{def}}{=} \frac{1}{2}\sum_{l=1}^{m}\{\mathscr{Q}_l^+(UV:W,X)_k\ s_k^+(\mathrm{loc}(U_k,V_k)-\mathrm{loc}(W_k,X_k))$$

$$+\mathcal{Q}_l^-(U,V:W,X)_k\, s_k^-(\mathrm{loc}(U_k,V_k)-\mathrm{loc}(W_k,X_k))$$
$$+(\mathrm{loc}(U_k,V_k)-\mathrm{loc}(W_k,X_k))s_k^+\mathcal{Q}_l^-(U,V:W,X)_k$$
$$+(\mathrm{loc}(U_k,V_k)-\mathrm{loc}(W_k,X_k))s_k^-\mathcal{Q}_l^+(U,V:W,X)_k\}. \tag{45}$$

4. New energy conserving schemes

In this section we propose two generic FDSs that inherit the energy conservation property for Eq. (2). $U_k^{(n)}$ means the approximation of $u(k\Delta x, n\Delta t)$ in this section. First, we propose a generic FDS that is implicit and uses the four-point discrete variational derivative described in Section 3.3. Almost known schemes that conserve energy for NLKGE are actual examples of this scheme. Second, we propose another one that is explicit and uses the two-point discrete variational derivative in Section 3.2. Only one scheme for NLKGE is known as an actual example of this scheme.

These two generic FDSs not only unify known schemes for NLKGE but produce new schemes for NLKGE, SKE, EE and other equations.

4.1. Implicit scheme

For the equation $\partial^2 u/\partial t^2 = -\delta G/\delta u$ in (2) we propose the following finite-difference scheme:

$$\delta_n^{\langle 2\rangle} U_k^{(n)} = -\left(\frac{\delta(G_\mathrm{d},\mathrm{loc})}{\delta(U^{(n+1)},U^{(n)}:U^{(n)},U^{(n-1)})}\right)_k, \quad 0\leqslant k\leqslant N,\ k\in\mathbb{Z},\ n\in\mathbb{N} \tag{46}$$

with discrete boundary conditions. We note that the proposed scheme (46) involves $(U_k^{(n+1)})_{k=-\beta}^{N+\beta}$, $(U_k^{(n)})_{k=-\beta}^{N+\beta}$ and $(U_k^{(n-1)})_{k=-\beta}^{N+\beta}$, where $(a_k)_{k=m_1}^{m_2} \stackrel{\mathrm{def}}{=} \{a_{m_1}, a_{m_1+1}, a_{m_1+2}, \ldots, a_{m_2}\}$,

$$\beta=\beta(G_\mathrm{d}) \stackrel{\mathrm{def}}{=} \begin{cases} 0: & g_l^+ = \text{const. and } g_l^- = \text{const. for } 1\leqslant {}^\forall l\leqslant m,\\ 1: & \text{not in above case and}\\ & g_l^+ = \text{const. or } g_l^- = \text{const. for } 1\leqslant {}^\forall l\leqslant m,\\ 2: & \text{otherwise.}\end{cases} \tag{47}$$

The discrete boundary conditions may be arbitrary under the following two constraints.

The first constraint: $(U_k^{(n+1)})_{k=-\beta}^{-1}$ and $(U_k^{(n+1)})_{k=N+1}^{N+\beta}$ must be described explicitly with $(U_k^{(n)})_{k=-\beta}^{N+\beta}$, $(U_k^{(n-1)})_{k=-\beta}^{N+\beta}$ and $(U_k^{(n+1)})_{k=0}^{N}$ through the discrete boundary conditions. This constraint is necessary for the well-posedness of the proposed scheme (46).

The second constraint: This corresponds to the boundary condition (3) in the continuous context. It is

$$\left[\frac{\partial(G_\mathrm{d},\mathrm{loc})}{\partial\delta U}(U^{(n+1)},U^{(n)}:U^{(n)},U^{(n-1)})_k\right]_{k=0}^{N} = 0. \tag{48}$$

We show that scheme (46) has the energy conservation property.

Theorem 2 (Energy conservation). *Let* $U_k^{(n)}$ *be computed through* (46) *and* (48). *Then the total energy* $\sum_{k=0}^{\prime\prime N}\{\frac{1}{2}(\delta_n^+U_k^{(n)})^2 + G_d(U^{(n+1)},U^{(n)})_k\}\Delta x$ *is independent of time step n.*

Proof.

$$
\begin{aligned}
&\frac{1}{\Delta t}\left[\sum_{k=0}^{N}{}'' \left\{\frac{1}{2}(\delta_n^+ U_k^{(n)})^2 + G_{\mathrm{d}}(U^{(n+1)}, U^{(n)})_k\right\}\Delta x \right.\\
&\qquad\left. -\sum_{k=0}^{N}{}'' \left\{\frac{1}{2}(\delta_n^+ U_k^{(n-1)})^2 + G_{\mathrm{d}}(U^{(n)}, U^{(n-1)})_k\right\}\Delta x\right]\\
&\quad = \sum_{k=0}^{N}{}'' \delta_n^{\langle 1\rangle} U_k^{(n)} \delta_n^{\langle 2\rangle} U_k^{(n)}\Delta x\\
&\qquad + \frac{1}{\Delta t}\sum_{k=0}^{N}{}'' \{G_{\mathrm{d}}(U^{(n+1)}, U^{(n)})_k - G_{\mathrm{d}}(U^{(n)}, U^{(n-1)})_k\}\Delta x\\
&\quad = \sum_{k=0}^{N}{}'' \delta_n^{\langle 1\rangle} U_k^{(n)} \delta_n^{\langle 2\rangle} U_k^{(n)}\Delta x\\
&\qquad + \sum_{k=0}^{N}{}'' \left(\frac{\delta(G_{\mathrm{d}}, \mathrm{loc})}{\delta(U^{(n+1)}, U^{(n)} : U^{(n)}, U^{(n-1)})}\right)_k \delta_n^{\langle 1\rangle} U_k^{(n)}\Delta x\\
&\qquad + \frac{1}{\Delta t}\left[\frac{\partial(G_{\mathrm{d}}, \mathrm{loc})}{\partial\delta U}(U^{(n+1)}, U^{(n)} : U^{(n)}, U^{(n-1)})_k\right]_{k=0}^{N}\\
&\quad = 0. \qquad (49)
\end{aligned}
$$

The second equality is derived from (44). The last is from scheme (46) and the discrete boundary condition (48). □

Remark 3. Note that (49) corresponds to (4) that means energy conservation property in the continuous context.

4.2. Explicit scheme

For the equation $\partial^2 u/\partial t^2 = -\delta G/\delta u$ in (2) we propose the following finite-difference scheme:

$$
\delta_n^{\langle 2+\rangle} U_k^{(n)} = -\left(\frac{\delta G_{\mathrm{d}}}{\delta(U^{(n+1)}, U^{(n)})}\right)_k, \quad 0 \leqslant k \leqslant N,\ k \in \mathbb{Z},\ n \in \mathbb{N} \qquad (50)
$$

with discrete boundary conditions. We note that the proposed scheme (50) involves $(U_k^{(n+2)})_{k=-\beta}^{N+\beta}$, $(U_k^{(n+1)})_{k=-\beta}^{N+\beta}$, $(U_k^{(n)})_{k=-\beta}^{N+\beta}$ and $(U_k^{(n-1)})_{k=-\beta}^{N+\beta}$.

The discrete boundary conditions may be arbitrary under the following two constraints.

The first constraint: $(U_k^{(n+2)})_{k=-\beta}^{-1}$ and $(U_k^{(n+2)})_{k=N+1}^{N+\beta}$ must be described explicitly with $(U_k^{(n+1)})_{k=-\beta}^{N+\beta}$, $(U_k^{(n)})_{k=-\beta}^{N+\beta}$, $(U_k^{(n-1)})_{k=-\beta}^{N+\beta}$ and $(U_k^{(n+2)})_{k=0}^{N}$ through the discrete boundary conditions. This constraint is necessary for the well-posedness of the proposed scheme (50).

The second constraint: This corresponds to the boundary condition (3) in the continuous context. It is

$$\left[\frac{\partial G_{\mathrm{d}}}{\partial \delta U}(U^{(n+1)}, U^{(n)})_k\right]_{k=0}^{N} = 0. \tag{51}$$

We show that scheme (50) has the energy conservation property.

Theorem 4 (Energy conservation). *Let* $U_k^{(n)}$ *be computed through* (50) *and* (51). *Then the total energy* $\sum''^{N}_{k=0}\{\frac{1}{2}(\delta_n^+ U_k^{(n)})(\delta_n^- U_k^{(n)}) + G_d(U^{(n)})_k\}\Delta x$ *is independent of time step n.*

Proof.

$$\begin{aligned}
&\frac{1}{\Delta t}\left[\sum_{k=0}^{N}{}'' \left\{\frac{1}{2}(\delta_n^+ U_k^{(n+1)})(\delta_n^- U_k^{(n+1)}) + G_{\mathrm{d}}(U^{(n+1)})_k\right\}\Delta x \right.\\
&\qquad \left. - \sum_{k=0}^{N}{}'' \left\{\frac{1}{2}(\delta_n^+ U_k^{(n)})(\delta_n^- U_k^{(n)}) + G_{\mathrm{d}}(U^{(n)})_k\right\}\Delta x\right]\\
&= \sum_{k=0}^{N}{}'' \delta_n^+ U_k^{(n)} \delta_m^{\langle 2+\rangle} U_k^{(n)} \Delta x\\
&\quad + \frac{1}{\Delta t}\sum_{k=0}^{N}{}'' \{G_{\mathrm{d}}(U^{(n+1)})_k - G_{\mathrm{d}}(U^{(n)})_k\}\Delta x\\
&= \sum_{k=0}^{N}{}'' \delta_n^+ U_k^{(n)} \delta_m^{\langle 2+\rangle} U_k^{(n)} \Delta x\\
&\quad + \sum_{k=0}^{N}{}'' \left(\frac{\delta G_{\mathrm{d}}}{\delta(U^{(n+1)}, U^{(n)})}\right)_k \delta_n^+ U_k^{(n)} \Delta x\\
&\quad + \frac{1}{\Delta t}\left[\frac{\partial G_{\mathrm{d}}}{\partial \delta U}(U^{(n+1)}, U^{(n)})_k\right]_{k=0}^{N}\\
&= 0.
\end{aligned} \tag{52}$$

The second equality is derived from (34). The last is from scheme (50) and the discrete boundary condition (51). □

5. Applications

Some examples using the proposed schemes are shown in this section.

5.1. The nonlinear wave equation

We consider the nonlinear wave equation (8) and (9) as specific examples of the target equation in (2). Fermi et al. obtain numerical solutions of these equations and study behavior of the energy in their famous work [17]. Energy function G for (8) is

$$G(u,u_x) = \frac{1}{2}(u_x)^2 + \frac{\varepsilon}{6}(u_x)^3 \tag{53}$$

and energy function for (9) is

$$G(u,u_x) = \frac{1}{2}(u_x)^2 + \frac{\varepsilon}{12}(u_x)^4. \tag{54}$$

From the proposed explicit energy conserving scheme (50) with the choice of

$$G_{\mathrm{d}}(U)_k \stackrel{\mathrm{def}}{=} \frac{1}{2}\left(\frac{(\delta_k^+ U_k)^2 + (\delta_k^- U_k)^2}{2}\right) + \frac{\varepsilon}{6}\left(\frac{(\delta_k^+ U_k)^3 + (\delta_k^- U_k)^3}{2}\right), \tag{55}$$

we obtain a new explicit energy conserving scheme for (8),

$$\begin{aligned} \delta_n^{\langle 2+\rangle} U_k^{(n)} = {} & \frac{1}{2}\delta_k^{\langle 2\rangle} U_k^{(n+1)} \left\{1 + \varepsilon\delta_k^{\langle 1\rangle}\left(\frac{2U_k^{(n+1)} + U_k^{(n)}}{3}\right)\right\} \\ & + \frac{1}{2}\delta_k^{\langle 2\rangle} U_k^{(n)} \left\{1 + \varepsilon\delta_k^{\langle 1\rangle}\left(\frac{2U_k^{(n)} + U_k^{(n+1)}}{3}\right)\right\}. \end{aligned} \tag{56}$$

From the proposed explicit energy conserving scheme (50) with the choice of

$$G_{\mathrm{d}}(U)_k \stackrel{\mathrm{def}}{=} \frac{1}{2}\left(\frac{(\delta_k^+ U_k)^2 + (\delta_k^- U_k)^2}{2}\right) + \frac{\varepsilon}{12}\left(\frac{\left(\delta_k^+ U_k\right)^4 + \left(\delta_k^- U_k\right)^4}{2}\right), \tag{57}$$

we obtain a new explicit energy conserving scheme for (9),

$$\delta_n^{\langle 2+\rangle} U_k^{(n)} = \delta_k^{\langle 2\rangle} \mu_n^+ U_k^{(n)} + \frac{\varepsilon}{3}\left\{\frac{A(U^{(n+1)}, U^{(n)})_{k+1/2} - A(U^{(n+1)}, U^{(n)})_{k-1/2}}{\Delta x}\right\}, \tag{58}$$

where

$$A(U,V)_{k+1/2} \stackrel{\mathrm{def}}{=} \frac{1}{4}\sum_{j=0}^{3}(\delta_k^+ U_k)^j(\delta_k^+ V_k)^{3-j}. \tag{59}$$

5.2. The nonlinear string vibration equation

We consider the nonlinear string vibration equation (10) as a specific example of the target equation in (2) where

$$G(u,u_x) = \sqrt{1 + (u_x)^2}. \tag{60}$$

Eq. (10) describes elastic string motions for which changes are not small in tension [8].

From the proposed explicit energy conserving scheme (50) with the choice of

$$G_{\mathrm{d}}(U)_k \stackrel{\mathrm{def}}{=} \frac{\sqrt{1+(\delta_k^+ U_k)^2}+\sqrt{1+(\delta_k^- U_k)^2}}{2}, \tag{61}$$

we obtain a new explicit energy conserving scheme for (10),

$$\delta_n^{\langle 2+\rangle} U_k^{(n)} = \frac{B(U^{(n+1)},U^{(n)})_{k+1/2} - B(U^{(n+1)},U^{(n)})_{k-1/2}}{\Delta x}, \tag{62}$$

where

$$B(U,V)_{k+1/2} \stackrel{\mathrm{def}}{=} \frac{\delta_k^+((U_k+V_k)/2)}{\frac{1}{2}(\sqrt{1+(\delta_k^+ U_k)^2}+\sqrt{1+(\delta_k^+ V_k)^2})}. \tag{63}$$

5.3. The nonlinear Klein–Gordon equation

We consider the nonlinear Klein–Gordon equation (12) as a specific example of the target equation in (2) where

$$G(u,u_x) = \tfrac{1}{2}(u_x)^2 + \phi(u). \tag{64}$$

This is a well-known nonlinear equation which has soliton solutions and includes linear wave equation, the sine-Gordon equation, the double sine-Gordon equation and the phi-4 equation. Numerical solution of this equation is relatively difficult and studies on numerical analysis are [1–7,10,11, 13–16,21,23–26,30–32].

The study [26] by Perring and Skyrme is the first study on numerical solution of the sine-Gordon equation. Ablowitz use fourth degree FDS in [4], symplectic Runge–Kutta method based on Fourier spectral discretization in [1], the Hirota scheme in [2] and symplectic method in [3] for the sine-Gordon equation. The Hirota FDS proposed in [21] is "completely integrable discretization for the sine-Gordon equation" but we must take $\Delta x = \Delta t$. In [5] Ben-Yu introduce Strauss scheme and propose a energy conserving scheme. The Strauss FDS in [30] is energy conserving but Li notes that the scheme is not unconditionally stable in [25]. Djidjeli shows an explicit scheme where space dimension is two and obtain stability criterion by linear stability analysis in [10]. Duncan compares his scheme with Strauss scheme and some symplectic schemes in [11]. In [15] Evans uses Gear–Nordesieck predictor–corrector algorithm to obtain numerical solution. Fei proposes two energy conserving schemes in [16]. Lee use FEM and show stability criterion and convergence in [24]. Vu-Quoc and Li propose some energy-conserving FDSs and momentum-conserving FDSs in [25,31]. In [32] Zaki propose a leap-frog method based on B-spline method and show stability criterion.

In many studies all calculus are not completely discrete, for example, energy of numerical solution is calculated through integral not summation. In the literature, we can find the following five schemes as energy conserving and completely discrete schemes. As described in introduction, all of the five schemes can be derived from the proposed schemes (46) or (50).

Strauss scheme [30]:

$$\delta_n^{\langle 2\rangle} U_k^{(n)} = \delta_k^{\langle 2\rangle} U_k^{(n)} - \frac{\mathrm{d}\phi}{\mathrm{d}(U_k^{(n+1)},U_k^{(n-1)})}. \tag{65}$$

This scheme is a special case of the proposed implicit scheme (46) with

$$G_{\mathrm{d}}(U,V)_k = \frac{1}{2}\left(\frac{\delta_k^+ U_k \delta_k^+ V_k + \delta_k^- U_k \delta_k^- V_k}{2}\right) + \frac{\phi(U_k)+\phi(V_k)}{2}. \tag{66}$$

Ben-Yu scheme [5]:

$$\delta_n^{\langle 2\rangle} U_k^{(n)} = \delta_k^{\langle 2\rangle} s_n^{\langle 1\rangle} U_k^{(n)} - \frac{\mathrm{d}\phi}{\mathrm{d}(U_k^{(n+1)}, U_k^{(n-1)})} \tag{67}$$

This scheme is a special case of the proposed implicit scheme (46) with

$$G_{\mathrm{d}}(U,V)_k = \frac{1}{2}\left(\frac{(\delta_k^+ U_k)^2 + (\delta_k^- U_k)^2 + (\delta_k^+ V_k)^2 + (\delta_k^- V_k)^2}{4}\right) + \frac{\phi(U_k)+\phi(V_k)}{2}. \tag{68}$$

Fei implicit scheme [16]:

$$\delta_n^{\langle 2\rangle} U_k^{(n)} = \delta_k^{\langle 2\rangle} U_k^{(n)} - \frac{\mathrm{d}\phi}{\mathrm{d}(\frac{1}{2}(U_k^{(n+1)} + U_k^{(n)}), \frac{1}{2}(U_k^{(n)} + U_k^{(n-1)}))}. \tag{69}$$

This scheme is a special case of the proposed implicit scheme (46) with

$$G_{\mathrm{d}}(U,V)_k = \frac{1}{2}\left(\frac{\delta_k^+ U_k \delta_k^+ V_k + \delta_k^- U_k \delta_k^- V_k}{2}\right) + \phi\left(\frac{U_k + V_k}{2}\right). \tag{70}$$

Li scheme [25]:

$$\delta_n^{\langle 2\rangle} U_k^{(n)} = \delta_k^{\langle 2\rangle} \mu_n^{\langle 1\rangle} U_k^{(n)} - \frac{\mathrm{d}\phi}{\mathrm{d}(U_k^{(n+1)}, U_k^{(n-1)})}. \tag{71}$$

This scheme is a special case of the proposed implicit scheme (46) with

$$G_{\mathrm{d}}(U,V)_k = \frac{1}{2}\left(\frac{(\delta_k^+((U_k+V_k)/2))^2 + (\delta_k^-((U_k+V_k)/2))^2}{2}\right) + \frac{\phi(U_k)+\phi(V_k)}{2}. \tag{72}$$

Fei explicit scheme [16]:

$$\delta_n^{\langle 2+\rangle} U_k^{(n)} = \delta_k^{\langle 2\rangle} \mu_n^+ U_k^{(n)} - \frac{\mathrm{d}\phi}{\mathrm{d}(U_k^{(n+1)}, U_k^{(n)})}. \tag{73}$$

This scheme is a special case of the proposed explicit scheme (50) with

$$G_{\mathrm{d}}(U)_k = \frac{1}{2}\left(\frac{(\delta_k^+ U_k)^2 + (\delta_k^- U_k)^2}{2}\right) + \phi(U_k). \tag{74}$$

Note that when $\phi = 0$, i.e. NLKGE (12) is linear wave equation, the Li scheme (71) is unconditionally stable [27, p. 264].

In addition to the above five schemes, we can make energy conserving new schemes for NLKGE from (46) or (50). For example, a new implicit scheme

$$\delta_n^{\langle 2\rangle} U_k^{(n)} = (\delta_k^{\langle 1\rangle})^2 \mu_n^{\langle 1\rangle} U_k^{(n)} - \frac{\mathrm{d}\phi}{\mathrm{d}(U_k^{(n+1)}, U_k^{(n-1)})} \tag{75}$$

is derived from (46) where

$$G_d(U,V)_k = \frac{1}{2}\left(\delta_k^{\langle 1\rangle}\left(\frac{U_k+V_k}{2}\right)\right)^2 + \frac{\phi(U_k)+\phi(V_k)}{2}. \tag{76}$$

The following new explicit scheme

$$\delta_n^{\langle 2+\rangle}U_k^{(n)} = s_k^{\langle 1\rangle}\delta_k^{\langle 2\rangle}\mu_n^+ U_k^{(n)} - \frac{\mathrm{d}\phi}{\mathrm{d}(U_k^{(n+1)},U_k^{(n)})} \tag{77}$$

is derived from (50) where

$$G_d(U)_k = \tfrac{1}{2}(\delta_k^+ U_k)(\delta_k^- U_k) + \phi(U_k). \tag{78}$$

Another new explicit scheme

$$\delta_n^{\langle 2+\rangle}U_k^{(n)} = (\delta_k^{\langle 1\rangle})^2\mu_n^+ U_k^{(n)} - \frac{\mathrm{d}\phi}{\mathrm{d}(U_k^{(n+1)},U_k^{(n)})} \tag{79}$$

is derived from (50) where

$$G_d(U)_k = \tfrac{1}{2}(\delta_k^{\langle 1\rangle}U_k)^2 + \phi(U_k). \tag{80}$$

Let us turn to numerical solutions of the above schemes. We obtain numerical solution for NLKGE using some of the above schemes. We take sine-Gordon equation in (11) as the NLKGE. The initial state is

$$u(x,0) = 4\arctan\left(\exp\left(\frac{x}{\sqrt{1-v^2}}\right)\right), \tag{81}$$

where $v = 0.2$ and $x \in [a,b]$ to be specified later. The exact solution for this initial state is known as

$$u(x,t) = 4\arctan\left(\exp\left(\frac{x-vt}{\sqrt{1-v^2}}\right)\right). \tag{82}$$

The energy $E^{\mathrm{TRUE}} \stackrel{\mathrm{def}}{=} \int\{\frac{1}{2}(u_t)^2 + G\}\mathrm{d}x$ for the exact solution is approximated as

$$\begin{aligned} E^{\mathrm{TRUE}} &\cong 4\frac{1+v^2}{\sqrt{1-v^2}} - (b-a) + 4\sqrt{1-v^2}\left(\frac{1}{1+\mathrm{e}^{2a/\sqrt{1-v^2}}} - \frac{1}{1+\mathrm{e}^{2b/\sqrt{1-v^2}}}\right) \\ &\cong \frac{8}{\sqrt{1-v^2}} - (b-a). \end{aligned} \tag{83}$$

In this case we take $[a,b] = [-10,10]$ and then $E^{\mathrm{TRUE}} = -11.83503\cdots$. The momentum $M^{\mathrm{TRUE}} \stackrel{\mathrm{def}}{=} \int u_x u_t \,\mathrm{d}x$ for the exact solution is approximated as

$$M^{\mathrm{TRUE}} \cong -\frac{8v}{\sqrt{1-v^2}} \tag{84}$$

and $M^{\mathrm{TRUE}} = -1.632993\cdots$ in this case. To obtain numerical solutions we take $\Delta x = 0.5$, $\Delta t = 0.025$ and

$$U_{-j}^{(n)} \stackrel{\mathrm{def}}{=} U_j^{(n)}, \quad U_{N+j}^{(n)} \stackrel{\mathrm{def}}{=} U_{N-j}^{(n)}, \quad 1 \leqslant j \leqslant N \tag{85}$$

for boundary conditions.

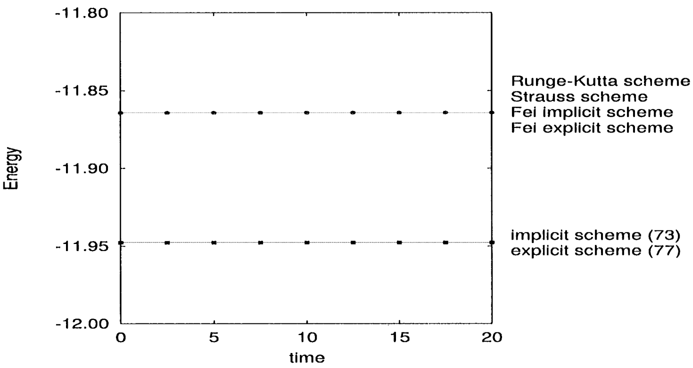

Fig. 1. Energy of numerical solutions calculated by energy conserving schemes for SGE.

Among the schemes mentioned above, we employ the Strauss scheme (65), the Fei implicit scheme (69), the Fei explicit scheme (73), the implicit scheme (75) and the explicit scheme (79). The fourth-order Runge–Kutta scheme is also employed for comparison. Specifically, the Runge–Kutta scheme is applied to ODE which is discretized in space by finite-difference method from the sine-Gordon equation as

$$\frac{\mathrm{d}}{\mathrm{d}t}U_k = V_k, \tag{86}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}V_k = \delta_k^{\langle 2\rangle} U_k - \sin U_k, \quad 0 \leqslant k \leqslant N, \tag{87}$$

where $U_k(t)$ and $V_k(t)$ are intended to approximate to $u(k\Delta x, t)$ and $\mathrm{d}u/\mathrm{d}t(k\Delta x, t)$, respectively. The pointwise Newton method is used for the Strauss scheme and the Fei implicit scheme, and the vector Newton method with diagonal LU decomposition for the implicit scheme (75). Numerical solutions obtained by those schemes agree quite well with the exact solution, while the former four schemes are slightly better than the latter schemes (75) and (79). This is no surprise because the accuracy of space difference operators in the former schemes are better than the ones in the latter schemes. Recall that our main interest in this paper is to propose the generic FDSs not to analyze numerical properties of individual schemes and that the latter schemes (75) and (79) are introduced to indicate the possibility of the generic schemes and not intended to be used for NLKGE in practice.

Fig. 1 shows the time dependency of energy of numerical solutions calculated by energy conserving schemes. Fig. 2 shows the time dependency of momentum of those numerical solutions. Fig. 1 indicates that the energy of numerical solutions are conserved quite well.

Table 1 shows the computation time by each scheme using the SUN Ultra 1 model 170E (CPU: UltraSPARC, 167 MHz). Computation times listed in the table are the average in five calculations. The results indicate that the explicit schemes are much faster than the other schemes including the Runge–Kutta scheme.

The sensitivity of the schemes to the time mesh size Δt is also investigated. The approximate maximum Δt for stable numerical solutions is shown also in Table 1. The maximum for the implicit scheme (75) is smaller than the size for the other schemes. This is not for the stability but for the convergence in the vector Newton method. The maximum time mesh size of the other proposed

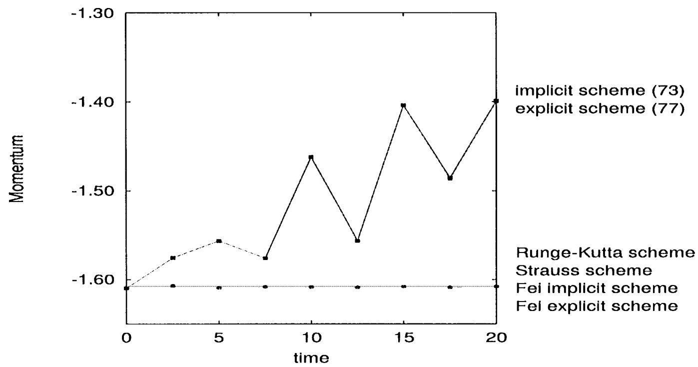

Fig. 2. Momentum of numerical solutions calculated by energy conserving schemes for SGE.

Table 1
Computation time and maximum Δt for each scheme

Scheme	Time (s)	Max Δt
Runge–Kutta scheme	17.68	0.7
Strauss scheme	13.19	0.5
Fei implicit scheme	14.36	0.5
Fei explicit scheme	5.97	0.4
The implicit scheme (75)	48.37	0.1
The explicit scheme (79)	4.48	0.8

schemes compares favorably with that of the Runge–Kutta scheme. This demonstrates the robustness of the proposed schemes against variations in time mesh size.

5.4. The Shimoji–Kawai equation

Here we consider the Shimoji–Kawai equation (13) as an example for the target equation in (2) where

$$G(u,u_x) = \tfrac{1}{2}(u_x)^4. \tag{88}$$

This is introduced in [29] by Shimoji and Kawai and they show multivalued exact solutions of the equation by a parametric equation.

For SKE from (50) we make a new explicit energy conserving scheme

$$\delta_n^{\langle 2+\rangle} U_k^{(n)} = \frac{1}{3}\left\{ \frac{A(U^{(n+1)},U^{(n)})_{k+1/2} - A(U^{(n+1)},U^{(n)})_{k-1/2}}{\Delta x} \right\}, \tag{89}$$

where $A(U,V)$ is defined in (59) and

$$G_{\mathrm{d}}(U)_k \stackrel{\mathrm{def}}{=} \frac{1}{12}\left\{ \frac{(\delta_k^+ U_k)^4 + (\delta_k^- U_k)^4}{2} \right\}. \tag{90}$$

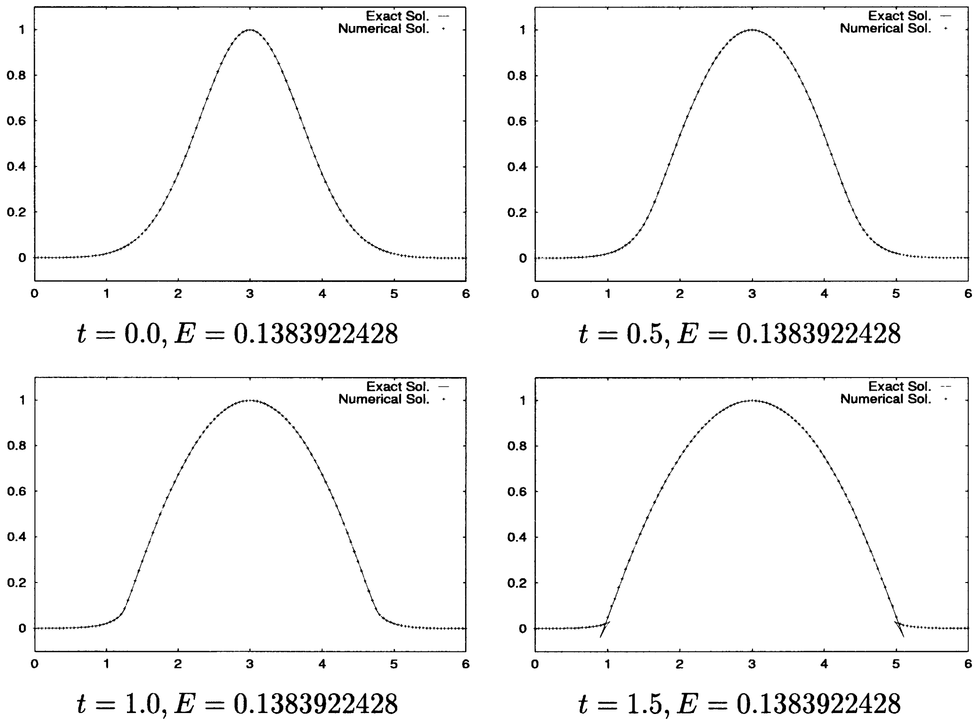

Fig. 3. Numerical solutions through the proposed energy conserving scheme (89) for SKE with initial state (91) and (92).

For numerical solutions parameters are $\Delta x = 0.05$, $\Delta t = 0.0001$ and boundary conditions are (85). The numerical investigation shows that the derived scheme (89) for SKE is quite promising in practice.

Fig. 3 shows numerical solutions for initial state

$$u(x,0) = \mathrm{e}^{-(x-3)^2}, \tag{91}$$

$$u_t(x,0) = 2(x-3)^2 \mathrm{e}^{-(x-3)^2}. \tag{92}$$

In the figures numerical solutions are indicated by points and exact solutions are indicated by lines. Energy values of numerical solutions are also indicated, to be compared with the values of exact solutions $0.1384729571\cdots$.

We consider another initial state. Fig. 4 shows numerical solutions for initial state

$$u(x,0) = \mathrm{e}^{-(x-3)^2}, \tag{93}$$

$$u_t(x,0) = -2(x-3)^2 \mathrm{e}^{-(x-3)^2}. \tag{94}$$

The energy of exact solution is also $0.1384729571\cdots$. For this initial state we can find that the exact solution becomes multivalued, for example, when $t = 1.5$ in Fig. 4. We can also find that the exact solution becomes slightly multivalued in Fig. 3 After $t = 0.5$ the numerical solution deviates from the exact solution considerably, but energy of the numerical solution agrees with that of the exact solution. To understand this phenomenon we should study more on this equation itself.

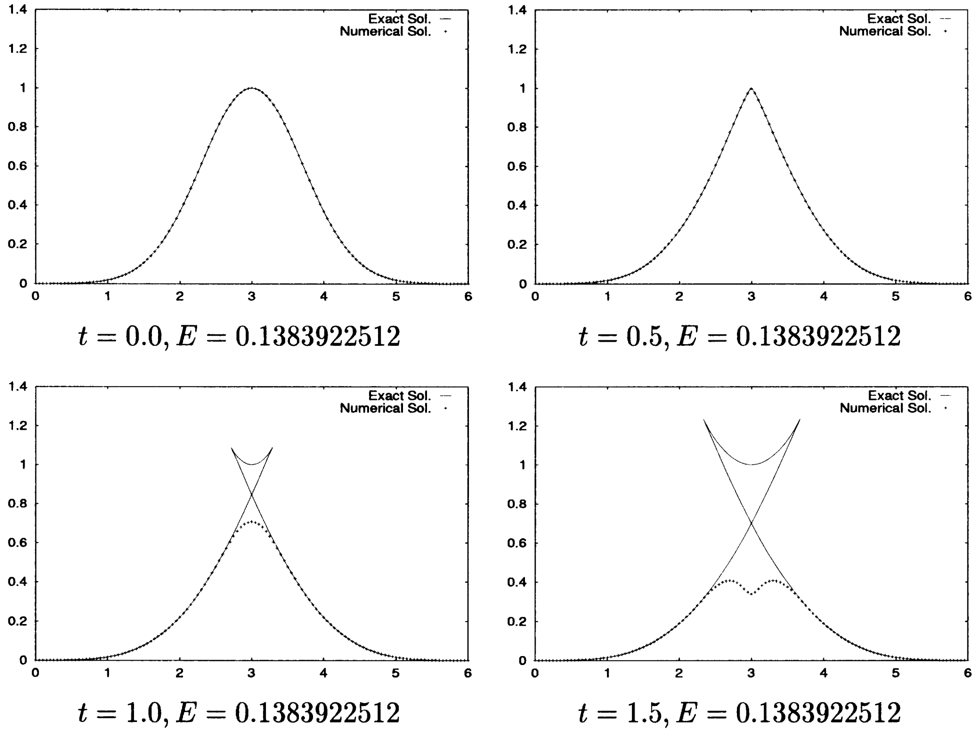

Fig. 4. Numerical solutions through the proposed energy conserving scheme (89) for SKE with initial state (93) and (94).

5.5. The Ebihara equation

Here we consider the Ebihara equation (14) as an example for the target equation in (2) where

$$G(u,u_x) = \frac{1}{2}x^{\alpha}(u_x)^2 + \frac{x^{-\gamma}}{2p+2}u^{2p+2}. \tag{95}$$

In [12] Ebihara investigates mathematical properties of this equation including the existence of global solutions. So far no explicit form of exact solution for this equation is yet known.

From the proposed explicit energy conserving scheme (50) with the choice of

$$G_{\mathrm{d}}(U)_k \stackrel{\mathrm{def}}{=} \frac{1}{2}(k\Delta x)^{\alpha}\left(\frac{(\delta_k^+U_k)^2 + (\delta_k^-U_k)^2}{2}\right) + \frac{(k\Delta x)^{-\gamma}}{2p+2}(U_k)^{2p+2}, \tag{96}$$

we yield a new explicit energy conserving scheme

$$\begin{aligned}\delta_n^{\langle 2+\rangle}U_k^{(n)} &= (k\Delta x)^{\alpha}\delta_k^{\langle 2\rangle}\mu_n^+U_k^{(n)} + \frac{(\delta_k^+(k\Delta x)^{\alpha})\delta_k^+\mu_n^+U_k^{(n)} + (\delta_k^-(k\Delta x)^{\alpha})\delta_k^-\mu_n^+U_k^{(n)}}{2} \\ &\quad - \frac{(k\Delta x)^{-\gamma}}{2p+2}\sum_{j=0}^{2p+1}(U_k^{(n+1)})^j(U_k^{(n)})^{2p+1-j}. \end{aligned} \tag{97}$$

6. Conclusion

We have proposed two general finite-difference schemes which inherit energy-conserving property from PDEs in (2). The proposed schemes are simple and applicable to many equations. Some actual example schemes are derived from the proposed general schemes and are shown to be competitive with existing schemes. This means that we may strongly expect that we can generate superior schemes for other PDEs easily.

When the space dimension is more than one, discrete calculus is much more difficult and complicated except when space axes are orthogonal to each other. A similar discrete calculus when the space dimension is two is exemplified in [19].

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References

[1] M.J. Ablowitz, B.M. Herbst, C.M. Schober, Numerical simulation of quasi-periodic solutions of the sine-Gordon equation, Physica D 87 (1995) 37–47.
[2] M.J. Ablowitz, B.M. Herbst, C.M. Schober, On the numerical solution of the sine-Gordon equation — I. Integrable discretizations and homoclinic manifolds, J. Comput. Phys. 126 (1996) 299–314.
[3] M.J. Ablowitz, B.M. Herbst, C.M. Schober, On the numerical solution of the sine-Gordon equation — II. Performance of numerical schemes, J. Comput. Phys. 131 (1997) 354–367.
[4] M.J. Ablowitz, M.D. Kruskal, J.F. Ladik, Solitary wave collisions, SIAM J. Appl. Math. 36 (1979) 428–437.
[5] G. Ben-Yu, P.J. Pascual, M.J. Rodriguez, L. Vázquez, Numerical solution of the sine-Gordon equation, Appl. Math. Comput. 18 (1986) 1–14.
[6] A.G. Bratsos, E.H. Twizell, A family of parametric finite-difference methods for the solution of the sine-Gordon equation, Appl. Math. Comput. 93 (1998) 117–137.
[7] R.K. Bullough, P.H. Caudrey, The multiple sine-Gordon equations in non-linear optics and in liquid ^{3}He, in: F. Calogero (Ed.), Nonlinear Evolution Equations Solvable by the Spectral Transform, Pitman, London, 1978, pp. 180–224.
[8] G.F. Carrier, On the non-linear vibration problem of the elastic string, Quart. Appl. Math. 3 (1945) 157–165.
[9] R. Courant, K.O. Friedrichs, H. Lewy, Über die Partiellen Differenzengleichungen der Mathematischen Physik, Math. Ann. 100 (1928) 32–74.
[10] K. Djidjeli, W.G. Price, E.H. Twizell, Numerical solutions of a damped sine-Gordon equation in two space variables, J. Eng. Math. 29 (1995) 347–369.
[11] D.B. Duncan, Symplectic finite difference approximations of the nonlinear Klein–Gordon equation, SIAM J. Numer. Anal. 34 (1997) 1742–1760.
[12] Y. Ebihara, Spherically symmetric solutions of some semilinear wave equations in: H. Kawarada, N. Kenmochi, N. Yanagihara (Eds.), Nonlinear Mathematical Problems in Industry II, Gakkotosho, Tokyo, 1993, pp. 431–434.
[13] J.C. Eilbeck, Numerical studies of solitons, in: A.R. Bishop, T. Schneider (Eds.), Solitons and Condensed Matter Physics, Springer, Berlin, 1978, pp. 28–43.
[14] M. Elgamal, S. Nakagiri, Weak solutions of sine-Gordon equation and their numerical analysis, in: Kohkyuuroku, Vol. 984, RIMS Kyoto University, Kyoto, 1997, pp. 123–137.
[15] W.A.B. Evans, M.D. Cunha, V.V. Konotop, L. Vázquez, Numerical study of various sine-Gordon “Breathers”, in: L. Vazquez et al. (Eds.), Nonlinear Klein–Gordon and Schrödinger systems: Theory and Applications, World Scientific, Singapore, 1996, pp. 293–302.

[16] Z. Fei, L. Vázquez, Two energy conserving numerical schemes for the sine-Gordon equation, Appl. Math. Comput. 45 (1991) 17–30.
[17] E. Fermi, J. Pasta, S. Ulam, Studies of non linear problems, Los Alamos Report, LA-1490 (1955) in: Collected Works of E. Fermi, Vol. 2, University of Chicago Press, Chicago, 1965, pp. 978–988.
[18] T. Flå, A numerical energy conserving method for the DNLS equation, J. Comput. Phys. 101 (1992) 71–79.
[19] D. Furihata, A stable and conservative finite difference scheme for the Cahn–Hilliard equation, Numer. Math., in press.
[20] D. Greenspan, Conservative numerical methods for $\ddot{x} = f(x)$, J. Comput. Phys. 56 (1984) 28–41.
[21] R. Hirota, Nonlinear partial difference equations III; discrete sine-Gordon equation, J. Phys. Soc. Jpn. 43 (1977) 2079–2086.
[22] R. Hirota, Difference analogues of nonlinear evolution equations in Hamiltonian form, Technical Report A-12, Department of Applied Mathematics, Hiroshima University, 1982.
[23] A.E. Kudryavtsev, Solitonlike solutions for a Higgs scalar field, JETP Lett. 22 (1975) 82–83.
[24] I.J. Lee, Numerical solution for nonlinear Klein–Gordon equation by collocation method with respect to spectral method, J. Korean Math. Soc. 32 (1995) 541–551.
[25] S. Li, L. Vu-Quoc, Finite difference calculus invariant structure of a class of algorithms for the nonlinear Klein–Gordon equation, SIAM J. Numer. Anal. 32 (1995) 1839–1875.
[26] J.K. Perring, T.H.R. Skyrme, A model unified field equation, Nucl. Phys. 31 (1962) 550–555.
[27] R.D. Richtmyer, K.W. Morton, Difference methods for initial-value problems, Wiley, New York, 1967.
[28] J.M. Sanz-Serna, Symplectic integrators for Hamiltonian problems: an overview, Acta Numer. 1 (1992) 243–286.
[29] S. Shimoji, T. Kawai, Multivalued solution on nonlinear wave equation, in: Y. Oyanagi (Ed.), Proceedings of the Numerical Analysis Symposium (Tokyo University, Tokyo, 1997), pp. 39–42 (in Japanese).
[30] W. Strauss, L. Vázquez, Numerical solution of a nonlinear Klein–Gordon equation, J. Comput. Phys. 28 (1978) 271–278.
[31] L. Vu-Quoc, S. Li, Invariant-conserving finite difference algorithms for the nonlinear Klein–Gordon equation, Comput. Methods Appl. Mech. Eng. 107 (1993) 341–349.
[32] S.I. Zaki, L.R.T. Gardner, G.A. Gardner, Numerical simulations of Klein–Gordon solitary-wave interactions, Nuovo Cimento Soc. Ital. Fis. B(12) 112 (1997) 1027–1036.