Chapter 10
An Energy-Preserving and Symmetric Scheme for Nonlinear Hamiltonian Wave Equations

In this chapter, we derive and analyse an energy-preserving and symmetric scheme for nonlinear Hamiltonian wave equations, which can exactly preserve the energy of the underlying Hamiltonian wave equations. To this end, we first define and discuss the bounded operator-argument functions on the underlying domain. We then introduce an operator-variation-of-constants formula, based on which we present an energy-preserving scheme for nonlinear Hamiltonian wave equations. The scheme preserves the energy of the original continuous Hamiltonian system exactly. In comparison with the existing work on this topic, such as the well-known Average Vector Field (AVF) formula for Hamiltonian ordinary differential equations, *the energy-preserving scheme avoids the semi-discretisation of spatial derivatives and exactly preserves the Hamiltonian of the original continuous Hamiltonian wave equation*. This point is very significant in comparison with the AVF formula, since *the AVF formula can preserve only the energy of Hamiltonian ordinary differential equations*. Hence, the main theme of this chapter is to establish a *scheme* which can exactly preserve the energy of the nonlinear Hamiltonian wave equation. The chapter is also accompanied by some examples.

10.1 Introduction

Nonlinear wave or heat equations arise frequently in a wide variety of applications, which can usually be expressed in suitable nonlinear Hamiltonian forms, and partial differential equations with a Hamiltonian structure are important in the study of solitons. Hamiltonian systems have some characteristic properties such as inner symmetries and energy conservation. However, there are no general methods guaranteed to find closed form solutions to nonlinear Hamiltonian systems. Over the last 20 years, geometric numerical integration has become an important area of numerical analysis and scientific computing. Structure-preserving integrators have received much attention in recent years and have applications in many areas of physics, such

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as molecular dynamics, fluid dynamics, celestial mechanics, and particle accelerators. An integrator is said to be *structure-preserving* if it preserves one or more physical/geometric properties of the system exactly. In this chapter, we pay attention to an energy-preserving scheme for the nonlinear Hamiltonian wave equation of the form

$$\begin{cases} u_{tt} - a^2 \Delta u = f(u), \quad t \geq t_0, \\ u(x, t_0) = \varphi_1(x), \ u_t(x, t_0) = \varphi_2(x), \end{cases} \tag{10.1}$$

where $\Delta = \partial_x^2$, and $f(u) = -V'(u)$ is the negative derivative of a potential function $V(u)$ with respect to u.

The nonlinear wave equation (10.1) in this chapter is assumed to be subject to the following periodic boundary condition

$$u(x, t) = u(x + \Gamma, t), \tag{10.2}$$

where Γ is the fundamental period in x.

It is known that Δ is an unbounded operator which is not defined for every $v \in L^2([x, x + \Gamma])$. In order to model periodic boundary conditions, we restrict ourselves to the case where Δ is defined on the domain

$$D(\Delta) = \{v(x) : \forall v \in L^2([x, x + \Gamma]) \text{ and } v(x) = v(x + \Gamma)\}. \tag{10.3}$$

We consider (10.1) with independent variables $(x, t) \in [x_l, x_r] \times \{t \geq t_0\}$ and suppose that $\Gamma = x_r - x_l$ is the period. Let $v = (u, p)^\intercal$ with $p = u_t$. The nonlinear wave equation (10.1) can be thought of as an infinite dimensional Hamiltonian system of the form

$$\partial_t v = J \frac{\delta H}{\delta v}, \quad \forall v \in \mathscr{B}. \tag{10.4}$$

This is equivalent to

$$\begin{cases} u_t = p, \\ p_t = a^2 \Delta u + f(u), \\ u(x, t_0) = \varphi_1(x), \ p(x, t_0) = \varphi_2(x), \end{cases} \tag{10.5}$$

where the Hamiltonian

$$H(u, p) := \frac{1}{2} \int_{x_l}^{x_r} \left[p^2 + a^2 u_x^2 + 2V(u) \right] \mathrm{d}x \tag{10.6}$$

is defined on the infinite dimensional "phase-space" $\mathscr{B} := \mathscr{V} \times L^2([x_l, x_r])$, where $\mathscr{V} = \left\{ u : u \in H^1([x_l, x_r]) \text{ and } u(x_l) = u(x_r) \right\}$, and the non-degenerate antisymmetric operator J represents a symplectic structure: the variables $v = (u, p)^\intercal$ are "Darboux coordinates" (see, e.g. [1]). The Hamiltonian system (10.4) preserves the energy (or the Hamiltonian) because J is skew-adjoint with respect to the L^2 inner product, i.e.,

$$\int_{x_l}^{x_r} uJu\,\mathrm{d}x = 0, \quad \forall u \in \mathscr{B}. \tag{10.7}$$

The conservation of the energy (or the Hamiltonian) is one of the most important properties of the nonlinear Hamiltonian wave equation (10.1), i.e.

$$E(t) = \frac{1}{2}\int_{x_l}^{x_r} \left[u_t^2(x,t) + a^2u_x^2(x,t) + 2V\big(u(x,t)\big)\right]\mathrm{d}x = E(t_0), \tag{10.8}$$

or

$$H(u,p) = H(u,p)\big|_{t=t_0}, \tag{10.9}$$

for the Hamiltonian system (10.5).

The nonlinear Hamiltonian wave equation (10.1) arises in a wide variety of application areas in science and engineering such as nonlinear optics, solid state physics and quantum field theory. Its description and understanding are of great importance both from the theoretical and practical point of view, and it has been investigated by many authors (see, e.g. [2, 8–11, 18, 26, 28, 35, 38]). This equation is the relativistic version of the Schrödinger equation [6, 7, 30]. Such a problem appears naturally in the study of some nonlinear dynamical problems of mathematical physics, including radiation theory, general relativity, the scattering and stability of kinks, vortices, and other coherent structures. This equation is the basis of much work in studying solitons and condensed matter physics, in investigating the interaction of solitons in collisionless plasma and the recurrence of initial states, in lattice dynamics, and in examining nonlinear phenomena.

Many authors have investigated energy preservation for semi-discrete Hamiltonian wave equations via classical spatial discretisation approximations. Usually, the semi-discrete systems are of the form

$$\begin{cases} y''(t) + My(t) = g(y(t)), \quad t \in [t_0, T], \\ y(t_0) = y_0, \quad y'(t_0) = y_0', \end{cases} \tag{10.10}$$

where $M \in \mathbb{R}^{m\times m}$ is a positive and semi-definite matrix (not necessarily diagonal or symmetric, in general). The solution of the system (10.10) exhibits nonlinear oscillations. When such oscillations occur, effective ODE solvers for (10.10) can be used, such as Gautschi-type methods (see, e.g. [16]), trigonometric Fourier collocation methods (see, e.g. [34]), and extended Runge–Kutta–Nyström (ERKN) methods (see, e.g. [42, 43]). With regard to the discrete energy-preserving method, the AVF formula is very popular (see, e.g. [3, 19, 21–25, 40]). However, the AVF formula cannot exactly preserve the energy of the original continuous Hamiltonian wave equation. In general, the discrete energy is different from the original energy of the continuous Hamiltonian wave equations. This means that the AVF formula based on classical discrete approximations cannot preserve the energy of the Hamiltonian wave equations exactly. This motivates an energy-preserving scheme for nonlinear Hamiltonian wave equations, which can exactly preserve the energy of the nonlinears Hamiltonian wave equation (10.1). *It should be noted that, in this chapter, all essential analytical features are present in the one-dimensional case* (10.1), *although the discussions are equally valid for high-dimensional nonlinear Hamiltonian wave equations*.

The outline of this chapter is as follows. Some preliminaries are given in Sect. 10.2. In Sect. 10.3, we introduce an operator-variation-of-constants formula for the nonlinear Hamiltonian wave equation (10.1), which is an analytical expression of the solution to the nonlinear Hamiltonian wave equation (10.1) expressed in a nonlinear integral equation. We then dicuss an energy-preserving scheme and analyse its properties in Sect. 10.4. Some illustrative examples are presented in Sect. 10.5. The last section is devoted to conclusions.

10.2 Preliminaries

This section presents some preliminaries in order to gain an insight into an exact energy-preserving scheme for the nonlinear Hamiltonian wave equation (10.1) subject to the periodic boundary condition (10.2).

To begin with, we define the following operator-argument functions:

$$\phi_j(\Delta) := \sum_{k=0}^{\infty} \frac{\Delta^k}{(2k+j)!}, \quad j = 0, 1, \ldots. \tag{10.11}$$

For example, Δ is the Laplace operator defined on $D(\Delta)$ in (10.3) and in this case, the operators defined by (10.11) is bounded on the subspace under the Sobolev norm $\|\cdot\|_{L^2 \leftarrow L^2}$ (see, e.g. [17, 20]). Accordingly, $\phi_j(\Delta)$ for $j = 0, 1, \ldots$ in (10.11) are called operator-argument functions. Besides, Δ can also be related to a linear mapping such as a positive semi-definite matrix $M \in \mathbb{R}^{m\times m}$ and in this particular case of $\Delta = -M$, (10.11) reduces to the matrix-valued functions which have been widely used in ARKN methods (Adapted Runge–Kutta–Nyström methods) and ERKN (Extended Runge–Kutta–Nyström methods) methods for the numerical solution of oscillatory or highly oscillatory differential equations (see, e.g. [12–14, 29, 31, 32, 40, 41, 43, 44]). These kinds of oscillatory problems have received a great deal of attention in the last few years (see, e.g. [4, 14–17, 34]).

In this chapter, some useful properties of these operator-argument functions are only sketched below for the sake of brevity.

Theorem 10.1 *For a symmetric negative (semi) definite operator Δ, the bounded ϕ-functions defined by (10.11) satisfy (9.10)–(9.14) in Chap. 9 and*

$$\begin{cases} \phi_0(m^2a^2\Delta)\phi_0(n^2a^2\Delta) + mna^2\Delta\phi_1(m^2a^2\Delta)\phi_1(n^2a^2\Delta) = \phi_0((m+n)^2a^2\Delta), \\ m\phi_0(n^2a^2\Delta)\phi_1(m^2a^2\Delta) + n\phi_0(m^2a^2\Delta)\phi_1(n^2a^2\Delta) = (m+n)\phi_1((m+n)^2a^2\Delta). \end{cases} \tag{10.12}$$

Proof These results are evident. □

Theorem 10.2 *Suppose that Δ is a Laplacian defined on the domain $D(\Delta)$. The bounded operator-argument functions ϕ_0 and ϕ_1 defined by (10.11) satisfy (9.9) in Chap. 9.*

Proof The results have been shown in Chap. 9. □

Some properties of the periodic functions are stated blow.

Theorem 10.3 *Assuming that $u(x,t)$, $v(x,t)$ are any sufficiently smooth periodic functions with respect to the variable x, i.e. $u(x+\Gamma,t) = u(x,t)$, and Γ is the fundamental period, then the following properties hold:*

(i) *For all $k, l = 0, 1, \ldots,$ we have*

$$\partial_x^k u(x+\Gamma,t) = \partial_x^k u(x,t), \quad \partial_t^l u(x+\Gamma,t) = \partial_t^l u(x,t). \tag{10.13}$$

(ii) *Applying integration by parts to the periodic functions $u(x,t)$, $v(x,t)$ yields*

$$\begin{aligned} &\int_{x_l}^{x_r} \partial_x^{2k} u(x,t)\cdot v(x,t)\mathrm{d}x = \int_{x_l}^{x_r} u(x,t)\cdot \partial_x^{2k} v(x,t)\mathrm{d}x, \\ &\int_{x_l}^{x_r} \partial_x^{2k+1} u(x,t)\cdot v(x,t)\mathrm{d}x = -\int_{x_l}^{x_r} u(x,t)\cdot \partial_x^{2k+1} v(x,t)\mathrm{d}x, \quad k = 0, 1, 2, \ldots, \end{aligned} \tag{10.14}$$

where the length $x_r - x_l$ of the interval $[x_l, x_r]$ is the period Γ or any nonnegative integer multiple of Γ.

(iii) *For any function $f(\cdot)$, the composite function $f\big(u(x,t)\big)$ is also a periodic function with respect to the variable x, and the fundamental period is Γ.*

10.3 Operator-Variation-of-Constants Formula for Nonlinear Hamiltonian Wave Equations

The next theorem presents the operator-variation-of-constants formula for the nonlinear Hamiltonian wave equation (10.1).

Theorem 10.4 *If $f(u)$ is continuous in (10.1) and Δ is the Laplace operator defined on the subspace $D(\Delta) \subset L^2$, then the exact solution of (10.1) and its derivative satisfy the following equations*

$$\begin{cases} u(x,t)=\phi_0\big((t-t_0)^2a^2\Delta\big)u(x,t_0)+(t-t_0)\phi_1\big((t-t_0)^2a^2\Delta\big)u_t(x,t_0)\\ \qquad\qquad +\displaystyle\int_{t_0}^{t}(t-\zeta)\phi_1\big((t-\zeta)^2a^2\Delta\big)\tilde{f}(\zeta)\mathrm{d}\zeta,\\ u_t(x,t)=(t-t_0)a^2\Delta\phi_1\big((t-t_0)^2a^2\Delta\big)u(x,t_0)+\phi_0\big((t-t_0)^2a^2\Delta\big)u_t(x,t_0)\\ \qquad\qquad +\displaystyle\int_{t_0}^{t}\phi_0\big((t-\zeta)^2a^2\Delta\big)\tilde{f}(\zeta)\mathrm{d}\zeta, \end{cases} \tag{10.15}$$

for $x\in[x_l,x_r],\ t_0,\ t\in(-\infty,+\infty)$*, where* $\tilde{f}(\zeta)=f\big(u(x,\zeta)\big)$*, and the bounded operator-argument functions* $\phi_0(\cdot)$ *and* $\phi_1(\cdot)$ *are defined by (10.11).*

Proof (10.15) solves the Eq. (10.1) exactly. In fact, this can be verified by directly inserting the formula (10.15) into the wave equation (10.1). The details of the proof for this theorem can be found in Appendix A of this chapter. □

Moreover, it can be proved that the operator-variation-of-constants formula (10.15) for the nonlinear Hamiltonian wave equation (10.1) is completely consistent with Dirichlet boundary conditions, Neumann boundary conditions, and Robin boundary conditions, respectively, under suitable assumptions. Readers are referred to the recent papers by Wu et al. [37, 39].

Let $u^n(x)=u(x,t_n)$ and $u_t^n(x)=u_t(x,t_n)$ represent the exact solution of (10.1) and its derivative with respect to t at $t=t_n$. It follows immediately from (10.15) with the change of variable $\xi=t_n+hz$ that

$$\begin{cases} u^{n+1}(x)=\ \phi_0\big(h^2a^2\Delta\big)u^n(x)+h\phi_1\big(h^2a^2\Delta\big)u_t^n(x)\\ \qquad\qquad +h^2\int_0^1(1-z)\phi_1\big((1-z)^2h^2a^2\Delta\big)f\big(u(x,t_n+hz)\big)\mathrm{d}z,\\ u_t^{n+1}(x)=\ ha^2\Delta\phi_1\big(h^2a^2\Delta\big)u^n(x)+\phi_0\big(h^2a^2\Delta\big)u_t^n(x)\\ \qquad\qquad +h\int_0^1\phi_0\big((1-z)^2h^2a^2\Delta\big)f\big(u(x,t_n+hz)\big)\mathrm{d}z, \end{cases} \tag{10.16}$$

where h is a time stepsize.

It is noted that the Eq. (10.15) or (10.16) is not a closed-form solution to the nonlinear Hamiltonian wave equation (10.1), but a nonlinear integral equation. In order to gain an energy-preserving scheme for (10.1), a further analysis based on (10.16) is still required.

10.4 Exact Energy-Preserving Scheme for Nonlinear Hamiltonian Wave Equations

In this section we establish an exact energy-preserving scheme for nonlinear Hamiltonian wave equations.

In light of the operator-variation-of-constants formula (10.16), it is natural to consider the following scheme:

$$\begin{cases} u^{n+1}(x) = \phi_0\big(h^2a^2\Delta\big)u^n(x) + h\phi_1\big(h^2a^2\Delta\big)u_t^n(x) + h^2 I_1(x), \\ u_t^{n+1}(x) = ha^2\Delta\phi_1\big(h^2a^2\Delta\big)u^n(x) + \phi_0\big(h^2a^2\Delta\big)u_t^n(x) + hI_2(x), \end{cases} \tag{10.17}$$

where h is the stepsize, and $I_1(x),\ I_2(x)$ are undetermined functions such that the following condition of energy preservation

$$E(t_{n+1}) = E(t_n) \quad \text{or} \quad H(u^{n+1}, p^{n+1}) = H(u^n, p^n),$$

is satisfied exactly, where $p = u_t$. It follows from (10.17) that

$$\begin{cases} u_x^{n+1}(x) = \phi_0\big(h^2a^2\Delta\big)u_x^n(x) + h\partial_x\phi_1\big(h^2a^2\Delta\big)u_t^n(x) + h^2\partial_x I_1(x), \\ u_t^{n+1}(x) = ha^2\partial_x\phi_1\big(h^2a^2\Delta\big)u_x^n(x) + \phi_0\big(h^2a^2\Delta\big)u_t^n(x) + hI_2(x). \end{cases} \tag{10.18}$$

To begin with, we compute

$$H(u^{n+1}, p^{n+1}) = H(u^{n+1}, u_t^{n+1}) = \frac{1}{2}\int_{x_l}^{x_r} \big[(u_t^{n+1}(x))^2 + a^2(u_x^{n+1}(x))^2 + 2V(u^{n+1}(x))\big]\mathrm{d}x. \tag{10.19}$$

Inserting (10.18) into (10.19), a careful calculation yields

$$\begin{aligned} H(u^{n+1}, u_t^{n+1}) &= \frac{1}{2}\int_{x_l}^{x_r} \big[\phi_0\big(h^2a^2\Delta\big)u_t^n \cdot \phi_0\big(h^2a^2\Delta\big)u_t^n + a^2h\partial_x\phi_1\big(h^2a^2\Delta\big)u_t^n \cdot h\partial_x\phi_1\big(h^2a^2\Delta\big)u_t^n\big]\mathrm{d}x \\ &+ \frac{a^2}{2}\int_{x_l}^{x_r} \big[ha^2\partial_x\phi_1\big(h^2a^2\Delta\big)u_x^n \cdot h\partial_x\phi_1\big(h^2a^2\Delta\big)u_x^n + \phi_0\big(h^2a^2\Delta\big)u_x^n \cdot \phi_0\big(h^2a^2\Delta\big)u_x^n\big]\mathrm{d}x \\ &+ \int_{x_l}^{x_r} \big[ha^2\partial_x\phi_1\big(h^2a^2\Delta\big)u_x^n \cdot \phi_0\big(h^2a^2\Delta\big)u_t^n + a^2\phi_0\big(h^2a^2\Delta\big)u_x^n \cdot h\partial_x\phi_1\big(h^2a^2\Delta\big)u_t^n\big]\mathrm{d}x \\ &+ \frac{1}{2}\int_{x_l}^{x_r} \big[\phi_0\big(h^2a^2\Delta\big)u_t^n \cdot hI_2(x) + a^2h\partial_x\phi_1\big(h^2a^2\Delta\big)u_t^n \cdot h^2\partial_x I_1(x)\big]\mathrm{d}x \\ &+ a^2\int_{x_l}^{x_r} \big[h\partial_x\phi_1\big(h^2a^2\Delta\big)u_x^n \cdot hI_2(x) + \phi_0\big(h^2a^2\Delta\big)u_x^n(x) \cdot h^2\partial_x I_1(x)\big]\mathrm{d}x \\ &+ \frac{1}{2}\int_{x_l}^{x_r} \big[h^2I_2(x) \cdot I_2(x) + a^2h^4\partial_x I_1(x) \cdot \partial_x I_1(x)\big]\mathrm{d}x + \int_{x_l}^{x_r} V(u^{n+1}(x))\mathrm{d}x. \end{aligned} \tag{10.20}$$

Applying Theorem 10.3 to (10.20) gives

$$\begin{aligned}H(u^{n+1},u_t^{n+1})=&\frac{1}{2}\int_{x_l}^{x_r}\big[\phi_0^2\big(h^2a^2\varDelta\big)-h^2a^2\varDelta\phi_1^2\big(h^2a^2\varDelta\big)\big]u_t^n\cdot u_t^n\mathrm{d}x\\&+\frac{a^2}{2}\int_{x_l}^{x_r}\big[\phi_0^2\big(h^2a^2\varDelta\big)-h^2a^2\varDelta\phi_1^2\big(h^2a^2\varDelta\big)\big]u_x^n\cdot u_x^n\mathrm{d}x\\&+a^2h\int_{x_l}^{x_r}\big[\partial_x\phi_1\big(h^2a^2\varDelta\big)\phi_0\big(h^2a^2\varDelta\big)-\phi_0\big(h^2a^2\varDelta\big)\partial_x\phi_1\big(h^2a^2\varDelta\big)\big]u_x^n\cdot u_t^n\mathrm{d}x\\&+\int_{x_l}^{x_r}\big[\phi_0\big(h^2a^2\varDelta\big)u_t^n\cdot hI_2(x)+a^2h\partial_x\phi_1\big(h^2a^2\varDelta\big)u_t^n\cdot h^2\partial_xI_1(x)\big]\mathrm{d}x\\&+a^2\int_{x_l}^{x_r}\big[h\partial_x\phi_1\big(h^2a^2\varDelta\big)u_x^n\cdot hI_2(x)+\phi_0\big(h^2a^2\varDelta\big)u_x^n(x)\cdot h^2\partial_xI_1(x)\big]\mathrm{d}x\\&+\frac{1}{2}\int_{x_l}^{x_r}\big[h^2I_2(x)\cdot I_2(x)+a^2h^4\partial_xI_1(x)\cdot\partial_xI_1(x)\big]\mathrm{d}x+\int_{x_l}^{x_r}V(u^{n+1}(x))\mathrm{d}x.\end{aligned}\tag{10.21}$$

On noticing Theorem 10.1, (10.21) reduces to

$$\begin{aligned}&H(u^{n+1},u_t^{n+1})=\frac{1}{2}\int_{x_l}^{x_r}\big[(u_t^n(x))^2+a^2(u_x^n(x))^2+2V(u^n(x))\big]\mathrm{d}x\\&+\int_{x_l}^{x_r}\big[\phi_0\big(h^2a^2\varDelta\big)u_t^n\cdot hI_2(x)+a^2h\partial_x\phi_1\big(h^2a^2\varDelta\big)u_t^n\cdot h^2\partial_xI_1(x)\big]\mathrm{d}x\\&+a^2\int_{x_l}^{x_r}\big[h\partial_x\phi_1\big(h^2a^2\varDelta\big)u_x^n\cdot hI_2(x)+\phi_0\big(h^2a^2\varDelta\big)u_x^n(x)\cdot h^2\partial_xI_1(x)\big]\mathrm{d}x\\&+\frac{1}{2}\int_{x_l}^{x_r}\big[h^2I_2(x)\cdot I_2(x)+a^2h^4\partial_xI_1(x)\cdot\partial_xI_1(x)\big]\mathrm{d}x+\int_{x_l}^{x_r}\big[V(u^{n+1}(x))-V(u^n(x))\big]\mathrm{d}x.\end{aligned}\tag{10.22}$$

In what follows, we calculate

$$\begin{aligned}V(u^{n+1})-V(u^n)=&\int_0^1\mathrm{d}V\big((1-\tau)u^n+\tau u^{n+1}\big)=-\int_0^1(u^{n+1}-u^n)\cdot f\big((1-\tau)u^n+\tau u^{n+1}\big)\mathrm{d}\tau\\\triangleq&-(u^{n+1}-u^n)\cdot I_f,\end{aligned}\tag{10.23}$$

where

$$I_f=\int_0^1 f\big((1-\tau)u^n+\tau u^{n+1}\big)\mathrm{d}\tau.$$

The first equation of (10.17) gives

$$\begin{aligned}u^{n+1}(x)-u^n(x)&=\big[\phi_0\big(h^2a^2\varDelta\big)-I\big]u^n(x)+h\phi_1\big(h^2a^2\varDelta\big)u_t^n(x)+h^2I_1(x)\\&=h^2a^2\partial_x\phi_2\big(h^2a^2\varDelta\big)u_x^n(x)+h\phi_1\big(h^2a^2\varDelta\big)u_t^n(x)+h^2I_1(x).\end{aligned}\tag{10.24}$$

Inserting (10.24) into (10.23) yields

$$V(u^{n+1})-V(u^n)=-h^2a^2\partial_x\phi_2\big(h^2a^2\varDelta\big)u_x^n(x)\cdot I_f-h\phi_1\big(h^2a^2\varDelta\big)u_t^n(x)\cdot I_f-h^2I_1(x)\cdot I_f.\tag{10.25}$$

Then the scheme (10.22) can be rewritten by

$$\begin{aligned}H(u^{n+1}, u_t^{n+1}) &= \frac{1}{2}\int_{x_l}^{x_r} \left[(u_t^n(x))^2 + a^2(u_x^n(x))^2 + 2V(u^n(x))\right]\mathrm{d}x + \mathscr{R}^n \\ &= H(u^n, u_t^n) + \mathscr{R}^n,\end{aligned} \tag{10.26}$$

where

$$\begin{aligned}\mathscr{R}^n =& h\int_{x_l}^{x_r} \left[\phi_0(h^2a^2\Delta)u_t^n(x)\cdot I_2(x) + a^2h^2\partial_x\phi_1(h^2a^2\Delta)u_t^n\cdot\partial_x I_1(x) - \phi_1(h^2a^2\Delta)u_t^n(x)\cdot I_f\right]\mathrm{d}x \\ &+ a^2h^2\int_{x_l}^{x_r} \left[\partial_x\phi_1(h^2a^2\Delta)u_x^n\cdot I_2(x) + \phi_0(h^2a^2\Delta)u_x^n(x)\cdot\partial_x I_1(x) - \partial_x\phi_2(h^2a^2\Delta)u_x^n(x)\cdot I_f\right]\mathrm{d}x \\ &+ h^2\int_{x_l}^{x_r} \left[\frac{1}{2}\left(I_2(x)\cdot I_2(x) + h^2a^2\partial_x I_1(x)\cdot\partial_x I_1(x)\right) - I_1(x)\cdot I_f\right]\mathrm{d}x.\end{aligned} \tag{10.27}$$

It follows from the results of Theorem 10.3 that

$$\begin{aligned}\mathscr{R}^n =& h\int_{x_l}^{x_r} \left[\phi_0(h^2a^2\Delta)I_2(x) - h^2a^2\Delta\phi_1(h^2a^2\Delta)I_1(x) - \phi_1(h^2a^2\Delta)I_f\right]\cdot u_t^n(x)\mathrm{d}x \\ &+ a^2h^2\int_{x_l}^{x_r} \left[\Delta\phi_1(h^2a^2\Delta)I_2(x) - \Delta\phi_0(h^2a^2\Delta)I_1(x) - \Delta\phi_2(h^2a^2\Delta)I_f\right]\cdot u_x^n(x)\mathrm{d}x \\ &+ h^2\int_{x_l}^{x_r} \left[\frac{1}{2}\left(I_2(x)\cdot I_2(x) - h^2a^2\Delta I_1(x)\cdot I_1(x)\right) - I_1(x)\cdot I_f\right]\mathrm{d}x.\end{aligned} \tag{10.28}$$

The above analysis gives the following important theorem immediately.

Theorem 10.5 *The scheme (10.17) exactly preserves the energy (10.8) or the Hamiltonian (10.9), i.e.,*

$$E(t_{n+1}) = E(t_n) \quad or \quad H(u^{n+1}, p^{n+1}) = H(u^n, p^n), \quad n = 0, 1, \ldots, \tag{10.29}$$

if and only if $\mathscr{R}^n = 0$.

Based on Theorem 10.1, the following theorem gives a sufficient condition for the scheme (10.17) to be energy-preserving exactly.

Theorem 10.6 *If*

$$\begin{aligned}I_1(x) &= \phi_2(h^2a^2\Delta)\int_0^1 f\left((1-\tau)u^n(x) + \tau u^{n+1}(x)\right)\mathrm{d}\tau, \\ I_2(x) &= \phi_1(h^2a^2\Delta)\int_0^1 f\left((1-\tau)u^n(x) + \tau u^{n+1}(x)\right)\mathrm{d}\tau,\end{aligned} \tag{10.30}$$

then the scheme (10.17) exactly preserves the energy (10.8) or the Hamiltonian (10.9).

Proof It is clear from (10.28) that if the following three equations

$$\phi_0\big(h^2a^2\Delta\big)I_2(x) - h^2a^2\Delta\phi_1\big(h^2a^2\Delta\big)I_1(x) = \phi_1\big(h^2a^2\Delta\big)I_f, \tag{10.31}$$

$$\phi_1\big(h^2a^2\Delta\big)I_2(x) - \phi_0\big(h^2a^2\Delta\big)I_1(x) = \phi_2\big(h^2a^2\Delta\big)I_f, \tag{10.32}$$

$$\frac{1}{2}\int_{x_l}^{x_r}\big(I_2(x)\cdot I_2(x) - h^2a^2\Delta I_1(x)\cdot I_1(x)\big)\mathrm{d}x = \int_{x_l}^{x_r} I_1(x)\cdot I_f\mathrm{d}x, \tag{10.33}$$

are satisfied, then $\mathscr{R}^n = 0$ for $n = 0, 1, \ldots$. Hence, we have

$$E(t_{n+1}) = E(t_n) \quad \text{or} \quad H(u^{n+1}, p^{n+1}) = H(u^n, p^n).$$

The difference of (10.31) times $\phi_1\big(h^2a^2\Delta\big)$ and (10.32) times $\phi_0\big(h^2a^2\Delta\big)$ is

$$\big[\phi_0^2\big(h^2a^2\Delta\big) - h^2a^2\Delta\phi_1^2\big(h^2a^2\Delta\big)\big]I_1(x) = \big[\phi_1^2\big(h^2a^2\Delta\big) - \phi_0\big(h^2a^2\Delta\big)\phi_2\big(h^2a^2\Delta\big)\big]I_f.$$

Likewise, the difference of (10.31) times $\phi_0\big(h^2a^2\Delta\big)$ and (10.32) times $h^2a^2\phi_1\big(h^2a^2\Delta\big)$ gives

$$\begin{aligned}&\big[\phi_0^2\big(h^2a^2\Delta\big) - h^2a^2\Delta\phi_1^2\big(h^2a^2\Delta\big)\big]I_2(x)\\ &= \big[\phi_0\big(h^2a^2\Delta\big)\phi_1\big(h^2a^2\Delta\big) - h^2a^2\Delta\phi_1\big(h^2a^2\Delta\big)\phi_2\big(h^2a^2\Delta\big)\big]I_f.\end{aligned}$$

Using Theorem 10.1, we obtain

$$I_1(x) = \phi_2\big(h^2a^2\Delta\big)I_f, \quad I_2(x) = \phi_1\big(h^2a^2\Delta\big)I_f. \tag{10.34}$$

It can be verified that under the condition (10.34) and Theorem 10.2, the equation (10.33) is also valid. Therefore, (10.30) are sufficient conditions for (10.17) to be an energy-preserving scheme. □

We are now in a position to present the following energy-preserving scheme for Hamiltonian PDEs.

Definition 10.1 The exact energy-preserving scheme for the nonlinear Hamiltonian wave equation (10.1) is defined by

$$\begin{cases} u^{n+1}(x) = \phi_0\big(h^2a^2\Delta\big)u^n(x) + h\phi_1\big(h^2a^2\Delta\big)u_t^n(x)\\ \quad + h^2\phi_2\big(h^2a^2\Delta\big)\displaystyle\int_0^1 f\big((1-\tau)u^n(x) + \tau u^{n+1}(x)\big)\mathrm{d}\tau,\\ u_t^{n+1}(x) = ha^2\Delta\phi_1\big(h^2a^2\Delta\big)u^n(x) + \phi_0\big(h^2a^2\Delta\big)u_t^n(x)\\ \quad + h\phi_1\big(h^2a^2\Delta\big)\displaystyle\int_0^1 f\big((1-\tau)u^n(x) + \tau u^{n+1}(x)\big)\mathrm{d}\tau, \end{cases} \tag{10.35}$$

where $h > 0$ is a time stepsize, $\phi_0(h^2a^2\Delta)$, $\phi_1(h^2a^2\Delta)$, and $\phi_2(h^2a^2\Delta)$ are bounded operator-argument functions defined by (10.11).

Since there is a very close similarity between the behaviour of solutions of reversible and Hamiltonian systems [27], in what follows, we show the symmetry of the energy-preserving scheme (10.35).

Theorem 10.7 *The energy-preserving scheme (10.35) is symmetric in time.*

Proof It follows from exchanging $u^{n+1}(x) \leftrightarrow u^n(x),\ u_t^{n+1}(x) \leftrightarrow u_t^n(x)$ and replacing h by $-h$ in (10.35) that

$$\begin{aligned} u^n(x) &= \phi_0\big(h^2a^2\Delta\big)u^{n+1}(x) - h\phi_1\big(h^2a^2\Delta\big)u_t^{n+1}(x) \\ &+ h^2\phi_2\big(h^2a^2\Delta\big)\int_0^1 f\big((1-\tau)u^{n+1}(x) + \tau u^n(x)\big)\mathrm{d}\tau, \\ u_t^n(x) &= -ha^2\Delta\phi_1\big(h^2a^2\Delta\big)u^{n+1}(x) + \phi_0\big(h^2a^2\Delta\big)u_t^{n+1}(x) \\ &- h\phi_1\big(h^2a^2\Delta\big)\int_0^1 f\big((1-\tau)u^{n+1}(x) + \tau u^n(x)\big)\mathrm{d}\tau. \end{aligned} \tag{10.36}$$

From (10.36) and Theorem 10.1, it follows that

$$\begin{aligned} u^{n+1}(x) &= \phi_0\big(h^2a^2\Delta\big)u^n(x) + h\phi_1\big(h^2a^2\Delta\big)u_t^n(x) \\ &+ h^2\phi_2\big(h^2a^2\Delta\big)\int_0^1 f\big((1-\tau)u^{n+1}(x) + \tau u^n(x)\big)\mathrm{d}\tau, \\ u_t^{n+1}(x) &= ha^2\Delta\phi_1\big(h^2a^2\Delta\big)u^n(x) + \phi_0\big(h^2a^2\Delta\big)u_t^n(x) \\ &+ h\phi_1\big(h^2a^2\Delta\big)\int_0^1 f\big((1-\tau)u^{n+1}(x) + \tau u^n(x)\big)\mathrm{d}\tau. \end{aligned} \tag{10.37}$$

Letting $\xi = 1 - \tau$, we have

$$\begin{aligned} &\int_0^1 f\big((1-\tau)u^{n+1}(x) + \tau u^n(x)\big)\mathrm{d}\tau = \int_0^1 f\big(\xi u^{n+1}(x) + (1-\xi)u^n(x)\big)\mathrm{d}\xi \\ &= \int_0^1 f\big((1-\tau)u^n(x) + \tau u^{n+1}(x)\big)\mathrm{d}\tau, \end{aligned}$$

which shows (10.37) is exactly the same as (10.35).

Therefore, the conclusion of the theorem is proved. □

Remark 10.1 The extension of the scheme (10.35) to the general high-dimensional nonlinear Hamiltonian wave equation

$$\begin{cases} u_{tt}(X,t) - a^2\Delta u(X,t) = f\big(u(X,t)\big), & X \in \Omega \subseteq \mathbb{R}^d,\ t_0 < t \le T, \\ u(X,t_0) = \varphi_1(X),\ u_t(X,t_0) = \varphi_2(X), & x \in \Omega \cup \partial\Omega, \end{cases} \tag{10.38}$$

with the corresponding periodic boundary conditions, is straightforward (see [20]), where

$$\Delta = \sum_{i=1}^{d} \partial_{x_i}^2.$$

Remark 10.2 It is noted that the new approach described above for dealing with (10.1) is totally different from classical discrete approximations such as variational methods, and the method of lines (see, e.g. [26]), since the semidiscretisation of the spatial derivative is now avoided. Compared with classical discrete approximations, this approach to solving (10.1) is exact for the space variable x.

Remark 10.3 It can be observed that when the solution of the initial-boundary value problem (10.1) and (10.2) is independent of the spatial variable x, the system (10.1) becomes a Hamiltonian ordinary differential equation and, in this case, (10.35) reduces to the average vector field (AVF) method. Besides, when the spatial interval is divided into a set of finite points with a fixed spatial stepsize via the classical discrete approximations, then the $-\Delta$ is replaced by a symmetric semi-definite positive matrix which is from a discrete operator, such as the second-order central difference operator, (10.35) reduces to the adapted average vector field (AAVF) methods [44]. In other words, the exact energy-preserving scheme (10.35) is an essential extension of AVF to Hamiltonian wave equations based on the operator-variation-of-constants formula (10.15).

Theorem 10.8 *If $V = V(\alpha u)$, where $\alpha \neq 0$, then*

$$\int_0^1 f\big((1-\tau)u^n(x) + \tau u^{n+1}(x)\big)\mathrm{d}\tau = \frac{-1}{u^{n+1}(x) - u^n(x)}\Big(V(\alpha u^{n+1}(x)) - V(\alpha u^n(x))\Big).$$

Proof

$$\begin{aligned}
&\int_0^1 f\big((1-\tau)u^n(x) + \tau u^{n+1}(x)\big)\mathrm{d}\tau = -\int_0^1 \alpha V'\Big(\alpha\big((1-\tau)u^n(x) + \tau u^{n+1}(x)\big)\Big)\mathrm{d}\tau \\
&= \frac{-\alpha}{\alpha\left(u^{n+1}(x) - u^n(x)\right)}\int_0^1 \frac{\mathrm{d}V\Big(\alpha\big((1-\tau)u^n(x) + \tau u^{n+1}(x)\big)\Big)}{\mathrm{d}\tau}\mathrm{d}\tau \\
&= \frac{-1}{u^{n+1}(x) - u^n(x)}\Big(V\left(\alpha u^{n+1}(x)\right) - V\left(\alpha u^n(x)\right)\Big).
\end{aligned}$$

□

From Theorem 10.8 we obtain the main result of this chapter.

Theorem 10.9 *An exact energy-preserving and symmetric scheme for the nonlinear Hamiltonian wave equation (10.1) is given by*

$$\begin{cases} u^{n+1}(x) = \phi_0\big(h^2a^2\Delta\big)u^n(x) + h\phi_1\big(h^2a^2\Delta\big)u_t^n(x) - h^2\phi_2\big(h^2a^2\Delta\big)J_n(x), \\ u_t^{n+1}(x) = ha^2\Delta\phi_1\big(h^2a^2\Delta\big)u^n(x) + \phi_0\big(h^2a^2\Delta\big)u_t^n(x) - h\phi_1\big(h^2a^2\Delta\big)J_n(x), \end{cases} \tag{10.39}$$

where $h > 0$ is a time stepsize, $\phi_0(h^2a^2\Delta)$, $\phi_1(h^2a^2\Delta)$, $\phi_2(h^2a^2\Delta)$ are bounded operator-argument functions defined by (10.11)*, and*

$$J_n(x) = \frac{V\big(u^{n+1}(x)\big) - V\big(u^n(x)\big)}{u^{n+1}(x) - u^n(x)}. \tag{10.40}$$

Here, it can be observed that, if $u^{n+1}(x) - u^n(x) = 0$*, then* $J_n(x)$ *in* (10.39) *is* $\frac{0}{0}$*, which can be understood as*

$$J_n(x) = \frac{\mathrm{d}V\big(u^n(x)\big)}{\mathrm{d}u} = -f\big(u^n(x)\big). \tag{10.41}$$

Proof The conclusion of the theorem can be proved directly by applying Theorem 10.8 to the energy-preserving scheme (10.35). □

Theorem 10.9 establishes the exact energy-preserving scheme (10.39) for the nonlinear Hamiltonian wave equation (10.1) with the periodic boundary condition (10.2). In the special case $f(u) = \alpha(x)$, that is $V(u) = -\alpha(x)u + \beta(x)$ and $J_n(x) = -\alpha(x)$, the formula (10.39) yields the exact solution of the underlying problem.

If $f(u) = 0$, then (10.1) becomes the homogeneous linear wave equation:

$$\begin{cases} u_{tt} - a^2 \Delta u = 0, \\ u(x, t_0) = \varphi_1(x), \ \ u_t(x, t_0) = \varphi_2(x), \end{cases} \tag{10.42}$$

and accordingly, from Theorem 10.1, (10.39) reduces to

$$\begin{cases} u^{n+1}(x) = \phi_0\big(h^2a^2\Delta\big)u^n(x) + h\phi_1\big(h^2a^2\Delta\big)u_t^n(x) \\ \qquad\qquad = \phi_0\big((n+1)^2h^2a^2\Delta\big)\varphi_1(x) + (n+1)h\phi_1\big((n+1)^2h^2a^2\Delta\big)\varphi_2(x), \\ u_t^{n+1}(x) = ha^2\Delta\phi_1\big(h^2a^2\Delta\big)u^n(x) + \phi_0\big(h^2a^2\Delta\big)u_t^n(x) \\ \qquad\qquad = (n+1)ha^2\Delta\phi_1\big((n+1)^2h^2a^2\Delta\big)\varphi_1(x) + \phi_0\big((n+1)^2h^2a^2\Delta\big)\varphi_2(x), \end{cases} \tag{10.43}$$

which exactly integrates the homogeneous linear wave equation (10.42). This implies that (10.43) possesses an additional advantage of energy preservation and quadratic invariant preservation for the homogeneous wave equation (10.42). Besides, compared with the well-known D'Alembert, Poisson and Kirchhoff formulas, *the formula* (10.43) *is independent of the computation of integrals and presents an exact closed-form solution to* (10.42).

10.5 Illustrative Examples

With regard to applications of the scheme (10.39) or (10.43), we now give some illustrative examples.

Problem 10.1 Consider the homogeneous linear wave equation

$$\begin{cases} u_{tt} = u_{xx}, \quad x \in (0, 2), \ t > 0, \\ u(x, 0) = \sin(\pi x), \ u_t(x, 0) = -\dfrac{1}{9}\sin(\pi x), \end{cases} \tag{10.44}$$

subject to the periodic boundary conditions $u(L, t) = u(0, t)$ where the period $L = 2$.

After a careful calculation, it is easy to see that (10.43) directly gives the analytic solution of Problem 10.1 and its derivative

$$\begin{cases} u(x, t) = \sin(\pi x)\cos(\pi t) - \dfrac{1}{9\pi}\sin(\pi x)\sin(\pi t), \\ u_t(x, t) = -\pi \sin(\pi x)\sin(\pi t) - \dfrac{1}{9}\sin(\pi x)\cos(\pi t), \end{cases} \tag{10.45}$$

on noticing that

$$\phi_0(t^2\frac{\partial^2}{\partial x^2})\sin(\pi x) = \sin(\pi x)\cos(\pi t),$$

$$t\phi_1(t^2\frac{\partial^2}{\partial x^2})\big(-\frac{1}{9}\sin(\pi x)\big) = -\frac{1}{9\pi}\sin(\pi x)\sin(\pi t),$$

and

$$t\frac{\partial^2}{\partial x^2}\phi_1(t^2\frac{\partial^2}{\partial x^2})\sin(\pi x) = -\pi\sin(\pi x)\sin(\pi t).$$

Problem 10.2 We consider the following two dimensional homogenous periodic wave equation

$$\begin{cases} u_{tt} - a^2(u_{xx} + u_{yy}) = 0, \ (x, y) \in (0, 2) \times (0, 2), t > 0, \\ u|_{t=0} = \sin(3\pi x)\sin(4\pi y), \ u_t|_{t=0} = 0. \end{cases} \tag{10.46}$$

Applying the formula (10.43) ($\Delta = \partial_x^2 + \partial_y^2$ in this case) to (10.46) leads to

$$\begin{cases} u(x, y, t) = \phi_0\big(t^2a^2\Delta\big)\sin(3\pi x)\sin(4\pi y), \\ u_t(x, y, t) = ta^2\Delta\phi_1\big(t^2a^2\Delta\big)\sin(3\pi x)\sin(4\pi y). \end{cases} \tag{10.47}$$

It follows from a simple calculation that

$$\begin{cases} u(x, y, t) = \sin(3\pi x)\sin(4\pi y)\cos(5t), \\ u_t(x, y, t) = -5\sin(3\pi x)\sin(4\pi y)\sin(5t). \end{cases} \tag{10.48}$$

Problem 10.3 Consider the following non-homogeneous linear periodic wave equation

$$\begin{cases} u_{tt} - u_{xx} = \cos x, \ x \in \left(\dfrac{\pi}{4}, 2\pi + \dfrac{\pi}{4}\right), \ t > 0, \\ u|_{t=0} = \sin x, \ u_t|_{t=0} = 0. \end{cases} \tag{10.49}$$

Applying (10.39) to (10.49) gives

$$\begin{cases} u(x,t) = \phi_0(t^2\Delta)\sin x + t^2\phi_2(t^2\Delta)\cos x, \\ u_t(x,t) = t\Delta\phi_1(t^2\Delta)\sin x + t\phi_1(t^2\Delta)\cos x. \end{cases} \tag{10.50}$$

Then a simple calculation yields

$$\begin{cases} u(x,t) = (\sin x - \cos x)\cos t + \cos x, \\ u_t(x,t) = -(\sin x - \cos x)\sin t, \end{cases} \tag{10.51}$$

which is exactly the solution of the problem (10.49).

Remark 10.4 The main purpose of this chapter is to establish a general framework for an exact energy-preserving scheme for nonlinear Hamiltonian wave equations, although we cannot achieve a closed-form solution for the nonlinear Hamiltonian wave equation (10.1). Consequently, we do not consider further computational issues in detail in this chapter.

10.6 Conclusions and Discussions

Energy-preserving schemes have a long history, and can date back to Courant, Friedrichs, and Lewy's work [5]. In this chapter, we considered the properties of energy-preserving schemes and presented an exact energy-preserving scheme for the nonlinear Hamiltonian wave equation (10.1) equipped with the periodic boundary condition (10.2), which is in fact identical to the infinite dimensional nonlinear Hamiltonian system (10.4) or (10.5). We first defined the bounded operator-argument functions (10.11) and analysed their properties, then established an operator-variation-of-constants formula for the nonlinear Hamiltonian wave equation (10.1). The proposed energy-preserving scheme is based on the operator-variation-of-constants formula which avoids the semidiscretisation of the spatial derivative and exactly preserves the energy of the original continuous Hamiltonian wave equation (10.1). This energy-preserving scheme (10.35) is a significant generalisation of the AVF formula and the AAVF formula (see, e.g. [33, 40]) as stated in Remark 10.3, since both the AVF formula and AAVF formula can preserve only the semi-discrete energy of the continuation Hamiltonian PDEs (10.1). In fact, both the AVF formula and AAVF formula are designed specially for Hamiltonian ordinary differential equations. In applications, such Hamiltonian ODEs in time can be obtained from Hamiltonian PDEs by the discretisation of the spatial derivative via classical discrete approximations such as variational methods, and the method of lines. Furthermore, we have also derived an exact energy-preserving and symmetric scheme (10.39) for the nonlinear Hamiltonian wave equation (10.1) with the periodic boundary condition (10.2), which avoids the evaluation of the integral

$$\int_0^1 f\big((1-\tau)u^n(x) + \tau u^{n+1}(x)\big)\mathrm{d}\tau$$

in the exact energy-preserving scheme (10.35). Therefore, *we have in fact derived an exact energy-preserving and symmetric scheme* (10.39) *for the nonlinear Hamiltonian wave equation* (10.1), although the closed form solution to (10.1) is not accessible (even though it exists).

Last but not least, the extension of scheme (10.35) to the general high-dimensional nonlinear wave equation (10.38) is straightforward, as stated in Remark 10.1. All essential analytical features presented for (10.1) are applicable to high-dimensional nonlinear Hamiltonian wave equations (10.38).

It should also be noted that the operator-variation-of-constants formula for wave equations makes it possible to systematically incorporate the inner structure properties of the original continuous system into numerical schemes in the design of structure-preserving integrators for nonlinear wave equations. Chapter 11 will try to demonstrate this point.

The material of this chapter is based on the work by Wu and Liu [36].

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