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Well-Posedness and the Energy and Charge Conservation for Nonlinear Wave Equations in Discrete Space-Time

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Abstract. We consider the discretization problem for $\mathbf{U}(1)$-invariant nonlinear wave equations in any dimension. We show that the classical finite-difference scheme used by Strauss and Vazquez (in J. Comput. Phys. **28**, 271–278 (1978)) conserves the positive-definite discrete analog of the energy if the grid ratio satisfies $dt/dx \leqslant 1/\sqrt{n}$, where dt and dx are the mesh sizes of the time and space variables and n is the spatial dimension. We also show that, if the grid ratio is $dt/dx = 1/\sqrt{n}$, then there is a discrete analog of charge, and this discrete analog is conserved.

We prove the existence and uniqueness of solutions to the discrete Cauchy problem. We use energy conservation to obtain a priori bounds for finite energy solutions, thus showing that the Strauss–Vazquez finite-difference scheme for the nonlinear Klein-Gordon equation with positive nonlinear term in the Hamiltonian is conditionally stable.

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1. INTRODUCTION

We study the $\mathbf{U}(1)$-invariant nonlinear wave equation discretized in space and time. Our objective is to find a stable finite-difference scheme for numerical simulation of the nonlinear wave processes, which corresponds to a well-posed Cauchy problem and provides us with a priori energy bounds.

The discretized models are widely studied in applied mathematics and in theoretical physics. Such models originally arose in condensed matter theory, due to atoms in a crystal forming a lattice. These models now occupy a prominent place in theoretical physics, partially because some of these models (like the Ising model) are exactly solvable. Lattice models are also used to describe polymers.

The paper [6] is fundamental for considering energy-conserving difference schemes for the nonlinear Klein–Gordon equations and nonlinear wave equations. The importance of having conserved quantities in the numerical scheme was illustrated by noticing that instability can occur for a finite-difference scheme which does not conserve energy. The authors suggested an implicit difference scheme and wrote out the expression for the energy conserved by that scheme. This finite-difference scheme was favorably compared with three other schemes in [3]. The higher-dimensional analog of the Strauss–Vazquez scheme and the corresponding energy-momentum tensor was represented in [5]. The general theory of finite-difference schemes for the nonlinear Klein-Gordon equation aimed at energy conservation was developed in [4] and [2]. In the paper [1], energy preserving schemes are constructed for a wide class of second-order nonlinear Hamiltonian systems of wave equations.

The Strauss–Vazquez finite-difference scheme over schemes in [4] and [2] is important, because it admits an easy solution algorithm. Namely, the discrete scheme involves the value of the unknown function at the "next" moment of time only at a single lattice point, and can be solved (numerically) with respect to the value at that point (see Remark 2.2 below). At the same time, the corresponding discrete energy for that scheme (see (2.23) below) contains quadratic terms that are not positive definite, showing that the scheme is not *unconditionally stable*.

We use the same finite-difference scheme as Strauss and Vazquez [6]. We show that, under the condition $dt/dx \leqslant 1/\sqrt{n}$ imposed on the grid ratio, where n is the number of spatial dimensions,

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the expression for the conserved discrete energy is positive definite, providing one with a priori energy estimates in the case of the discrete nonlinear Klein–Gordon equation. Moreover, under the assumption $dt/dx = 1/\sqrt{n}$ on the grid ratio, we show that the equation possesses a conserved discrete charge. The continuous limits of our discrete versions for the energy and charge coincide with the energy and charge in the continuous case.

Let us stress that the positive definiteness of energy enables one to obtain a priori bounds for the norm of the solution. Such a priori bounds are of utmost importance for applications. Numerically, these bounds indicate the stability of the finite-difference scheme in question.

The discrete charge conservation does not seem to be particularly important on its own; however, it could be regarded as an indication that the $\mathbf{U}(1)$-invariance of the continuous equation is in a sense compatible with the chosen discretization procedure (see the discussion in [4, Sec. 1]).

In Section 2, we formulate our main results. We establish the existence of solutions to the corresponding discrete Cauchy problem and analyze the uniqueness of solutions. We show that, for confining polynomial potentials, uniqueness holds if the mesh size is sufficiently small. Moreover, we describe a class of polynomial nonlinearities for which the value of the mesh size can readily be specified. We also study charge conservation. The proofs related to the well-posedness are presented in Section 3.

2. MAIN RESULTS

2.1. Continuous Case

Let us first consider the $\mathbf{U}(1)$-invariant nonlinear wave equation

$$\ddot{\psi}(x,t) = \Delta\psi(x,t) - 2\partial_\lambda v(x, |\psi(x,t)^2|)\psi(x,t), \qquad x \in \mathbb{R}^n, \tag{2.1}$$

where $\psi(x,t) \in \mathbb{C}^N$, $N \geqslant 1$, and $v(x,\lambda)$ is such that $v \in C(\mathbb{R}^n \times \mathbb{R})$ and $v(x,\cdot) \in C^2(\mathbb{R})$ for each $x \in \mathbb{R}^n$. Equation (2.1) can be represented in the Hamiltonian form with the Hamiltonian

$$\mathcal{E}(\psi,\dot{\psi}) = \int_{\mathbb{R}^n} \Big[\frac{|\dot{\psi}^2|}{2} + \frac{|\nabla\psi^2|}{2} + v(x, |\psi(x,t)^2|)\Big]\,dx, \tag{2.2}$$

where $|\psi^2| = \bar{\psi}\cdot\psi$ for $\psi \in \mathbb{C}^N$. The value of the Hamiltonian functional $\mathcal{E}$ and the value of the charge functional

$$\mathcal{Q}(\psi,\dot{\psi}) = \frac{i}{2}\int_{\mathbb{R}^n} \big(\bar{\psi}\cdot\dot{\psi} - \dot{\bar{\psi}}\cdot\psi\big)\,dx \tag{2.3}$$

are formally conserved for solutions to (2.1). A particular case of (2.1) is the nonlinear Klein–Gordon equation with $v(x,\lambda) = \frac{m^2}{2}\lambda + z(x,\lambda)$ and $m > 0$,

$$\ddot{\psi} = \Delta\psi - m^2\psi - 2\partial_\lambda z(x,|\psi^2|)\psi, \qquad x \in \mathbb{R}^n, \quad t \in \mathbb{R}. \tag{2.4}$$

If $z(x,\lambda) \geqslant 0$ for all $x \in \mathbb{R}^n$ and $\lambda \geqslant 0$, then the conservation of energy

$$\int_{\mathbb{R}^n} \Big[\frac{|\dot{\psi}^2|}{2} + \frac{|\nabla\psi^2|}{2} + \frac{m^2|\psi^2|}{2} + z(x,|\psi^2|)\Big]\,dx$$

yields an a priori estimate for the norm of the solution,

$$\int_{\mathbb{R}^n} |\psi(x,t)^2|\,dx \leqslant \frac{2}{m^2}\mathcal{E}(\psi|_{t=0}, \dot{\psi}|_{t=0}). \tag{2.5}$$

2.2. Discretized Equation

Let us now describe the discretized equation. Let $(X,T)\in\mathbb{Z}^n\times\mathbb{Z}$ be a point of the space-time lattice. We always indicate the temporal dependence by superscripts and the spatial dependence by subscripts. Let $V_X(\lambda)=v(\varepsilon X,\lambda)$ be a function on $\mathbb{Z}^n\times\mathbb{R}$ such that $V_X\in C^2(\mathbb{R})$ for each $X\in\mathbb{Z}^n$. Write

$$B_X(\lambda,\mu):=(V_X(\lambda)-V_X(\mu))/(\lambda-\mu),\qquad \lambda,\,\mu\in\mathbb{R},\quad X\in\mathbb{Z}^n, \tag{2.6}$$

and consider the standard implicit finite-difference scheme for (2.1) [6],

$$\frac{\psi_X^{T+1}-2\psi_X^T+\psi_X^{T-1}}{\tau^2}=\sum_{j=1}^n\frac{\psi_{X+e_j}^T-2\psi_X^T+\psi_{X-e_j}^T}{\varepsilon^2}-B_X(|\psi_X^{T+1}|^2,|\psi_X^{T-1}{}^2|)(\psi_X^{T+1}+\psi_X^{T-1}), \tag{2.7}$$

where $\psi_X^T\in\mathbb{C}^N$, $N\geqslant 1$, is defined on the lattice $(X,T)\in\mathbb{Z}^n\times\mathbb{Z}$ and

$$e_1=(1,0,0,0,\dots)\in\mathbb{Z}^n,\qquad e_2=(0,1,0,0,\dots)\in\mathbb{Z}^n,\qquad \text{and so on.} \tag{2.8}$$

Remark 2.1. The continuous limit of (2.7) is given by (2.1), with εX corresponding to $x\in\mathbb{R}^n$ and τT corresponding to $t\in\mathbb{R}$. Since $\partial_\lambda V_X(\lambda)=B_X(\lambda,\lambda)$, the continuous limit of the last term on the right-hand side of (2.7) coincides with the right-hand side of (2.1).

Assume that ψ_X^T takes values in $\mathbb{C}^N$ with $N\geqslant 1$.

Remark 2.2. An advantage of the Strauss–Vazquez finite-difference scheme (2.7) over other energy-preserving schemes discussed in [4, 2] is that, at the moment $T+1$, relation (2.7) involves only the value of the function ψ at the point X, allowing one to implement a simple solution algorithm even in higher-dimensional cases.

2.3. Well-Posedness

Denote by ψ^T the function ψ defined on the lattice $(X,T)\in\mathbb{Z}^n\times\mathbb{Z}$ at the moment $T\in\mathbb{Z}$.

Theorem 2.3. (Existence of solutions) *Assume that*

$$k_1:=\inf_{X\in\mathbb{Z}^n,\lambda\geqslant 0}\partial_\lambda V_X(\lambda)>-\infty. \tag{2.9}$$

If the value of k_1 in (2.9) is negative, take $\tau_1=\sqrt{-1/k_1}$; if $k_1\geqslant 0$, take $\tau_1=+\infty$. Then for any $\tau\in(0,\tau_1)$ and any $\varepsilon>0$, there is a global solution ψ^T, $T\in\mathbb{Z}$, to the Cauchy problem for equation (2.7) with arbitrary initial data ψ^0, ψ^1 (which stand for ψ^T at $T=0$ and $T=1$).

Moreover, if $(\psi^0,\psi^1)\in l^2(\mathbb{Z}^n)\times l^2(\mathbb{Z}^n)$, then $\psi^T\in l^2(\mathbb{Z}^n)$ for all $T\in\mathbb{Z}$.

Remark 2.4. In this theorem we do not claim that $|\psi^T{}_{l^2(\mathbb{Z}^n)}|$ is uniformly bounded for all $T\in\mathbb{Z}$. For a priori estimates concerning $|\psi^T{}_{l^2(\mathbb{Z}^n)}|$, see Theorem 2.13 below.

One can readily see that any X-independent polynomial potential of the form

$$V_X(\lambda)=V(\lambda)=\sum_{q=0}^p C_q\lambda^{q+1},\qquad C_q\in\mathbb{R},\qquad C_p>0 \tag{2.10}$$

satisfies (2.9). Note that, since $\lim\limits_{\lambda\to+\infty}V(\lambda)=+\infty$, this potential is confining.

Remark 2.5. Note that, if $V_X(\lambda)$ is given by (2.10), it follows from the small Bézout theorem that $B_X(\lambda,\mu)=(V_X(\lambda)-V_X(\mu))/(\lambda-\mu)$ is a polynomial of λ and μ with real coefficients.

Theorem 2.6. (Uniqueness of solutions) *Assume that the functions $K_X^{\pm}(\lambda,\mu)=B_X(\lambda,\mu)+2\partial_\lambda B_X(\lambda,\mu)(\lambda\pm\sqrt{\lambda\mu})$ are bounded below and let*

$$k_2:=\inf_{\pm,\,X\in\mathbb{Z}^n,\,\lambda\geqslant 0,\,\mu\geqslant 0}K_X^{\pm}(\lambda,\mu)>-\infty. \tag{2.11}$$

If the value of k_2 *in* (2.11) *satisfies* $k_2 < 0$, *take* $\tau_2 = \sqrt{-1/k_2}$; *if* $k_2 \geqslant 0$, *take* $\tau_2 = +\infty$. *Then for any* $\tau \in (0, \tau_2)$ *and any* $\varepsilon > 0$, *there is a solution to the Cauchy problem for equation* (2.7) *with arbitrary initial data* (ψ^0, ψ^1), *and this solution is unique.*

Remark 2.7. Note that, since $K_X^-(\lambda, \lambda) = B_x(\lambda, \lambda) = \partial_\lambda W_x(\lambda)$, it follows that the values of k_1 and k_2 from Theorem 2.3 and Theorem 2.6, whenever $k_2 > -\infty$, are related by $k_2 \leqslant k_1$, and therefore, the values of τ_1 and τ_2 in these theorems are related by $\tau_2 \leqslant \tau_1$.

Theorem 2.8. (Existence and uniqueness for polynomial nonlinearities)

(1) *Condition* (2.11) *holds for any confining polynomial potential* (2.10).

(2) *Assume that*

$$V_X(\lambda) = \sum_{q=0}^{4} C_{X,q} \lambda^{q+1}, \qquad X \in \mathbb{Z}^n, \quad \lambda \geqslant 0, \tag{2.12}$$

where $C_{X,q} \geqslant 0$ *for* $X \in \mathbb{Z}^n$ *and* $1 \leqslant q \leqslant 4$, *and* $C_{X,0}$ *are uniformly bounded below,*

$$k_3 := \inf_{X \in \mathbb{Z}^n} C_{X,0} > -\infty. \tag{2.13}$$

If the value of k_3 *in* (2.13) *satisfies* $k_3 < 0$, *take* $\tau_3 = \sqrt{-1/k_3}$; *if* $k_3 \geqslant 0$, *take* $\tau_3 = +\infty$. *Then for any* $\tau \in (0, \tau_3)$ *and any* $\varepsilon > 0$, *there is a solution to the Cauchy problem for equation* (2.7) *with arbitrary initial data* (ψ^0, ψ^1), *and this solution is unique.*

Thus, even though the potential (2.10) satisfies conditions (2.9) and (2.11) in Theorem 2.3 and Theorem 2.6, it could be difficult to specify the corresponding values τ_1 and τ_2 explicitly. Yet, the second part of Theorem 2.8 gives a simple description of a class of X-dependent polynomials $V_X(\lambda)$ for which the range of admissible $\tau > 0$ can be readily specified.

We prove the existence and uniqueness results stated in Theorems 2.3, 2.6, and 2.8 in Section 3.

2.4. Energy Conservation

Theorem 2.9. (Energy conservation) *Suppose* ψ *is a solution to equation* (2.7) *such that* $\psi^T \in l^2(\mathbb{Z}^n)$ *for all* $T \in \mathbb{Z}$. *Then the discrete energy*

$$E^T = \sum_{X \in \mathbb{Z}^n} \Big[\Big(\frac{1}{\tau^2} - \frac{n}{\varepsilon^2}\Big) \frac{|\psi_X^{T+1} - \psi_X^T|^2}{2} + \sum_{j=1}^{n} \sum_{\pm} \frac{\big|\psi_X^{T+1} - \psi_{X \pm e_j}^T\big|^2}{4\varepsilon^2} + \frac{V_X(|\psi_X^{T+1}|^2) + V_X(|\psi_X^T|^2)}{2} \Big] \varepsilon^n \tag{2.14}$$

is conserved.

Remark 2.10. The discrete energy is positive definite if the grid ratio satisfies the condition

$$\tau/\varepsilon \leqslant 1/\sqrt{n}. \tag{2.15}$$

Remark 2.11. The continuous limit of the discrete energy E^T defined in (2.14) coincides with the energy functional (2.2) of the continuous nonlinear wave equation (2.1).

Remark 2.12. If ψ^0 and $\psi^1 \in l^2(\mathbb{Z}^n)$, then, by Theorem 2.3, we also have $\psi^T \in l^2(\mathbb{Z}^n)$ for all $T \in \mathbb{Z}$ as long as $\inf_{X \in \mathbb{Z}^n, \lambda \geqslant 0} \partial_\lambda V_X(\lambda) > -\infty$.

Proof. For any u, $v \in \mathbb{C}^N$, we have the identity

$$|u|^2 - |v|^2 = \mathrm{Re}\left[(\bar{u} - \bar{v}) \cdot (u + v)\right]. \tag{2.16}$$

Applying (2.16), we obtain

$$\sum_{X \in \mathbb{Z}^n} \big(|\psi_X^{T+1} - \psi_X^T|^2 - |\psi_X^T - \psi_X^{T-1}|^2\big) = \mathrm{Re} \sum_{X \in \mathbb{Z}^n} \big(\bar{\psi}_X^{T+1} - \bar{\psi}_X^{T-1}\big) \cdot \big(\psi_X^{T+1} - 2\psi_X^T + \psi_X^{T-1}\big). \tag{2.17}$$

Using (2.16), we also derive the following identity for any function $\psi_X^T \in \mathbb{C}^N$:

$$\sum_{X\in\mathbb{Z}^n}\sum_{j=1}^{n}\Big[|\psi_X^{T+1}-\psi_{X-e_j}|^{T^2}-|\psi_{X-e_j}^T-\psi_X^{T-1}|^2+|\psi_X^{T+1}-\psi_{X+e_j}^T|^2-|\psi_{X+e_j}^T-\psi_X^{T-1}|^2\Big]$$

$$=\mathrm{Re}\sum_{X\in\mathbb{Z}^n}\sum_{j=1}^{n}\Big[(\bar\psi_X^{T+1}-\bar\psi_X^{T-1})\cdot(\psi_X^{T+1}-2\psi_{X\pm e_j}^T+\psi_X^{T-1})$$

$$+(\bar\psi_X^{T+1}-\bar\psi_X^{T-1})\cdot(\psi_X^{T+1}-2\psi_{X+e_j}^T+\psi_X^{T-1})\Big]$$

$$=\mathrm{Re}\sum_{X\in\mathbb{Z}^n}(\bar\psi_X^{T+1}-\bar\psi_X^{T-1})\cdot\Big[2n\big(\psi_X^{T+1}-2\psi_X^T+\psi_X^{T-1}\big)-2\sum_{j=1}^{n}\big(\psi_{X+e_j}^T-2\psi_X^T+\psi_{X-e_j}^T\big)\Big]. \tag{2.18}$$

Further, (2.6) together with (2.16) imply that

$$V_X(|\psi_X^{T+1}|^2)-V_X(|\psi_X^{T-1}|^2)=\mathrm{Re}\big[(\bar\psi_X^{T+1}-\bar\psi_X^{T-1})\cdot(\psi_X^{T+1}+\psi_X^{T-1})\big]B_X(|\psi_X^{T+1}|^2,|\psi_X^{T-1}|^2). \tag{2.19}$$

Taking into account (2.17), (2.18), and (2.19), we see that

$$\frac{E^T-E^{T-1}}{\varepsilon^n}=\sum_{X\in\mathbb{Z}^n}\Big[\Big(\frac{1}{\tau^2}-\frac{n}{\varepsilon^2}\Big)\frac{|\psi_X^{T+1}-\psi_X^T|^2-|\psi_X^T-\psi_X^{T-1}|^2}{2}$$

$$+\sum_{j=1}^{n}\sum_{\pm}\frac{|\psi_X^{T+1}-\psi_{X\pm e_j}^T|^2-|\psi_{X\pm e_j}^T-\psi_X^{T-1}|^2}{4\varepsilon^2}+\frac{V_X(|\psi_X^{T+1}|^2)-V_X(|\psi_X^{T-1}|^2)}{2}\Big]$$

$$=\mathrm{Re}\sum_{X\in\mathbb{Z}^n}(\bar\psi_X^{T+1}-\bar\psi_X^{T-1})\cdot\Big[\Big(\frac{1}{\tau^2}-\frac{n}{\varepsilon^2}\Big)\frac{\psi_X^{T+1}-2\psi_X^T+\psi_X^{T-1}}{2}$$

$$+\frac{n\big(\psi_X^{T+1}-2\psi_X^T+\psi_X^{T-1}\big)-\sum_{j=1}^n\big(\psi_{X+e_j}^T-2\psi_X^T+\psi_{X-e_j}^T\big)}{2\varepsilon^2}$$

$$+\frac{\psi_X^{T+1}+\psi_X^{T-1}}{2}B_X(|\psi_X^{T+1}|^2,|\psi_X^{T-1}|^2)\Big].$$

The expression in the square brackets adds up to zero due to (2.7). It follows that $E^T=E^{T-1}$ for all $T\in\mathbb{Z}$.

2.5. A Priori Estimates

Theorem 2.13. *(A priori estimates) Assume that $\varepsilon>0$ and $\tau>0$ satisfy $\tau/\varepsilon\leqslant 1/\sqrt{n}$. Assume that*

$$V_X(\lambda)=(m^2/2)\lambda+W_X(\lambda), \tag{2.20}$$

where $m>0$, and the function $W_X\in C^2(\mathbb{R})$ satisfies $W_X(\lambda)\geqslant 0$ for $\lambda\geqslant 0$ and for every $X\in\mathbb{Z}^n$. Then any solution ψ_X^T to the Cauchy problem (2.7) with arbitrary initial data $(\psi^0,\psi^1)\in l^2(\mathbb{Z}^n)\times l^2(\mathbb{Z}^n)$ satisfies the a priori estimate

$$\|\psi^T\|_{l^2}^2\varepsilon^n\leqslant 4E^0/m^2, \tag{2.21}$$

where E^0 is the energy (2.14) of the solution ψ_X^T at the moment $T=0$.

Proof. This immediately follows from the conservation of the energy (2.14) with $V_X(\lambda)$ given by (2.20),

$$E^T=\sum_{X\in\mathbb{Z}^n}\Big[\Big(\frac{1}{\tau^2}-\frac{n}{\varepsilon^2}\Big)\frac{|\psi_X^{T+1}-\psi_X^T|^2}{2}+\sum_{j=1}^{n}\frac{|\psi_X^{T+1}-\psi_{X-e_j}^T|^2+|\psi_X^{T+1}-\psi_{X+e_j}^T|^2}{4\varepsilon^2}$$

$$+\frac{m^2(|\psi_X^{T+1}|^2+|\psi_X^T|^2)}{4}+\frac{W_X(|\psi_X^{T+1}|^2)+W_X(|\psi_X^T|^2)}{2}\Big]\varepsilon^n.$$

Remark 2.14. In the continuous limit as $\varepsilon \to 0$, relation (2.21) is similar to the a priori estimate (2.5) for the solutions to the continuous nonlinear Klein-Gordon equation (2.4).

Remark 2.15. In [6], for $\psi_X^T \in \mathbb{R}$, $(X,T) \in \mathbb{Z}\times\mathbb{Z}$ (in dimension $n=1$), the following expression for the discretized energy was introduced:

$$E_{SV}^T = \frac{1}{2}\sum_{X\in\mathbb{Z}^n}\Big[\frac{(\psi_X^{T+1}-\psi_X^T)^2}{\tau^2}+\frac{(\psi_{X+1}^{T+1}-\psi_X^{T+1})(\psi_{X+1}^T-\psi_X^T)}{\varepsilon^2}+V(|\psi_X^{T+1}|^2)+V(|\psi_X^T|^2)\Big]. \tag{2.22}$$

The presence of the second term, which is not positive definite, deprives one of the a priori l^2 bounds for ψ (such as the one stated in Theorem 2.13). In view of this, the Strauss–Vazquez finite-difference scheme for the nonlinear Klein–Gordon equation is *not unconditionally stable.* Other schemes (conditionally and unconditionally stable) were suggested in [4] and [2]. Now, due to the a priori bound (2.21), we derive that, as a matter of fact, the Strauss–Vazquez scheme is stable in n dimensions under the assumption that the grid ratio is $\tau/\varepsilon \leqslant 1/\sqrt{n}$. Note that, if $\psi \in \mathbb{R}$, then the Strauss–Vazquez energy (2.22) agrees with the energy defined in (2.14).

2.6. Charge Conservation

Consider charge conservation. We define a discrete charge under the following assumption.

Assumption 2.16.

$$\tau/\varepsilon = 1/\sqrt{n}. \tag{2.23}$$

Under Assumption 2.16, ψ_X^T drops out of equation (2.7); the latter can be represented as

$$\big(\psi_X^{T+1}+\psi_X^{T-1}\big)\big(1+\tau^2 B_X(|\psi_X^{T+1}|^2,|\psi_X^{T-1}|^2)\big)=\frac{1}{n}\sum_{j=1}^n(\psi_{X+e_j}^T+\psi_{X-e_j}^T). \tag{2.24}$$

Theorem 2.17. (Charge conservation) *Let Assumption* 2.16 *be satisfied. Let ψ be a solution to equation* (2.25) *such that $\psi^T \in l^2(\mathbb{Z}^n)$ for all $T\in\mathbb{Z}$ (see Theorem* 2.3*). Then the discrete charge*

$$Q^T=\frac{i}{4\tau}\sum_{X\in\mathbb{Z}^n}\big[\bar\psi_{X+e_j}^T\cdot\psi_X^{T+1}+\bar\psi_{X-e_j}^T\cdot\psi_X^{T+1}-\bar\psi_X^{T+1}\cdot\psi_{X+e_j}^T-\bar\psi_X^{T+1}\cdot\psi_{X-e_j}^T\big]\varepsilon^n \tag{2.25}$$

is conserved.

Remark 2.18. The continuous limit of the discrete charge Q defined in (2.25) coincides with the charge functional (2.3) of the continuous nonlinear wave equation (2.1).

Proof. Let us prove the charge conservation. Write

$$\frac{4\tau}{i\varepsilon^n}Q^T=\sum_{X\in\mathbb{Z}^n}\sum_{j=1}^n\sum_{\pm}\Big[\bar\psi_{X\pm e_j}^T\cdot\psi_X^{T+1}-\text{C. C.}\Big],$$

$$\frac{4\tau}{i\varepsilon^n}Q^{T-1}=\sum_{X\in\mathbb{Z}^n}\sum_{j=1}^n\sum_{\pm}\Big[\bar\psi_{X\pm e_j}^{T-1}\cdot\psi_X^T-\text{C. C.}\Big]=-\sum_{X\in\mathbb{Z}^n}\sum_{j=1}^n\sum_{\pm}\Big[\bar\psi_{X\pm e_j}^T\cdot\psi_X^{T-1}-\text{C. C.}\Big].$$

Therefore,

$$\begin{aligned}\frac{4\tau\big(Q^T-Q^{T-1}\big)}{i\varepsilon^n}&=\sum_{X\in\mathbb{Z}^n}\sum_{j=1}^n\sum_{\pm}\bar\psi_{X\pm e_j}^T\cdot(\psi_X^{T+1}+\psi_X^{T-1})-\text{C. C.}\\&=n\sum_{X\in\mathbb{Z}^n}\big(1+\tau^2B_X(|\psi_X^{T+1}|^2,|\psi_X^{T-1}|^2)\big)|\psi_X^{T+1}+\psi_X^{T-1}|^2-\text{C. C.}=0.\end{aligned} \tag{2.26}$$

To pass to the second line, we have used the complex conjugate of (2.24). This completes the proof of Theorem 2.17.

3. PROOF OF WELL-POSEDNESS AND UNIQUENESS RESULTS

Proof of Theorem 2.3. Represent equation (2.7) in the following form:

$$\big(\psi_X^{T+1}+\psi_X^{T-1}\big)\big(1+\tau^2 B_X(|\psi_X^{T+1}|^2,|\psi_X^{T-1}|^2)\big)=\frac{\tau^2}{\varepsilon^2}\sum_{j=1}^n\big(\psi_{X+e_j}^T-2\psi_X^T+\psi_{X-e_j}^T\big)+2\psi_X^T,$$
$$X\in\mathbb{Z}^n,\quad T\in\mathbb{Z}. \tag{3.1}$$

By (2.9) and by the choice of τ_1 in Theorem 2.3, for $\tau\in(0,\tau_1)$, we obtain

$$\inf_{X\in\mathbb{Z}^n,\lambda\geqslant 0}\big(1+\tau^2\partial_\lambda V_X(\lambda)\big)>0. \tag{3.2}$$

Since

$$\inf_{X\in\mathbb{Z}^n,\,\lambda\geqslant 0,\,\mu\geqslant 0}B_X(\lambda,\mu)=\inf_{X\in\mathbb{Z}^n,\,\lambda\geqslant 0,\,\mu\geqslant 0}\frac{V_X(\lambda)-V_X(\mu)}{\lambda-\mu}=\inf_{X\in\mathbb{Z}^n,\,\lambda\geqslant 0}\partial_\lambda V_X(\lambda), \tag{3.3}$$

inequality (3.2) yields

$$c:=\inf_{X\in\mathbb{Z}^n,\lambda\geqslant 0,\mu\geqslant 0}\big(1+\tau^2 B_X(\lambda,\mu)\big)>0. \tag{3.4}$$

Let us show that equation (3.1) allows us to find ψ_X^{T+1}, for any given $X\in\mathbb{Z}^n$ and $T\in\mathbb{Z}$, if ψ^T and ψ^{T-1} are known. Equation (3.1) implies that

$$\big(1+\tau^2 B_X(|\psi_X^{T+1}|^2,|\psi_X^{T-1}|^2)\big)(\psi_X^{T+1}+\psi_X^{T-1})=\xi_X^T, \tag{3.5}$$

$$\xi_X^T:=\frac{\tau^2}{\varepsilon^2}\sum_{j=1}^n\big(\psi_{X+e_j}^T-2\psi_X^T+\psi_{X-e_j}^T\big)+2\psi_X^T\in\mathbb{C}^N. \tag{3.6}$$

If $\xi_X^T=0$, then there is a solution to (3.5) given by $\psi_X^{T+1}=-\psi_X^{T-1}$. Due to (3.4), this solution is unique. Let us now assume that $\xi_X^T\neq 0$. By (3.5), we must have

$$\psi_X^{T+1}+\psi_X^{T-1}=s\xi_X^T,\qquad\text{with some } s\in\mathbb{R}. \tag{3.7}$$

Introduce the function

$$f(s):=\big(1+\tau^2 B_X(|s\xi_X^T-\psi_X^{T-1}|^2,|\psi_X^{T-1}|^2)\big)s. \tag{3.8}$$

We do not indicate the dependence of f on ψ_X^{T-1}, ξ_X^T, and X, treating them as parameters. For $\xi_X^T\neq 0$, we can solve (3.5) by finding $s\in\mathbb{R}$ such that

$$f(s)=1. \tag{3.9}$$

Since $f(0)=0$, whereas $\lim_{s\to\infty}f(s)=+\infty$ by (3.4), one concludes that there is at least one solution $s>0$ to (3.9).

Let us prove that, if $(\psi^0,\psi^1)\in l^2(\mathbb{Z}^n)\times l^2(\mathbb{Z}^n)$, then $||\psi^T||_{l^2(\mathbb{Z}^n)}$ remains finite (however, not necessarily uniformly bounded) for all $T\in\mathbb{Z}$. It follows from (3.4) and (3.5) that

$$|\psi_X^{T+1}|\leqslant\frac{1}{c}|\xi_X^T|+|\psi_X^{T-1}|. \tag{3.10}$$

Since $||\xi^T||_{l^2(\mathbb{Z}^n)}\leqslant\left(\frac{4\tau^2}{\varepsilon^2}+2\right)||\psi^T||_{l^2(\mathbb{Z}^n)}$ by (3.6), relation (3.10) implies the estimate

$$||\psi^{T+1}||_{l^2(\mathbb{Z}^n)}\leqslant\frac{1}{c}\left(\frac{4\tau^2}{\varepsilon^2}+2\right)||\psi^T||_{l^2(\mathbb{Z}^n)}+||\psi^{T-1}||_{l^2(\mathbb{Z}^n)}, \tag{3.11}$$

and, by recursion, $||\psi^T||_{l^2(\mathbb{Z}^n)}$ is finite for all $T \geqslant 0$. The case $T \leqslant 0$ can be completed in the same way.

Now we turn to the uniqueness of solutions to the Cauchy problem for equation (2.7).

Proof of Theorem 2.6. Note first that, by Remark 2.7, the values τ_1 in Theorem 2.3 and τ_2 in Theorem 2.6 satisfy the inequality $\tau_2 \leqslant \tau_1$. Therefore, the existence of a solution ψ_X^T to the Cauchy problem for equation (2.7) follows from Theorem 2.3.

We claim that this solution ψ_X^T is unique. If in (3.6), one has

$$\xi_X^T := \frac{\tau^2}{\varepsilon^2}\sum_{j=1}^{n}(\psi_{X+e_j}^T - 2\psi_X^T + \psi_{X-e_j}^T) + 2\psi_X^T = 0,$$

then, by (3.4), the only solution ψ_X^{T+1} to (3.5) is given by $\psi_X^{T+1} = -\psi_X^{T-1}$. Now consider the case $\xi_X^T \neq 0$. By (3.5), (3.7), and (3.8), it suffices to prove the uniqueness of a solution to (3.9). To this end, it suffices to show that

$$f'(s) > 0, \qquad s \in \mathbb{R}. \tag{3.12}$$

The explicit expression for $f'(s)$ is

$$1+\tau^2 B_X(|s\xi_X^T-\psi_X^{T-1}|^2, |\psi_X^{T-1}|^2)+\tau^2\partial_\lambda B_X(|s\xi_X^T-\psi_X^{T-1}|^2, |\psi_X^{T-1}|^2)(-2\,\mathrm{Re}(\bar\psi_X^{T-1}\cdot\xi_X^T)+2|\xi_X^T|^2 s)s. \tag{3.13}$$

Using relation (3.7), we can derive the identity

$$(-2\,\mathrm{Re}(\bar\psi_X^{T-1}\cdot\xi_X^T)+2|\xi_X^T|^2 s)s = 2\Big|s\xi_X^T - \frac{\psi_X^{T-1}}{2}\Big|^2 - \frac{|\psi_X^{T-1}|^2}{2} = 2\Big|\psi_X^{T+1} + \frac{\psi_X^{T-1}}{2}\Big|^2 - \frac{|\psi_X^{T-1}|^2}{2}$$

and rewrite expression (3.13) for $f'(s)$ in the form

$$f'(s) = 1+\tau^2\Big[B_X(|\psi_X^{T+1}|^2, |\psi_X^{T-1}|^2) + 2\partial_\lambda B_X(|\psi_X^{T+1}|^2, |\psi_X^{T-1}|^2)\Big(|\psi_X^{T+1} + \frac{\psi_X^{T-1}}{2}|^2 - \frac{|\psi_X^{T-1}|^2}{4}\Big)\Big]. \tag{3.14}$$

Write $\lambda = |\psi_X^{T+1}|^2$, $\mu = |\psi_X^{T-1}|^2$. Since $\lambda - \sqrt{\lambda\mu} + \frac{\mu}{4} \leqslant |\psi_X^{T+1} + \frac{\psi_X^{T-1}}{2}|^2 \leqslant \lambda + \sqrt{\lambda\mu} + \frac{\mu}{4}$, we see that

$$f'(s) \geqslant 1+\tau^2 \min_{\pm} \inf_{X\in\mathbb{Z}^n,\,\lambda\geqslant 0,\,\mu\geqslant 0} K_X^{\pm}(\lambda,\mu) \quad \text{with} \quad K_X^{\pm}(\lambda,\mu) = B_X(\lambda,\mu)+2\partial_\lambda B_X(\lambda,\mu)(\lambda\pm\sqrt{\lambda\mu}). \tag{3.15}$$

By (2.11) and by our choice of τ_2 in Theorem 2.6, for any $\tau \in (0,\tau_2)$, we have

$$\kappa := \inf_{X\in\mathbb{Z}^n,\,\lambda\geqslant 0,\,\mu\geqslant 0}\{1+\tau^2 K_X^{\pm}(\lambda,\mu)\} > 0;$$

then, by (3.15), $f'(s) \geqslant \kappa$, where $\kappa > 0$. It follows that, for $\xi_X^T \neq 0$, there is a unique s solving (3.9). Hence, there is a unique solution ψ_X^{T+1} to equation (3.5) for the given values ψ_X^{T-1} and ξ_X^T. This completes the proof of the theorem.

Proof of Theorem 2.8. We claim that condition (2.11) in Theorem 2.6 is satisfied by any polynomial potential of the form (2.10). Inequality (2.11) is satisfied if the highest-order term in $V(\lambda)$ contributes a strictly positive expression. More precisely, we must prove the following result.

Lemma 3.1. *Let* $V(\lambda) = \lambda^{p+1}$, *and let* $B(\lambda,\mu) = \frac{\lambda^{p+1}-\mu^{p+1}}{\lambda-\mu}$, $p \geqslant 0$. *Then the following inequality holds*:

$$\inf_{\lambda\geqslant 0,\,\mu\geqslant 0,\,\lambda^2+\mu^2=1}\Big[B(\lambda,\mu)+2\partial_\lambda B(\lambda,\mu)(\lambda\pm\sqrt{\lambda\mu})\Big] > 0. \tag{3.16}$$

Proof. Since B and $\partial_\lambda B$ are strictly positive for $\lambda^2+\mu^2>0$, the inequality (3.16) is nontrivial for the minus sign in (3.16) and only for $\mu>\lambda$. We have,

$$B(\lambda,\mu)=\frac{\mu^{p+1}-\lambda^{p+1}}{\mu-\lambda},$$

$$\partial_\lambda B(\lambda,\mu)=\frac{-(p+1)\lambda^p(\mu-\lambda)-\lambda^{p+1}+\mu^{p+1}}{(\mu-\lambda)^2}=\frac{\mu^{p+1}-(p+1)\lambda^p\mu+p\lambda^{p+1}}{(\mu-\lambda)^2}.$$

Let $z\geqslant 0$ satisfy $z^2=\lambda/\mu$. We must show that

$$\frac{1-z^{2p+2}}{1-z^2}+2\frac{1-(p+1)z^{2p}+pz^{2p+2}}{(1-z^2)^2}(z^2-z)>0,\qquad 0\leqslant z<1,\tag{3.17}$$

or equivalently,

$$(1+z)(1-z^{2p+2})-2z\big(1-(p+1)z^{2p}+pz^{2p+2}\big)>0.$$

The left-hand side becomes

$$(1+z)(1-z^{2p+2})-2z\big(1-z^{2p+2}-(p+1)(z^{2p}-z^{2p+2})\big)=(1-z)(1-z^{2p+2})+2z(p+1)(z^{2p}-z^{2p+2}),$$

which is clearly strictly positive for all $0\leqslant z<1$ and $p\geqslant 0$, thus proving (3.17).

This completes the proof of the first part of Theorem 2.8; we now turn to the second part.

Lemma 3.2. (Uniqueness criterion) *Assume that, for a particular $\tau>0$ and for all $\lambda\geqslant 0$, $\mu\geqslant 0$, $X\in\mathbb{Z}^n$, the following inequalities hold:*

$$1+\tau^2\inf_{X\in\mathbb{Z}^n,\,\lambda\geqslant 0,\,\mu\geqslant 0}\Big(B_X(\lambda,\mu)-\partial_\lambda B_X(\lambda,\mu)\frac{\mu}{2}\Big)>0;\tag{3.18}$$

$$\inf_{X\in\mathbb{Z}^n,\,\lambda\geqslant 0,\,\mu\geqslant 0}\partial_\lambda B_X(\lambda,\mu)\geqslant 0.\tag{3.19}$$

Then, for arbitrary initial data (ψ^0,ψ^1), there is a solution ψ_X^T to the Cauchy problem for equation (2.7)*, and this solution is unique.*

Proof of Lemma 3.2. Inequalities (3.18) and (3.19) imply that

$$1+\tau^2\inf_{X\in\mathbb{Z}^n,\,\lambda\geqslant 0}B_X(\lambda,\lambda)>0,$$

and hence, by the same argument as in Theorem 2.3, there is a solution ψ_X^T. Relation (3.14) shows that $f'(s)\geqslant c$ for some $c>0$. The rest of the proof is the same as for Theorem 2.6.

In the second part of Theorem 2.8, we assume that

$$V_X(\lambda)=\sum_{q=0}^{4}C_{X,q}\lambda^{q+1},\qquad X\in\mathbb{Z}^n,\quad \lambda\geqslant 0,\tag{3.20}$$

where $C_{X,q}\geqslant 0$ for $X\in\mathbb{Z}^n$ and $1\leqslant q\leqslant 4$, and

$$k_3=\inf_{X\in\mathbb{Z}^n}C_{X,0}>-\infty.\tag{3.21}$$

We see that the term $C_{X,0}\lambda$ in $V_X(\lambda)$ contributes the expression $b_{X,0}(\lambda,\mu)=C_{X,0}$ to $B_X(\lambda,\mu)$, whereas every term in $V_X(\lambda)$ of the form $C_{X,q}\lambda^{q+1}$ with $1\leqslant q\leqslant 4$ and $C_{X,q}\geqslant 0$ contributes the expression $C_{X,q}b_q(\lambda,\mu)$ with

$$b_q(\lambda,\mu)=\sum_{k=0}^{q}\lambda^{q-k}\mu^k$$

to $B_X(\lambda,\mu)$. For $\tau\in(0,\tau_3)$, with $\tau_3=\sqrt{-1/k_3}$ for $k_3<0$ and $\tau_3=+\infty$ for $k_3\geqslant 0$, one has

$$1+\tau^2\inf_{X\in\mathbb{Z}^n}C_{X,0}>0.\tag{3.22}$$

Lemma 3.3. *For* $1 \leqslant q \leqslant 4$, $b_q(\lambda, \mu) = \sum_{k=0}^{q} \lambda^{q-k} \mu^k$ *satisfies the inequality*

$$b_q(\lambda, \mu) \geqslant \partial_\lambda b_q(\lambda, \mu) \frac{\mu}{2} \qquad \textit{for all} \;\; \lambda,\, \mu \geqslant 0.$$

By (3.22) and Lemma 3.3, condition (3.18) is satisfied. Since $C_{X,q} \geqslant 0$ for $1 \leqslant q \leqslant 4$, each term $C_{X,q} b_q(\lambda, \mu)$ satisfies condition (3.19). Therefore, by Lemma 3.2, there is a unique solution ψ_X^T to the Cauchy problem for equation (2.7). This completes the proof of Theorem 2.8.

4. CONCLUSION

We have found out that the Straus–Vazquez finite-difference scheme [6] for the $\mathbf{U}(1)$-invariant nonlinear wave equation in spatial dimension n with grid ratio satisfying the condition $\tau/\varepsilon \leqslant 1/\sqrt{n}$ admits a positive-definite discrete analog of energy, and this energy is conserved. The result holds in any spatial dimension $n \geqslant 1$ for fields with values in $\mathbb{C}^N$, $N \geqslant 1$. In the case of the nonlinear Klein–Gordon equation with positive potential, this provides a priori bounds for the solution, showing that the finite-difference scheme is stable.

We have found out that, for the grid ratio $\tau/\varepsilon = 1/\sqrt{n}$, this finite-difference scheme also preserves the discrete charge.

We have proved that the solution of the corresponding Cauchy problem exists and is unique for a broad class of nonlinearities. In particular, this is the case for any confining polynomial potential if the discretization is sufficiently small. Finally, we indicated a class of polynomials for which the size of the discretization can readily be specified.

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