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Dissipative or Conservative Finite-Difference Schemes for Complex-Valued Nonlinear Partial Differential Equations[1]

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We propose a new procedure for designing finite-difference schemes that inherit energy conservation or dissipation property from complex-valued nonlinear partial differential equations (PDEs), such as the nonlinear Schrödinger equation, the Ginzburg–Landau equation, and the Newell–Whitehead equation. The procedure is a complex version of the procedure that Furihata has recently presented for real-valued nonlinear PDEs. Furthermore, we show that the proposed procedure can be modified for designing "linearly implicit" finite-difference schemes that inherit energy conservation or dissipation property.

Key Words: finite-difference method; energy conservation; energy dissipation; nonlinear partial differential equation; nonlinear Schrödinger equation; Ginzburg–Landau equation; Newell–Whitehead equation; linearly implicit scheme.

1. INTRODUCTION

The first purpose of this paper is to propose a procedure for designing by rote finite-difference schemes that inherit energy conservation or dissipation property from "complex-valued" nonlinear partial differential equations (PDEs). As for "real-valued" nonlinear PDEs, recently Furihata has presented a procedure of the same type [5]. He considered the real-valued PDEs of the form

$$\frac{\partial u}{\partial t} = \left(\frac{\partial}{\partial u}\right)^{\alpha} \frac{\delta G}{\delta u} \qquad (\alpha : \text{nonnegative integer}), \tag{1}$$

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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 the variational derivative of $G(u, u_x)$ for u. He evolved a method of designing finite-difference schemes that inherit energy conservation or dissipation property from the PDEs (1) by inventing "discrete variational derivatives," i.e., a rigorous discretization of variational derivatives, which implies that inherited properties are satisfied exactly. An essential feature of the derived finite-difference schemes is that the inherited properties are kept even if the time mesh size changes in the time evolution process, which enables us to use some appropriate time mesh size adaptive methods to obtain numerical solutions.

We here take the same approach as Furihata does. The PDEs that we treat in this paper are of the form

$$\mathrm{i}\frac{\partial u}{\partial t} = -\frac{\delta G}{\delta \bar{u}} \tag{2}$$

or

$$\frac{\partial u}{\partial t} = -\frac{\delta G}{\delta \bar{u}}, \tag{3}$$

where $u = u(x, t)$ is a complex-valued function, $G = G(u, u_x)$ is a function of both u and $u_x = \partial u/\partial x$, and $\delta G/\delta \bar{u}$ is the complex variational derivative of $G(u, u_x)$ for $\bar{u}$. As is shown in Section 2, under certain boundary conditions, the solutions of the PDEs (2) enjoy the so-called "energy conservation property," i.e., $\frac{\partial}{\partial t}\int G\,dx = 0$, and the solutions of the PDEs (3) enjoy the so-called "energy dissipation property," i.e., $\frac{\partial}{\partial t}\int G\,dx \leq 0$. In this paper we provide a procedure for designing the finite-difference schemes that inherit the above properties for PDE (2) or (3) by devising "complex discrete variational derivatives," i.e., a rigorous discretization of complex variational derivatives. The derived schemes have the feature that the inherited properties are kept even if the time mesh size changes in the time evolution process. Because of these properties the derived schemes are expected to be numerically stable, yield solutions converging to PDE solutions, and be sufficiently flexible to be treated.

The second, somewhat additional, purpose of this paper is to show that the proposed procedure can be modified for designing "linearly implicit" finite-difference schemes that inherit energy conservation or dissipation property for the PDE (2) or (3) whose nonlinear terms are of the form $|u|^{2s}u$ (s: integer). A fundamental notion employed in the modification is "multiple points complex discrete variational derivative," which is a generalization of the complex discrete variational derivative. Since the derived schemes are linearly implicit, we only need to solve a linear system at each time step. It should be noted, however, that the derived linearly implicit schemes lose the feature the schemes derived by the first proposed procedure possess, that is, the inherited properties are no longer kept if the time mesh size changes in the time evolution process.

This paper is organized as follows. In Section 2 we define the target complex-valued PDEs and review their properties. In Section 3 the notation we employ in this paper is defined and some discrete calculus including the definition of the complex discrete variational derivative is described. In Section 4 a procedure for designing the conservative or dissipative finite-difference schemes is presented. In Section 5, following the proposed procedure we present schemes for some example equations, such as the nonlinear Schrödinger equation (NLS equation for short), the complex-valued time-dependent Ginzburg–Landau equation (CGL equation), and the Newell–Whitehead equation (NW equation). In Section 6 we modify the procedure for designing the linearly implicit conservative or dissipative finite-difference schemes, and following the modified procedure we design linearly implicit schemes for the odd-order NLS equation, the CGL equation, and the NW equation. We also show numerical results for the NW equation, which demonstrates that the derived linearly implicit scheme has some good features. Section 7 is the conclusion.

2. COMPLEX VARIATIONAL DERIVATIVE AND TARGET EQUATIONS

In this section we define the target equations and briefly review their properties (dissipation or conservation of energy). To this end, we commence by defining the complex variational derivative.

2.1. *Complex Variational Derivative*

Let $u : [0, \infty) \times [0, L] \to \mathbf{C}$ be a smooth function (say $u(\cdot, x) \in C^3[0, \infty)$, and $u(t, \cdot) \in C^4[0, L]$) and $G(u, u_x)$ be a real-valued functional of u and u_x, where u_x denotes $\partial u/\partial x$ and so on. $G(u, u_x)$ can be written as a function of four real variables (Reu, Imu, Reu_x, Imu_x) and we assume that G is C^1 with respect to the four components. We define another real-valued functional $H(u)$ as

$$H(u) \stackrel{\mathrm{d}}{\equiv} \int_0^L G(u, u_x)\,\mathrm{d}x. \tag{4}$$

The "variation" of $H(u)$ is defined with the Gâteaux derivative of $H(u)$ as

$$\begin{aligned}
\delta H(u; \eta) &= \lim_{\varepsilon \to 0} \int_0^L \frac{G(u + \varepsilon\eta, u_x + \varepsilon\eta_x) - G(u, u_x)}{\varepsilon}\,\mathrm{d}x \\
&= \int_0^L \left\{ \frac{\partial G}{\partial u}\eta + \frac{\partial G}{\partial \overline{u}}\overline{\eta} + \frac{\partial G}{\partial u_x}\eta_x + \frac{\partial G}{\partial \overline{u_x}}\overline{\eta_x} \right\} \mathrm{d}x \\
&= \int_0^L \left\{ \left(\frac{\partial G}{\partial u} - \frac{\mathrm{d}}{\mathrm{d}x}\frac{\partial G}{\partial u_x} \right)\eta + \left(\frac{\partial G}{\partial \overline{u}} - \frac{\mathrm{d}}{\mathrm{d}x}\frac{\partial G}{\partial \overline{u_x}} \right)\overline{\eta} \right\} \mathrm{d}x + \left[\frac{\partial G}{\partial u_x}\eta + \frac{\partial G}{\partial \overline{u_x}}\overline{\eta} \right]_0^L,
\end{aligned} \tag{5}$$

where $\eta : [0, \infty) \times [0, L] \to \mathbf{C}$ is a smooth function, $\varepsilon \in \mathbf{R}$, and $\overline{u}$ is complex conjugate of u. By the assumption on G the partial derivatives are well defined. The "complex variational derivative of G" is defined as what is enclosed in $(\cdot)$ on the right-hand side of (5), i.e.,

$$\frac{\delta G}{\delta u} \stackrel{\mathrm{d}}{\equiv} \frac{\partial G}{\partial u} - \frac{\mathrm{d}}{\mathrm{d}x}\frac{\partial G}{\partial u_x}, \tag{6}$$

$$\frac{\delta G}{\delta \overline{u}} \stackrel{\mathrm{d}}{\equiv} \frac{\partial G}{\partial \overline{u}} - \frac{\mathrm{d}}{\mathrm{d}x}\frac{\partial G}{\partial \overline{u_x}}. \tag{7}$$

Here it is worthy of attention that the variational derivatives are complex conjugates of each other, that is,

$$\overline{\frac{\delta G}{\delta u}} = \frac{\delta G}{\delta \overline{u}}. \tag{8}$$

2.2. *Target Equations*

The equations that we treat in this paper are those which are defined with the complex variational derivatives of G, and they are classified into two types: conservative type and dissipative type.

Conservative type. The equations are defined as

$$\mathrm{i}\frac{\partial u}{\partial t} = -\frac{\delta G}{\delta \overline{u}} \qquad (x \in [0, L], t > 0), \tag{2}$$

where $\mathrm{i} = \sqrt{-1}$. In physical contexts G is often called "free energy" or "local energy," and H is called "global energy." The equation is called "conservative" because it conserves the global energy H, as can be easily seen as

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}H(u) &= \int_0^L \left\{ \frac{\delta G}{\delta u}\frac{\partial u}{\partial t} + \frac{\delta G}{\delta \overline{u}}\frac{\partial \overline{u}}{\partial t} \right\} \mathrm{d}x + \left[\frac{\partial G}{\partial u_x}\frac{\partial u}{\partial t} + \frac{\partial G}{\partial \overline{u_x}}\frac{\partial \overline{u}}{\partial t} \right]_0^L \\ &= \int_0^L \left(-\mathrm{i}\left|\frac{\delta G}{\delta u}\right|^2 + i\left|\frac{\delta G}{\delta u}\right|^2 \right) \mathrm{d}x \\ &= 0, \end{aligned} \tag{9}$$

under the boundary condition which satisfies

$$\left[\frac{\partial G}{\partial u_x}\frac{\partial u}{\partial t} + \frac{\partial G}{\partial \overline{u_x}}\frac{\partial \overline{u}}{\partial t} \right]_0^L = 0. \tag{10}$$

We note that the periodic boundary condition or the zero Dirichlet condition satisfies (10).

As a typical example of (2), the NLS equation

$$\mathrm{i}\frac{\partial u}{\partial t} = -u_{xx} - \gamma|u|^{p-1}u \qquad (x \in [0, L], t > 0, \gamma \in \mathbf{R}, p = 3, 4, \ldots), \tag{11}$$

is well known.

Dissipative type. The equations are defined as

$$\frac{\partial u}{\partial t} = -\frac{\delta G}{\delta \overline{u}} \qquad (x \in [0, L], t > 0). \tag{3}$$

This equation dissipates the global energy H under the condition (10) as follows:

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}H(u) &= \int_0^L \frac{\mathrm{d}}{\mathrm{d}t}G(u, u_x)\,\mathrm{d}x \\ &= \int_0^L \left\{ \frac{\partial G}{\partial u}\frac{\partial u}{\partial t} + \frac{\partial G}{\partial \overline{u}}\frac{\partial \overline{u}}{\partial t} + \frac{\partial G}{\partial u_x}\frac{\partial u_x}{\partial t} + \frac{\partial G}{\partial \overline{u_x}}\frac{\partial \overline{u_x}}{\partial t} \right\} \mathrm{d}x \\ &= \int_0^L \left\{ \frac{\delta G}{\delta u}\frac{\partial u}{\partial t} + \frac{\delta G}{\delta \overline{u}}\frac{\partial \overline{u}}{\partial t} \right\} \mathrm{d}x + \left[\frac{\partial G}{\partial u_x}\frac{\partial u}{\partial t} + \frac{\partial G}{\partial \overline{u_x}}\frac{\partial \overline{u}}{\partial t} \right]_0^L \\ &= -2\int_0^L \left|\frac{\delta G}{\delta u}\right|^2 \mathrm{d}x \\ &\leq 0. \end{aligned} \tag{12}$$

The variational formulation (3) means that the dynamics of u is expressed as the gradient flow of $G(u)$, that is, u goes down along the steepest descent path of $G(u)$ [10].

As examples of (3), there is the well known real-coefficient CGL equation

$$\frac{\partial u}{\partial t} = pu_{xx} + q|u|^2u + ru \qquad (x \in [0, L], t > 0,\ p > 0, q < 0, r \in \mathbf{R}), \tag{13}$$

and the NW equation

$$\frac{\partial u}{\partial t}(t, x, y) = \mu u - |u|^2 u + \left(\frac{\partial}{\partial x} - \frac{\mathrm{i}}{2k_c}\frac{\partial^2}{\partial y^2}\right)^2 u \qquad \begin{pmatrix} (x, y) \in [0, L_x] \times [0, L_y], \\ t > 0, \\ \mu, k_c \in \mathbf{R}. \end{pmatrix}. \tag{14}$$

Note that the latter is two-dimensional in space variables.

3. DISCRETE SYMBOLS

In this section we describe the discrete symbols and the formulas employed in this paper. We also define the complex discrete variational derivatives which are the discrete analogues of the complex variational derivatives (6) and (7).

3.1. *Basic Symbols and Formulas*

Throughout this paper we use the notation below.

We denote the numerical solution as

$$U_k^{(m)} \simeq u(k\Delta x, m\Delta t) \qquad (k \in \mathbf{Z}, m = 0, 1, 2, \ldots), \tag{15}$$

where Δx and $\Delta t > 0$ are the mesh sizes in x and t, respectively. The time step (m) is omitted unless indispensable.

We use the following difference operators:

$$\delta_k^+ U_k \stackrel{\mathrm{d}}{\equiv} \frac{U_{k+1} - U_k}{\Delta x}, \tag{16}$$

$$\delta_k^- U_k \stackrel{\mathrm{d}}{\equiv} \frac{U_k - U_{k-1}}{\Delta x}, \tag{17}$$

$$\delta_k^{\langle 1\rangle} U_k \stackrel{\mathrm{d}}{\equiv} \frac{U_{k+1} - U_{k-1}}{2\Delta x}, \tag{18}$$

$$\delta_k^{\langle 2\rangle} U_k \stackrel{\mathrm{d}}{\equiv} \frac{U_{k+1} - 2U_k + U_{k-1}}{\Delta x^2}, \tag{19}$$

$$\delta_k^{\langle 4\rangle} U_k \stackrel{\mathrm{d}}{\equiv} \frac{U_{k+2} - 4U_{k+1} + 6U_k - 4U_{k-1} + U_{k-2}}{\Delta x^4}. \tag{20}$$

The following formula is analogous to the integration-by-parts formula in usual calculus and holds for any two sequences U_k and V_k (for proof, see [5]),

$$\sum_{k=o}^{N}{}'' U_k(\delta_k^+ V_k)\Delta x + \sum_{k=0}^{N}{}'' (\delta_k^- U_k) V_k \Delta x = \left[\frac{U_k V_{k+1} + U_{k-1} V_k}{2}\right]_{k=0}^{N}, \tag{21}$$

where $\sum''^{N}_{k=0} U_k \Delta x = (\frac{1}{2}U_0 + U_1 + \cdots + U_{N-1} + \frac{1}{2}U_N)\Delta x$ (trapezoidal rule) and $[U_k]_{k=0}^{N} \stackrel{\mathrm{d}}{\equiv} U_N - U_0$. By repeatedly using the above formula, we can also derive higher order summation-by-parts formulas.

3.2. *Complex Discrete Variational Derivative*

In this section we provide the definition of the complex discrete variational derivatives which should be a discrete analogue of the variational derivatives (6) and (7).

Let us assume that $G_{\mathrm{d}} : \mathbf{C}^{N+1} \to \mathbf{R}^{N+1}$, which is a discrete approximation of G, is in the separated form

$$G_{\mathrm{d}}(\boldsymbol{U})_k = \sum_{l=1}^{M} |p_l(U_k)|^{N_l^P} |q_l^+(\delta_k^+ U_k)|^{N_l^+} |q_l^-(\delta_k^- U_k)|^{N_l^-}, \tag{22}$$

where $M \in \{1, 2, 3, \ldots\}$, $N_l^P, N_l^+, N_l^- \in \{2, 3, 4, \ldots\}$, and $p_l, q_l^+, q_l^- : \mathbf{C} \to \mathbf{C}$ are assumed to be analytic functions which satisfy $p_l(\overline{u}) = \overline{p_l(u)}$, $q_l^+(\overline{u}) = \overline{q_l^+(u)}$, and $q_l^-(\overline{u}) = \overline{q_l^-(u)}$ $(u \in \mathbf{C})$.[2] Hereafter we abbreviate $|p_l(U_k)|^{N_l^P}$ as $P_l(U_k)$, $|q_l^+(\delta_k^+ U_k)|^{N_l^+}$ as $Q_l^+(U_k)$, and $|q_l^-(\delta_k^- U_k)|^{N_l^-}$ as $Q_l^-(U_k)$. $H_{\mathrm{d}} : \mathbf{C}^{N+1} \to \mathbf{R}$, which should be the discrete version of H, is defined accordingly as

$$H_{\mathrm{d}}(\boldsymbol{U}) \stackrel{\mathrm{d}}{\equiv} \sum_{k=0}^{N}{}'' G_{\mathrm{d}}(\boldsymbol{U})_k \Delta x. \tag{23}$$

To follow the variation calculation (5), let us consider the difference of H_{d} at the different points U and V,

$$\begin{aligned}
&H_{\mathrm{d}}(\boldsymbol{U}) - H_{\mathrm{d}}(\boldsymbol{V})\\
&= \sum_{k=0}^{N}{}'' \{G_{\mathrm{d}}(\boldsymbol{U})_k - G_{\mathrm{d}}(\boldsymbol{V})_k\}\Delta x\\
&= \sum_{k=0}^{N}{}'' \Bigg\{ \left(\frac{\partial G_{\mathrm{d}}}{\partial(\boldsymbol{U}, \boldsymbol{V})}\right)_k (U_k - V_k) + \left(\frac{\partial G_{\mathrm{d}}}{\partial(\overline{\boldsymbol{U}, \boldsymbol{V}})}\right)_k (\overline{U_k - V_k})\\
&\quad + \left(\frac{\partial G_{\mathrm{d}}}{\partial \delta^+(\boldsymbol{U}, \boldsymbol{V})}\right)_k (\delta_k^+ U_k - \delta_k^+ V_k) + \left(\frac{\partial G_{\mathrm{d}}}{\partial \delta^+(\overline{\boldsymbol{U}, \boldsymbol{V}})}\right)_k (\overline{\delta_k^+ U_k} - \overline{\delta_k^+ V_k})\\
&\quad + \left(\frac{\partial G_{\mathrm{d}}}{\partial \delta^-(\boldsymbol{U}, \boldsymbol{V})}\right)_k (\delta_k^- U_k - \delta_k^- V_k) + \left(\frac{\partial G_{\mathrm{d}}}{\partial \delta^-(\overline{\boldsymbol{U}, \boldsymbol{V}})}\right)_k (\overline{\delta_k^- U_k} - \overline{\delta_k^- V_k}) \Bigg\} \Delta x\\
&= \sum_{k=0}^{N}{}'' \Bigg[\Bigg\{ \left(\frac{\partial G_{\mathrm{d}}}{\partial(\boldsymbol{U}, \boldsymbol{V})}\right)_k - \delta_k^- \left(\frac{\partial G_{\mathrm{d}}}{\partial \delta^+(\boldsymbol{U}, \boldsymbol{V})}\right)_k - \delta_k^+ \left(\frac{\partial G_{\mathrm{d}}}{\partial \delta^-(\boldsymbol{U}, \boldsymbol{V})}\right)_k \Bigg\} (U_k - V_k)\\
&\quad + \Bigg\{ \left(\frac{\partial G_{\mathrm{d}}}{\partial(\overline{\boldsymbol{U}, \boldsymbol{V}})}\right)_k - \delta_k^- \left(\frac{\partial G_{\mathrm{d}}}{\partial \delta^+(\overline{\boldsymbol{U}, \boldsymbol{V}})}\right)_k - \delta_k^+ \left(\frac{\partial G_{\mathrm{d}}}{\partial \delta^-(\overline{\boldsymbol{U}, \boldsymbol{V}})}\right)_k \Bigg\} (\overline{U_k - V_k}) \Bigg] \Delta x\\
&\quad + \left[\left(\frac{\partial G_{\mathrm{d}}}{\partial \delta(\boldsymbol{U}, \boldsymbol{V})}\right)_k \right]_{k=0}^{N},
\end{aligned} \tag{24}$$

[2] This assumption means that we restrict the possible form of $G(u, u_x)$ to $G(u, u_x) = \sum_{l=1}^{M} |p_l(U_k)|^{N_l^P} |q_l(u_x)|^{N_l}$, where q_l and N_l are defined similarly as above. Though it could be more general, we do this to keep the discussion simple and to give the explicit forms of the complex discrete variational derivative.

where

$$\left(\frac{\partial G_{\mathrm{d}}}{\partial(\boldsymbol{U},\boldsymbol{V})}\right)_k \stackrel{\mathrm{d}}{\equiv} \left(\frac{Q_l^+(U_k)Q_l^-(U_k)+Q_l^+(V_k)Q_l^-(V_k)}{2}\right) \times \left(\frac{p_l(U_k)-p_l(V_k)}{U_k-V_k}\right) f\left(N_l^P;\, p_l(U_k),\, p_l(V_k)\right) \tag{25a}$$

$$\left(\frac{\partial G_{\mathrm{d}}}{\partial\delta^+(\boldsymbol{U},\boldsymbol{V})}\right)_k \stackrel{\mathrm{d}}{\equiv} \left(\frac{P_l(U_k)+P_l(V_k)}{2}\right)\left(\frac{Q_l^-(U_k)+Q_l^-(V_k)}{2}\right) \times \left(\frac{q_l^+(\delta_k^+U_k)-q_l^+(\delta_k^+V_k)}{\delta_k^+U_k-\delta_k^+V_k}\right) f(N_l^+;\, q_l^+(\delta_k^+U_k),\, q_l^+(\delta_k^+V_k)) \tag{25b}$$

$$\left(\frac{\partial G_{\mathrm{d}}}{\partial\delta^-(\boldsymbol{U},\boldsymbol{V})}\right)_k \stackrel{\mathrm{d}}{\equiv} \left(\frac{P_l(U_k)+P_l(V_k)}{2}\right)\left(\frac{Q_l^+(U_k)+Q_l^+(V_k)}{2}\right) \times \left(\frac{q_l^-(\delta_k^-U_k)-q_l^-(\delta_k^-V_k)}{\delta_k^-U_k-\delta_k^-V_k}\right) f(N_l^-;\, q_l^-(\delta_k^-U_k),\, q_l^-(\delta_k^-V_k)) \tag{25c}$$

$$\begin{aligned}\left(\frac{\partial G_{\mathrm{d}}}{\partial\delta(\boldsymbol{U},\boldsymbol{V})}\right)_k = \frac{1}{2}\Bigg\{&\left(\frac{\partial G_{\mathrm{d}}}{\partial\delta^+(\boldsymbol{U},\boldsymbol{V})}\right)_k (U_{k+1}-V_{k+1}) + \left(\frac{\partial G_{\mathrm{d}}}{\partial\delta^+(\boldsymbol{U},\boldsymbol{V})}\right)_{k-1}(U_k-V_k)\\ &+\left(\frac{\partial G_{\mathrm{d}}}{\partial\delta^+(\overline{\boldsymbol{U}},\overline{\boldsymbol{V}})}\right)_k (\overline{U_{k+1}-V_{k+1}}) + \left(\frac{\partial G_{\mathrm{d}}}{\partial\delta^+(\overline{\boldsymbol{U}},\overline{\boldsymbol{V}})}\right)_{k-1}(\overline{U_k-V_k})\\ &+\left(\frac{\partial G_{\mathrm{d}}}{\partial\delta^-(\boldsymbol{U},\boldsymbol{V})}\right)_k (U_{k-1}-V_{k-1}) + \left(\frac{\partial G_{\mathrm{d}}}{\partial\delta^-(\boldsymbol{U},\boldsymbol{V})}\right)_{k+1}(U_k-V_k)\\ &+\left(\frac{\partial G_{\mathrm{d}}}{\partial\delta^-(\overline{\boldsymbol{U}},\overline{\boldsymbol{V}})}\right)_k (\overline{U_{k-1}-V_{k-1}}) + \left(\frac{\partial G_{\mathrm{d}}}{\partial\delta^-(\overline{\boldsymbol{U}},\overline{\boldsymbol{V}})}\right)_{k+1}(\overline{U_k-V_k})\Bigg\},\end{aligned} \tag{26}$$

and

$$f(n; z_1, z_2) \stackrel{\mathrm{d}}{\equiv} \begin{cases} \dfrac{\overline{z_1+z_2}}{2}(|z_1|^{n-2}+|z_1|^{n-4}|z_2|^2+\cdots+|z_2|^{n-2}), & n : \text{even},\\[2ex] \dfrac{\overline{z_1+z_2}}{2}\,\dfrac{|z_1|^{n-1}+|z_1|^{n-2}|z_2|+\cdots+|z_2|^{n-1}}{|z_1|+|z_2|}, & n : \text{odd}.\end{cases} \tag{27}$$

In the second equality of (24), a trivial equality $\alpha\beta-\xi\eta=\frac{1}{2}(\alpha-\xi)(\beta+\eta)+\frac{1}{2}(\alpha+\xi)(\beta-\eta)$ which holds for any $\alpha,\beta,\xi,\eta\in\mathbf{C}$ is repeatedly used. In the third equality, the summation-by-parts formula (21) is applied. $\partial G_{\mathrm{d}}/\partial(\boldsymbol{U},\boldsymbol{V}) : \mathbf{C}^{N+1}\times\mathbf{C}^{N+1}\to\mathbf{C}^{N+1}$ corresponds to $\partial G/\partial u$, and both $\partial G_{\mathrm{d}}/\partial\delta^+(\boldsymbol{U},\boldsymbol{V}) : \mathbf{C}^{N+1}\times\mathbf{C}^{N+1}\to\mathbf{C}^{N+1}$ and $\partial G_{\mathrm{d}}/\partial\delta^-(\boldsymbol{U},\boldsymbol{V}) : \mathbf{C}^{N+1}\times\mathbf{C}^{N+1}\to\mathbf{C}^{N+1}$ correspond to $\partial G/\partial u_x$.

Now we define the complex discrete variational derivatives (corresponding to (6) and (7)) as follows:

$$\left(\frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U},\boldsymbol{V})}\right)_k \stackrel{\mathrm{d}}{\equiv} \left(\frac{\partial G_{\mathrm{d}}}{\partial(\boldsymbol{U},\boldsymbol{V})}\right)_k - \delta_k^-\left(\frac{\partial G_{\mathrm{d}}}{\partial\delta^+(\boldsymbol{U},\boldsymbol{V})}\right)_k - \delta_k^+\left(\frac{\partial G_{\mathrm{d}}}{\partial\delta^-(\boldsymbol{U},\boldsymbol{V})}\right)_k \tag{28}$$

$$\left(\frac{\delta G_{\mathrm{d}}}{\delta(\overline{\boldsymbol{U}},\overline{\boldsymbol{V}})}\right)_k \stackrel{\mathrm{d}}{\equiv} \left(\frac{\partial G_{\mathrm{d}}}{\partial(\overline{\boldsymbol{U}},\overline{\boldsymbol{V}})}\right)_k - \delta_k^-\left(\frac{\partial G_{\mathrm{d}}}{\partial\delta^+(\overline{\boldsymbol{U}},\overline{\boldsymbol{V}})}\right)_k - \delta_k^+\left(\frac{\partial G_{\mathrm{d}}}{\partial\delta^-(\overline{\boldsymbol{U}},\overline{\boldsymbol{V}})}\right)_k. \tag{29}$$

Note that the complex discrete variational derivatives are complex conjugates of each other (corresponding to (8)), that is,

$$\overline{\left(\frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U},\boldsymbol{V})}\right)_k} = \left(\frac{\delta G_{\mathrm{d}}}{\delta(\overline{\boldsymbol{U}},\overline{\boldsymbol{V}})}\right)_k. \tag{30}$$

It should be noted that when

$$\left[\left(\frac{\partial G_{\mathrm{d}}}{\partial\delta(\boldsymbol{U},\boldsymbol{V})}\right)_k\right]_{k=0}^{N} = 0, \tag{31}$$

which is the discrete analogue of (10), is satisfied, the boundary effect vanishes in the right-hand-most side of (24):

$$\begin{aligned}
&H_{\mathrm{d}}(\boldsymbol{U}) - H_{\mathrm{d}}(\boldsymbol{V})\\
&= \sum_{k=0}^{N}{}'' \Bigg[\left\{\left(\frac{\partial G_{\mathrm{d}}}{\partial(\boldsymbol{U},\boldsymbol{V})}\right)_k - \delta_k^-\left(\frac{\partial G_{\mathrm{d}}}{\partial\delta^+(\boldsymbol{U},\boldsymbol{V})}\right)_k - \delta_k^+\left(\frac{\partial G_{\mathrm{d}}}{\partial\delta^-(\boldsymbol{U},\boldsymbol{V})}\right)_k\right\}(U_k - V_k)\\
&\quad + \left\{\left(\frac{\partial G_{\mathrm{d}}}{\partial(\overline{\boldsymbol{U}},\overline{\boldsymbol{V}})}\right)_k - \delta_k^-\left(\frac{\partial G_{\mathrm{d}}}{\partial\delta^+(\overline{\boldsymbol{U}},\overline{\boldsymbol{V}})}\right)_k - \delta_k^+\left(\frac{\partial G_{\mathrm{d}}}{\partial\delta^-(\overline{\boldsymbol{U}},\overline{\boldsymbol{V}})}\right)_k\right\}(\overline{U_k - V_k})\Bigg]\Delta x\\
&= \sum_{k=0}^{N}{}'' \left[\left(\frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U},\boldsymbol{V})}\right)_k (U_k - V_k) + \left(\frac{\delta G_{\mathrm{d}}}{\delta(\overline{\boldsymbol{U}},\overline{\boldsymbol{V}})}\right)_k (\overline{U_k - V_k})\right]\Delta x.
\end{aligned} \tag{32}$$

Remark. In a more general case where G involves $u_{xx}, u_{xxx}, \ldots$, or where the space dimension is more than one, the discrete variational derivative of G can be defined in a similar manner. We omit its general form because it is too complicated to be explicitly written here. However, for a simple two-dimensional equation, i.e., the Newell–Whitehead equation where G involves $u_x, u_{xx}, u_{yy}, u_{xyy}$, and u_{yyyy}, a concrete form of the discrete variational derivative is given in Sections 5 and 6.

4. DESIGN OF SCHEMES

In this section we design the finite-difference schemes for the target equations (2) or (3) with the complex discrete variational derivatives and prove that the finite-difference schemes inherit the conservation or dissipation property.

First we define a discrete local energy G_{d}, and then define the finite-difference scheme for the conservative equation (2) by

$$\mathrm{i}\left(\frac{U_k^{(m+1)} - U_k^{(m)}}{\Delta t}\right) = -\left(\frac{\delta G_{\mathrm{d}}}{\delta\left(\overline{\boldsymbol{U}^{(m+1)}}, \overline{\boldsymbol{U}^{(m)}}\right)}\right)_k \tag{33}$$

and for the dissipative Eq. (3) by

$$\frac{U_k^{(m+1)} - U_k^{(m)}}{\Delta t} = -\left(\frac{\delta G_{\mathrm{d}}}{\delta\left(\overline{\boldsymbol{U}^{(m+1)}}, \overline{\boldsymbol{U}^{(m)}}\right)}\right)_k. \tag{34}$$

Furthermore, we discretize the boundary condition so that the resulting boundary condition satisfies

$$\left[\left(\frac{\partial G_{\mathrm{d}}}{\partial\delta\left(\boldsymbol{U}^{(m+1)}, \boldsymbol{U}^{(m)}\right)}\right)_k\right]_{k=0}^{N} = 0, \tag{35}$$

which is a discrete analogue of (10). For example, for the periodic boundary condition or the zero Dirichlet boundary condition, we set $U_0^{(m)} = U_N^{(m)}$ or $U_0^{(m)} = U_N^{(m)} = 0$, respectively.

These finite-difference schemes conserve or dissipate the discrete global energy.

THEOREM 4.1 (discrete energy conservation). *Let $\boldsymbol{U}^{(m)}$ be a solution of* (33) *with the boundary condition which satisfies* (35). *Then the global energy $H_{\mathrm{d}}(\boldsymbol{U}^{(m)})$ is conserved, that is*,

$$H_{\mathrm{d}}\left(\boldsymbol{U}^{(m)}\right) = H_{\mathrm{d}}\left(\boldsymbol{U}^{(0)}\right) \qquad (m = 1, 2, 3, \dots). \tag{36}$$

Proof.

$$\begin{aligned}
&\frac{1}{\Delta t}\left\{H_{\mathrm{d}}\left(\boldsymbol{U}^{(m+1)}\right) - H_{\mathrm{d}}\left(\boldsymbol{U}^{(m)}\right)\right\} \\
&= \frac{1}{\Delta t}\sum_{k=0}^{N}{}'' \left\{G_{\mathrm{d}}\left(\boldsymbol{U}^{(m+1)}\right)_k - G_{\mathrm{d}}\left(\boldsymbol{U}^{(m)}\right)_k\right\} \Delta x \\
&= \sum_{k=0}^{N}{}'' \left\{ \left(\frac{\delta G_{\mathrm{d}}}{\delta\left(\boldsymbol{U}^{(m+1)}, \boldsymbol{U}^{(m)}\right)}\right)_k \left(\frac{\overline{U_k^{(m+1)} - U_k^{(m)}}}{\Delta t}\right) \right. \\
&\quad \left. + \left(\frac{\delta G_{\mathrm{d}}}{\delta\left(\overline{\boldsymbol{U}^{(m+1)}}, \overline{\boldsymbol{U}^{(m)}}\right)}\right)_k \left(\frac{U_k^{(m+1)} - U_k^{(m)}}{\Delta t}\right) \right\} \Delta x \\
&= \sum_{k=0}^{N}{}'' \left\{ \mathrm{i}\left|\left(\frac{\delta G_{\mathrm{d}}}{\delta\left(\boldsymbol{U}^{(m+1)}, \boldsymbol{U}^{(m)}\right)}\right)_k\right|^2 - \mathrm{i}\left|\left(\frac{\delta G_{\mathrm{d}}}{\delta\left(\boldsymbol{U}^{(m+1)}, \boldsymbol{U}^{(m)}\right)}\right)_k\right|^2 \right\} \Delta x \\
&= 0.
\end{aligned} \tag{37}$$

■

THEOREM 4.2 (discrete energy dissipation). *Let $\boldsymbol{U}^{(m)}$ be a solution of* (34) *with the boundary condition which satisfies* (35). *Then the global energy $H_{\mathrm{d}}(\boldsymbol{U}^{(m)})$ dissipates, that is*,

$$H_{\mathrm{d}}\left(\boldsymbol{U}^{(m+1)}\right) \le H_{\mathrm{d}}\left(\boldsymbol{U}^{(m)}\right) \qquad (m = 0, 1, 2, \dots). \tag{38}$$

Proof.

$$\begin{aligned}
&\frac{1}{\Delta t}\left\{H_{\mathrm{d}}\left(\boldsymbol{U}^{(m+1)}\right) - H_{\mathrm{d}}\left(\boldsymbol{U}^{(m)}\right)\right\} \\
&= \frac{1}{\Delta t}\sum_{k=0}^{N}{}'' \left\{G_{\mathrm{d}}\left(\boldsymbol{U}^{(m+1)}\right)_k - G_{\mathrm{d}}\left(\boldsymbol{U}^{(m)}\right)_k\right\} \Delta x \\
&= \sum_{k=0}^{N}{}'' \left\{ \left(\frac{\delta G_{\mathrm{d}}}{\delta\left(\boldsymbol{U}^{(m+1)}, \boldsymbol{U}^{(m)}\right)}\right)_k \left(\frac{\overline{U_k^{(m+1)} - U_k^{(m)}}}{\Delta t}\right) \right. \\
&\quad \left. + \left(\frac{\delta G_{\mathrm{d}}}{\delta\left(\overline{\boldsymbol{U}^{(m+1)}}, \overline{\boldsymbol{U}^{(m)}}\right)}\right)_k \left(\frac{U_k^{(m+1)} - U_k^{(m)}}{\Delta t}\right) \right\} \Delta x \\
&= -2\sum_{k=0}^{N}{}'' \left|\left(\frac{\delta G_{\mathrm{d}}}{\delta\left(\boldsymbol{U}^{(m+1)}, \boldsymbol{U}^{(m)}\right)}\right)_k\right|^2 \Delta x \\
&\le 0.
\end{aligned} \tag{39}$$

■

Because of the nonlinearity in the PDE, (2) or (3), the derived schemes become nonlinear in general. Hence some time-consuming iterative solver such as the Newton method is required. But it does not necessarily imply that the all schemes are costly, since the time step width Δt in the schemes may be taken far larger than in the naive "fast" schemes.

It is also worth mentioning that Δt can be taken adaptively. In fact, Scheme (33) or (34) and the conservation theorem 4.1 or dissipation theorem 4.2 depend only on two consecutive time steps, and therefore a change of Δt does not destroy the dissipation or conservation property.

5. APPLICATIONS

In this section we present several applications.

5.1. *The NLS Equation*

There are many PDEs described in the form (2). Among them, the most prominent PDE is the nonlinear Schrödinger equation (NLS)

$$\mathrm{i}\frac{\partial u}{\partial t} = -u_{xx} - \gamma |u|^{p-1}u \qquad (x \in [0, L], t > 0, \gamma \in \mathbf{R}, p = 3, 4, \ldots). \tag{11}$$

The NLS equation is not only of physical interest in applications such as nonlinear optics and plasma physics, but also of mathematical interest because it may exhibit blowup or become chaotic. We refer the reader to the surveys [2, 15] and the references therein for physical and theoretical aspects of the NLS equation.

Up to the present many numerical studies have been done by various numerical methods, such as the finite-difference method and the finite-element method (see Taha [16] for a review). Delfour *et al.* [3] constructed a finite-difference scheme on the whole spatial domain and proved that it is conservative. Akrivis [1] discussed the Galerkin analogue of Delfour's scheme and showed the existence, uniqueness, and L^2 error estimate of the solution in the cubic case ($p = 3$). Fei [4] proposed a conservative linearly implicit finite-difference scheme, which can be regarded as a linear version of Delfour's scheme and showed the L^2 error estimate in the cubic case ($p = 3$).

We here consider the NLS equation (11) under the periodic boundary condition, i.e., for any $t > 0$,

$$\begin{cases} u(t, 0) = u(t, L), \\ \frac{\partial u}{\partial x}(t, 0) = \frac{\partial u}{\partial x}(t, L). \end{cases} \tag{40}$$

As is well known, the local energy $G(u, u_x)$ for the NLS equation is given as

$$G(u, u_x) = -|u_x|^2 + \frac{2\gamma}{p+1}|u|^{p+1}, \tag{41}$$

and accordingly the global energy $H(u)$ is given as

$$H(u) = \int_0^L \left(-|u_x|^2 + \frac{2\gamma}{p+1}|u|^{p+1} \right) \mathrm{d}x. \tag{42}$$

Following our proposed procedure, we first define the discrete local energy as

$$G_{\mathrm{d}}(\boldsymbol{U})_k \stackrel{\mathrm{d}}{\equiv} -\frac{|\delta_k^+ U_k|^2 + |\delta_k^- U_k|^2}{2} + \frac{2\gamma}{p+1}|U_k|^{p+1}. \tag{43}$$

Note that this G_{d} approximates $G(u, u_x)$ above, and it can be decomposed as assumed in (22). Calculating the complex discrete variational derivatives mechanically by (28), (29), and (25a), (25b), (25c), we have

$$\left(\frac{\delta G_{\mathrm{d}}}{\delta\left(\overline{\boldsymbol{U}^{(m+1)}}, \overline{\boldsymbol{U}^{(m)}}\right)}\right)_k = \delta_k^{\langle 2\rangle}\left(\frac{U_k^{(m+1)} + U_k^{(m)}}{2}\right) + \frac{2\gamma}{p+1}\left(\frac{\left|U_k^{(m+1)}\right|^{p+1} - \left|U_k^{(m)}\right|^{p+1}}{\left|U_k^{(m+1)}\right|^2 - \left|U_k^{(m)}\right|^2}\right)\left(\frac{U_k^{(m+1)} + U_k^{(m)}}{2}\right). \tag{44}$$

Then from (33) we obtain the finite-difference scheme:

$$\mathrm{i}\left(\frac{U_k^{(m+1)} - U_k^{(m)}}{\Delta t}\right) = -\delta_k^{\langle 2\rangle}\left(\frac{U_k^{(m+1)} + U_k^{(m)}}{2}\right) - \frac{2\gamma}{p+1}\left(\frac{\left|U_k^{(m+1)}\right|^{p+1} - \left|U_k^{(m)}\right|^{p+1}}{\left|U_k^{(m+1)}\right|^2 - \left|U_k^{(m)}\right|^2}\right)\left(\frac{U_k^{(m+1)} + U_k^{(m)}}{2}\right). \tag{45}$$

Here we impose the discrete periodic boundary condition

$$U_k^{(m)} = U_{k+N}^{(m)} \qquad (k \in \mathbf{Z}, m = 0, 1, 2, \ldots), \tag{46}$$

corresponding to the periodic boundary condition (40).

As the periodic boundary condition (46) satisfies (35), the conservation theorem 4.1 holds. Moreover, the scheme is “probability” conservative; i.e., it inherits a discrete analogue of the probability conservation law $\int_0^L |u|^2\,\mathrm{d}x = \mathrm{const.}$ [3]. With these properties the scheme is shown to be stable and L^2-convergent when $p = 3$. It is also shown that the same theorem and the same properties stand under the zero Dirichlet boundary condition. The details are beyond the scope of this paper and are therefore omitted here [9].

We should note that, for a simple case, i.e., the case where $L = +\infty$, Delfour *et al.* [3] proposed the same scheme as (45) with no mention of its derivation.

5.2. *The CGL Equation*

As noted earlier, the complex-valued Ginzburg–Landau equation (CGL) [7],

$$\frac{\partial u}{\partial t} = pu_{xx} + q|u|^2 u + ru \qquad (x \in [0, L], t > 0, p > 0, q < 0, r \in \mathbf{R}), \tag{13}$$

is an example of the dissipative equation (3). It describes evolution phenomena in the wide range of physical applications, such as fluid dynamics, pattern formation, and the theory of superconductivity. The CGL equation also attracts many mathematicians because it can be regarded as a dissipative version of the NLS equation, and may also exhibit blowup [7]. In these contexts many numerical experiments have been carried out. But they are mainly of physical interest, and few papers are devoted to the study of numerical Schemes [8, 11], especially to dissipative schemes.

We consider the CGL Eq. (13) under the periodic boundary condition (40). The local energy $G(u, u_x)$ is given as

$$G(u, u_x) = p|u_x|^2 - \frac{q}{2}|u|^4 - r|u|^2, \tag{47}$$

and accordingly the global energy $H(u)$ as

$$H(u) = \int_0^L \left(p|u_x|^2 - \frac{q}{2}|u|^4 - r|u|^2 \right) \mathrm{d}x. \tag{48}$$

Following our proposed procedure, we first define the discrete local energy as

$$G_{\mathrm{d}}(\boldsymbol{U})_k \stackrel{\mathrm{d}}{\equiv} p \left(\frac{|\delta_k^+ U_k|^2 + |\delta_k^- U_k|^2}{2} \right) - \frac{q}{2}|U_k|^4 - r|U_k|^2. \tag{49}$$

Consequently, the discrete variational derivative becomes

$$\left(\frac{\delta G_{\mathrm{d}}}{\delta\left(\overline{\boldsymbol{U}^{(m+1)}}, \overline{\boldsymbol{U}^{(M)}}\right)} \right)_k = -p\delta_k^{\langle 2\rangle} \left(\frac{U_k^{(m+1)} + U_k^{(m)}}{2} \right) - q \left(\frac{\left|U_k^{(m+1)}\right|^2 + \left|U_k^{(m)}\right|^2}{2} \right) \times \left(\frac{U_k^{(m+1)} + U_k^{(m)}}{2} \right) - r \left(\frac{U_k^{(m+1)} + U_k^{(m)}}{2} \right). \tag{50}$$

Finally from (34) we obtain the finite-difference scheme

$$\frac{U_k^{(m+1)} - U_k^{(m)}}{\Delta t} = p\delta_k^{\langle 2\rangle} \left(\frac{U_k^{(m+1)} + U_k^{(m)}}{2} \right) + q \left(\frac{\left|U_k^{(m+1)}\right|^2 + \left|U_k^{(m)}\right|^2}{2} \right) \times \left(\frac{U_k^{(m+1)} + U_k^{(m)}}{2} \right) + r \left(\frac{U_k^{(m+1)} + U_k^{(m)}}{2} \right). \tag{51}$$

Here we impose the discrete periodic boundary condition (46). Since the periodic boundary condition (46) satisfies (35), the dissipation theorem 4.2 holds.

This scheme seems not to have been pointed out explicitly in the literature, although it is just the CGL version of the Delfour scheme for the NLS Eq. [3]. It can be proved that the scheme is stable and L^2-convergent (the proof is omitted here).

5.3. *The NW Equation*

As stated earlier the Newell–Whitehead (NW) Eq. [12]

$$\frac{\partial u}{\partial t}(t, x, y) = \mu u - |u|^2 u + \left(\frac{\partial}{\partial x} - \frac{\mathrm{i}}{2k_c} \frac{\partial^2}{\partial y^2} \right)^2 u \qquad \left(\begin{array}{c} (x, y) \in [0, L_x] \times [0, L_y], \\ t > 0, \\ \mu, k_c \in \mathbf{R}, \end{array} \right) \tag{14}$$

is an example of the two-dimensional dissipative Eq. (3), which describes the generation of roll patterns in the Bénard convection flow. For the NW equation, there seem to be few studies on numerical schemes.

Here we consider the NW equation with the periodic boundary condition (40) imposed in both directions. It is well known that the local energy for the NW equation is

$$G(u, u_x, u_{yy}) = -\mu|u|^2 + \frac{1}{2}|u|^4 + \left|\frac{\partial u}{\partial x} - \frac{\mathrm{i}}{2k_c}\frac{\partial^2 u}{\partial y^2}\right|^2. \tag{52}$$

Integrating the local energy on the domain $[0, L_x] \times [0, L_y]$, we have the global energy for the NW equation:

$$H(u) = \int_0^{L_x}\int_0^{L_y}\left(-\mu|u|^2 + \frac{1}{2}|u|^4 + \left|\frac{\partial u}{\partial x} - \frac{\mathrm{i}}{2k_c}\frac{\partial^2 u}{\partial y^2}\right|^2\right)\mathrm{d}x\,\mathrm{d}y. \tag{53}$$

To derive a finite-difference scheme, we have to follow the proposed procedure, which was essentially formulated for the one-dimensional PDEs. But the procedure can also be applied to higher dimensional problems as long as they can be directly decomposed with the space variables. And the NW problem above is the case.

First, we define the discrete energy as

$$\begin{aligned} G_{\mathrm{d}}(\boldsymbol{U})_{k,l} &\stackrel{\mathrm{d}}{\equiv} -\mu|U_{k,l}|^2 + \frac{1}{2}|U_{k,l}|^4 \\ &\quad + \frac{1}{2}\left(\left|\delta_k^+ U_{k,l} - \frac{\mathrm{i}}{2k_c}\delta_l^{\langle 2\rangle}U_{k,l}\right|^2 + \left|\delta_k^- U_{k,l} - \frac{\mathrm{i}}{2k_c}\delta_l^{\langle 2\rangle}U_{k,l}\right|^2\right), \end{aligned} \tag{54}$$

and accordingly define the discrete global energy as

$$H_{\mathrm{d}}(\boldsymbol{U}) \stackrel{\mathrm{d}}{\equiv} \sum_{k=0}^{N_x}{}'' \sum_{l=0}^{N_y}{}'' G_{\mathrm{d}}(U)_{k,l}\,\Delta x\,\Delta y, \tag{55}$$

where N_x and N_y are the number of grid points in x and y, $\Delta x \stackrel{\mathrm{d}}{\equiv} L_x/N_x$, $\Delta y \stackrel{\mathrm{d}}{\equiv} L_y/N_y$, and the numerical solution $U_{k,l}^{(m)} \simeq u(m\Delta t, k\Delta x, l\Delta y)$ is now $\mathbf{C}^{(N_x+1)(N_y+1)}$ vector. The difference operators with the subscript l operate in l direction.

To define a discrete variational derivative we consider the difference $H_{\mathrm{d}}(\boldsymbol{U}) - H_{\mathrm{d}}(\boldsymbol{V})$ by analogy with the one-dimensional case as

$$\begin{aligned} H_{\mathrm{d}}(\boldsymbol{U}) - H_{\mathrm{d}}(\boldsymbol{V}) = \sum_{k=0}^{N_x}{}'' \sum_{l=0}^{N_y}{}'' \Bigg\{ &\left(\frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}, \boldsymbol{V})}\right)_{k,l}(U_{k,l} - V_{k,l}) \\ &+ \overline{\left(\frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}, \boldsymbol{V})}\right)_{k,l}}\,(\overline{U_{k,l} - V_{k,l}})\Bigg\}\Delta x\,\Delta y, \end{aligned} \tag{56}$$

where

$$\begin{aligned} \left(\frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}, \boldsymbol{V})}\right)_{k,l} &= -\mu\left(\frac{U_{k,l} + V_{k,l}}{2}\right) + \left(\frac{|U_{k,l}|^2 + |V_{k,l}|^2}{2}\right)\left(\frac{U_{k,l} + V_{k,l}}{2}\right) \\ &\quad - \left(\delta_k^{\langle 2\rangle} - \frac{\mathrm{i}}{k_c}\delta_k^{\langle 1\rangle}\delta_l^{\langle 2\rangle} - \frac{1}{4k_c^2}\delta_l^{\langle 4\rangle}\right)\left(\frac{U_{k,l} + V_{k,l}}{2}\right). \end{aligned} \tag{57}$$

In the calculation above we use the summation-by-parts formula in k and l directions separately.

Then we have a finite-difference scheme:

$$\begin{aligned}
&\frac{U_{k,l}^{(m+1)} - U_{k,l}^{(m)}}{\Delta t} \\
&\quad = -\left(\frac{\delta G_{\mathrm{d}}}{\delta\left(\overline{\boldsymbol{U}^{(m+1)}}, \overline{\boldsymbol{U}^{(m)}}\right)} \right)_{k,l} \\
&\quad = \mu \left(\frac{U_{k,l}^{(m+1)} + U_{k,l}^{(m)}}{2} \right) - \left(\frac{\left|U_{k,l}^{(m+1)}\right|^2 + \left|U_{k,l}^{(m)}\right|^2}{2} \right) \left(\frac{U_{k,l}^{(m+1)} + U_{k,l}^{(m)}}{2} \right) \\
&\qquad + \left(\delta_k^{\langle 2\rangle} - \frac{\mathrm{i}}{k_c} \delta_k^{\langle 1\rangle} \delta_l^{\langle 2\rangle} - \frac{1}{4k_c^2} \delta_l^{\langle 4\rangle} \right) \left(\frac{U_{k,l}^{(m+1)} + U_{k,l}^{(m)}}{2} \right).
\end{aligned} \tag{58}$$

We impose the discrete periodic boundary condition in both directions as

$$U_{k,l}^{(m)} = U_{k+N_x,l}^{(m)} = U_{k,l+N_y}^{(m)}. \tag{59}$$

It is easy to see that under the discrete periodic boundary condition (59) the dissipation property holds for the scheme.

6. MODIFIED PROCEDURE FOR DESIGNING LINEARLY IMPLICIT SCHEMES

In this section we modify the proposed procedure for designing linearly implicit finite-difference schemes that inherit energy conservation or dissipation property. For this purpose we introduce a fundamental notion multiple points complex discrete variational derivative, which is a generalization of the complex discrete variational derivative. The modified procedure can be applied to the PDE (2) or (3) whose nonlinear terms are of the form $|u|^{2s}u$ ($s = 1, 2, \ldots$), such as the odd-order nonlinear Schrödinger (NLS) equation, the complex-valued Ginzburg–Landau (CGL) equation, and the Newell–Whitehead (NW) equation.

6.1. *Linearly Implicit Scheme for the NLS Equation*

In this section we propose linearly implicit finite-difference schemes for the NLS equation. To illustrate the basic idea of the modified procedure, we first discuss the derivation of the linearly implicit scheme for the cubic NLS equation (a special case with $s = 1$). Next we generalize the process to cover the general cases ($s \geq 2$).

Let us consider the cubic NLS equation

$$\mathrm{i}\frac{\partial u}{\partial t} = -u_{xx} - \gamma|u|^2 u \qquad (x \in [0, L], t > 0, \gamma \in \mathbf{R}), \tag{60}$$

whose energy is now

$$G(u, u_x) = -|u_x|^2 + \frac{\gamma}{2}|u|^4. \tag{61}$$

To obtain a linearly implicit scheme, it is essential to understand the mechanism of how the nonlinearity in the energy is passed down to the equation through the variation calculation. In the cubic NLS equation, $|u|^4$ in the local energy G (61) is the source of the nonlinear term $|u|^2 u$ in the resulting Eq. (60). In general, the power of nonlinearity in the energy is always 1 higher than that of the resulting nonlinearity. Hence we easily come to the conclusion that if we want the resulting scheme to be linear we must reduce the power of nonlinearity in the energy to 2, at most. In the cubic NLS equation, for example, decomposing $|U_k^{(m)}|^4$ to $|U_k^{(m+1)}|^2|U_k^{(m)}|^2$ will suffice and the corresponding part of the discrete variation calculation becomes

$$\begin{aligned} &\left|U_k^{(m+1)}\right|^2\left|U_k^{(m)}\right|^2 - \left|U_k^{(m)}\right|^2\left|U_k^{(m-1)}\right|^2 \\ &= \left|U_k^{(m)}\right|^2 \left(\frac{U_k^{(m+1)} + U_k^{(m-1)}}{2}\right)\left(\overline{U_k^{(m+1)} - U_k^{(m-1)}}\right) \\ &\quad + \left|U_k^{(m)}\right|^2 \left(\frac{\overline{U_k^{(m+1)} + U_k^{(m-1)}}}{2}\right)\left(U_k^{(m+1)} - U_k^{(m-1)}\right). \end{aligned} \tag{62}$$

Now $|U_k^{(m)}|^2(U_k^{(m+1)} + U_k^{(m-1)})/2$, which is the approximation of $|u|^2 u$, is still on the order of $|u|^3$, but is *linear* with regard to the unknown variable $U_k^{(m+1)}$.

With this observation we can now construct a whole linearly implicit scheme for the cubic NLS equation. We define a discrete local energy with two consecutive numerical solutions as

$$\begin{aligned} G_{\mathrm{d}}\left(\boldsymbol{U}^{(m+1)}, \boldsymbol{U}^{(m)}\right)_k \stackrel{\mathrm{d}}{\equiv} &-\frac{\left|\delta_k^+ U_k^{(m+1)}\right|^2 + \left|\delta_k^- U_k^{(m+1)}\right|^2 + \left|\delta_k^+ U_k^{(m)}\right|^2 + \left|\delta_k^- U_k^{(m)}\right|^2}{4} \\ &+ \frac{\gamma}{2}\left|U_k^{(m+1)}\right|^2\left|U_k^{(m)}\right|^2, \end{aligned} \tag{63}$$

and accordingly the discrete global energy as

$$H_{\mathrm{d}}\left(\boldsymbol{U}^{(m+1)}, \boldsymbol{U}^{(m)}\right) \stackrel{\mathrm{d}}{\equiv} \sum_{k=0}^{N}{}'' G_{\mathrm{d}}\left(U^{(m+1)}, U^{(m)}\right)_k \Delta x. \tag{64}$$

Taking its variation we have

$$\begin{aligned} &H_{\mathrm{d}}\left(\boldsymbol{U}^{(m+1)}, \boldsymbol{U}^{(m)}\right) - H_{\mathrm{d}}\left(\boldsymbol{U}^{(m)}, \boldsymbol{U}^{(m-1)}\right) \\ &= \frac{\delta G_{\mathrm{d}}}{\delta\left(\boldsymbol{U}^{(m+1)}, \boldsymbol{U}^{(m)}, \boldsymbol{U}^{(m-1)}\right)_k} \frac{U_k^{(m+1)} - U_k^{(m-1)}}{2} \\ &\quad + \frac{\delta G_{\mathrm{d}}}{\delta\left(\overline{\boldsymbol{U}^{(m+1)}}, \overline{\boldsymbol{U}^{(m)}}, \overline{\boldsymbol{U}^{(m-1)}}\right)_k} \frac{\overline{U_k^{(m+1)} - U_k^{(m-1)}}}{2}, \end{aligned} \tag{65}$$

where

$$\begin{aligned} \frac{\delta G_{\mathrm{d}}}{\delta\left(\boldsymbol{U}^{(m+1)}, \boldsymbol{U}^{(m)}, \boldsymbol{U}^{(m-1)}\right)_k} = &\frac{1}{2}\delta_k^{\langle 2\rangle}\left(\overline{U_k^{(m+1)} + U_k^{(m-1)}}\right) \\ &+ \frac{\gamma}{2}\left|U_k^{(m)}\right|^2\left(\overline{U_k^{(m+1)} + U_k^{(m-1)}}\right) \end{aligned} \tag{66}$$

$$\frac{\delta G_{\mathrm{d}}}{\delta\left(\overline{\boldsymbol{U}^{(m+1)}}, \overline{\boldsymbol{U}^{(m)}}, \overline{\boldsymbol{U}^{(m-1)}}\right)_k} = \overline{\frac{\delta G_{\mathrm{d}}}{\delta\left(\boldsymbol{U}^{(m+1)}, \boldsymbol{U}^{(m)}, \boldsymbol{U}^{(m-1)}\right)_k}} \tag{67}$$

are "three points discrete variational derivatives," which is a generalization of the discrete variational derivatives defined in Section 4.

With these we can now define a linearly implicit finite-difference scheme as

$$\begin{aligned} \mathrm{i}\left(\frac{U_k^{(m+1)} - U_k^{(m-1)}}{2\Delta t}\right) &= -\frac{\delta G_{\mathrm{d}}}{\delta\left(\overline{\boldsymbol{U}^{(m+1)}}, \overline{\boldsymbol{U}^{(m)}}, \overline{\boldsymbol{U}^{(m-1)}}\right)_k} \\ &= -\frac{1}{2}\delta_k^{\langle 2\rangle}\left(U_k^{(m+1)} + U_k^{(m-1)}\right) - \frac{\gamma}{2}\left|U_k^{(m)}\right|^2\left(U_k^{(m+1)} + U_k^{(m-1)}\right). \end{aligned} \tag{68}$$

Because the scheme (68) is linear with respect to $U_k^{(m+1)}$, we need only to solve a linear system at each time step, and therefore it is much faster than the nonlinear scheme (45), which needs heavy iterative calculations.

The scheme conserves the discrete energy under the periodic boundary condition (the proof is omitted because it is straightforward by analogy).

THEOREM 6.1 (discrete energy conservation). *The solution of the linearly implicit scheme* (68) *conserves the discrete energy* H_{d} (64) *under the periodic boundary condition* (46). *That is*,

$$H_{\mathrm{d}}\left(\boldsymbol{U}^{(m+1)}, \boldsymbol{U}^{(m)}\right) = H_{\mathrm{d}}\left(\boldsymbol{U}^{(1)}, \boldsymbol{U}^{(0)}\right) \qquad (m = 1, 2, 3, \ldots). \tag{69}$$

The discrete probability conservation law and the stability and L^2-convergence of the solution can be also established, under the periodic or zero Dirichlet boundary condition.

It should be noted that the scheme (68) is the same one that Fei *et al.* [4] proposed on the whole spatial domain. They also proved that the scheme is energy- and probability-conserving, stable, and L^2-convergent on the whole spatial domain.

The above process can be easily extended to the general case of nonlinear terms $|u|^{2s}u$ $(s = 2, 3, \ldots)$. We just have to decompose $|U_k^{(m)}|^{2s+2}$ (in the energy) into $|U_k^{(m+1)}|^2$ $|U_k^{(m)}|^2 \cdots |U_k^{(m-s+1)}|^2$. As a result, the three points discrete variational derivative is further generalized to the *multiple* points discrete variational derivative which depends on three or more points.[3]

Here we present a linearly implicit finite-difference scheme for the odd-order NLS equation

$$\mathrm{i}\frac{\partial u}{\partial t} = -u_{xx} - \gamma|u|^{2s}u \qquad (x \in [0, L], t > 0, s = 2, 3, \ldots). \tag{70}$$

[3] In our notation "multiple points discrete variational derivative" denotes the three or more points one. The two points one are excluded from this definition, though "multiple" includes two in English and hence the definition is a little confusing. This is a matter of terminology.

For the odd-order NLS equation, the discrete local energy should be defined as

$$G_{\mathrm{d}}\left(\boldsymbol{U}^{(m+1)}, \boldsymbol{U}^{(m)}, \ldots, \boldsymbol{U}^{(m-s+1)}\right)_k \stackrel{\mathrm{d}}{\equiv} \frac{\left|\delta_k^{+} U_k^{(m+1)}\right|^2 + \left|\delta_k^{+} U_k^{(m)}\right|^2 + \cdots + \left|\delta_k^{+} U_k^{(m-s+1)}\right|^2}{2(s+1)} + \frac{\left|\delta_k^{-} U_k^{(m+1)}\right|^2 + \left|\delta_k^{-} U_k^{(m)}\right|^2 + \cdots + \left|\delta_k^{-} U_k^{(m-s+1)}\right|^2}{2(s+1)} + \frac{\gamma}{s+1}\left|U_k^{(m+1)}\right|^2\left|U_k^{(m)}\right|^2 \cdots \left|U_k^{(m-s+1)}\right|^2, \tag{71}$$

and accordingly the discrete global energy is defined as

$$H_{\mathrm{d}}\left(\boldsymbol{U}^{(m+1)}, \boldsymbol{U}^{(m)}, \ldots, \boldsymbol{U}^{(m-s+1)}\right) \stackrel{\mathrm{d}}{\equiv} \sum_{k=0}^{N}{}'' G_{\mathrm{d}}\left(\boldsymbol{U}^{(m+1)}, \boldsymbol{U}^{(m)}, \ldots, \boldsymbol{U}^{(m-s+1)}\right)_k \Delta x. \tag{72}$$

Through the discrete variation calculation we have

$$\mathrm{i}\left(\frac{U_k^{(m+1)} - U_k^{(m-s)}}{(s+1)\Delta t}\right) = \frac{\delta G_{\mathrm{d}}}{\delta(\overline{\boldsymbol{U}^{(m+1)}}, \overline{\boldsymbol{U}^{(m)}}, \ldots, \overline{\boldsymbol{U}^{(m-s)}})_k} = -\frac{1}{2}\delta_k^{\langle 2\rangle}\left(U_k^{(m+1)} + U_k^{(m-s)}\right) - \frac{\gamma}{2}\left|U_k^{(m)}\right|^2\left|U_k^{(m-1)}\right|^2 \cdots \left|U_k^{(m-s+1)}\right|^2\left(U_k^{(m+1)} + U_k^{(m-s)}\right). \tag{73}$$

The resulting scheme depends on the solutions at $s+2$ time steps and is linear to $U_k^{(m+1)}$. This scheme conserves the discrete energy under the periodic boundary condition as follows.

THEOREM 6.2 (discrete energy conservation). *The solution of the linearly implicit scheme* (73) *conserves the discrete energy* H_{d} (72) *under the periodic boundary condition* (46). *That is*, *for* $m = s, s+1, s+2, \ldots$

$$H_{\mathrm{d}}\left(\boldsymbol{U}^{(m+1)}, \boldsymbol{U}^{(m)}, \ldots, \boldsymbol{U}^{(m-s+1)}\right) = H_{\mathrm{d}}\left(\boldsymbol{U}^{(s)}, \boldsymbol{U}^{(s-1)}, \ldots, \boldsymbol{U}^{(0)}\right). \tag{74}$$

The proof is again trivial and hence omitted. This scheme also conserves a discrete analogue of the probability. This scheme seems to be new.

Remark. The resulting linearly implicit schemes have two minor drawbacks. First, it is not "self-starting," i.e., we need not only $\boldsymbol{U}^{(0)}$ but also $\boldsymbol{U}^{(1)}$ to start calculation. We must calculate $\boldsymbol{U}^{(1)}$ in advance by other integrating schemes such as the Euler or Runge–Kutta method. And second, the time mesh adaptive methods can no longer be used because the linearly implicit schemes depend on the numerical solutions at more than two time steps. But this is not much of a problem because the adaptive methods are less important in the fast linearly implicit schemes. This remark should be applied to all linearly implicit schemes mentioned in this paper.

6.2. *Linearly Implicit Scheme for the CGL Equation*

In this section we propose a linearly implicit scheme for the CGL equation

$$\frac{\partial u}{\partial t} = p u_{xx} + q|u|^2 u + r u \qquad (x \in [0, L], t > 0, p > 0, q < 0, r \in \mathbf{R}). \tag{13}$$

For the CGL equation, we define the discrete local energy as

$$H_{\mathrm{d}}\left(\boldsymbol{U}^{(m+1)}, \boldsymbol{U}^{(m)}\right) = \sum_{k=0}^{N}{}'' \left\{ \frac{p}{4}\left(\left|\delta_k^+ U_k^{(m+1)}\right|^2 + \left|\delta_k^+ U_k^{(m)}\right|^2 + \left|\delta_k^- U_k^{(m+1)}\right|^2 + \left|\delta_k^- U_k^{(m)}\right|^2\right) - \frac{q}{2}\left|U_k^{(m+1)}\right|^2\left|U_k^{(m)}\right|^2 - \frac{r}{2}\left(U_k^{(m+1)}\overline{U_k^{(m)}} + \overline{U_k^{(m+1)}}U_k^{(m)}\right)\right\}\Delta x. \quad (75)$$

From the discrete energy we obtain the finite-difference scheme as

$$\frac{U_k^{(m+1)} - U_k^{(m-1)}}{2\Delta t} = p\delta_k^{\langle 2\rangle}\left(\frac{U_k^{(m+1)} + U_k^{(m-1)}}{2}\right) + q\left|U_k^{(m)}\right|^2\left(\frac{U_k^{(m+1)} + U_k^{(m-1)}}{2}\right) + rU_k^{(m)}. \quad (76)$$

This scheme seems to be new.

The scheme dissipates the energy under the periodic boundary condition as follows.

THEOREM 6.3 (discrete energy dissipation). *Let* $\boldsymbol{U}^{(m)}$ *be a solution of* (76) *with the periodic boundary condition* (46). *Then the global energy* H_{d} (75) *dissipates, that is,*

$$H_{\mathrm{d}}\left(\boldsymbol{U}^{(m+1)}, \boldsymbol{U}^{(m)}\right) \le H_{\mathrm{d}}\left(\boldsymbol{U}^{(m)}, \boldsymbol{U}^{(m-1)}\right) \qquad (m = 1, 2, 3, \ldots). \quad (77)$$

6.3. *Linearly Implicit Scheme for the NW Equation*

In this section we propose a linearly implicit scheme for the NW equation. We also present a simple numerical example.

For the NW equation.

$$\frac{\partial u}{\partial t}(t, x, y) = \mu u - |u|^2 u + \left(\frac{\partial}{\partial x} - \frac{\mathrm{i}}{2k_c}\frac{\partial^2}{\partial y^2}\right)^2 u \qquad \begin{pmatrix} (x, y) \in [0, L_x] \times [0, L_y], \\ t > 0, \\ \mu, k_c \in \mathbf{R}, \end{pmatrix}, \quad (14)$$

we define the discrete energy as

$$H_{\mathrm{d}}\left(\boldsymbol{U}^{(m+1)}, \boldsymbol{U}^{(m)}\right) \stackrel{\mathrm{d}}{\equiv} \sum_{k=0}^{N_x}{}'' \sum_{l=0}^{N_y}{}'' \left\{ -\frac{\mu}{2}\left(U_{k,l}^{(m+1)}\overline{U_{k,l}^{(m)}} + \overline{U_{k,l}^{(m+1)}}U_{k,l}^{(m)}\right) + \frac{1}{2}\left|U_{k,l}^{(m+1)}\right|^2\left|U_{k,l}^{(m)}\right|^2 + \frac{1}{4}\left(\left|\delta_k^+ U_{k,l}^{(m+1)} - \frac{\mathrm{i}}{2k_c}\delta_l^{\langle 2\rangle}U_{k,l}^{(m+1)}\right|^2 + \left|\delta_k^+ U_{k,l}^{(m)} - \frac{\mathrm{i}}{2k_c}\delta_l^{\langle 2\rangle}U_{k,l}^{(m)}\right|^2\right) + \frac{1}{4}\left(\left|\delta_k^- U_{k,l}^{(m+1)} - \frac{\mathrm{i}}{2k_c}\delta_l^{\langle 2\rangle}U_{k,l}^{(m+1)}\right|^2 + \left|\delta_k^- U_{k,l}^{(m)} - \frac{\mathrm{i}}{2k_c}\delta_l^{\langle 2\rangle}U_{k,l}^{(m)}\right|^2\right)\right\}\Delta x\Delta y. \quad (78)$$

From the discrete energy we obtain the finite-difference scheme as

$$\frac{U_{k,l}^{(m+1)} - U_{k,l}^{(m-1)}}{2\Delta t} = \mu U_{k,l}^{(m)} - \left|U_{k,l}^{(m)}\right|^2 \left(\frac{U_{k,l}^{(m+1)} + U_{k,l}^{(m-1)}}{2}\right) + \left(\delta_k^{\langle 2\rangle} - \frac{\mathrm{i}}{k_c}\delta_k^{\langle 1\rangle}\delta_l^{\langle 2\rangle} - \frac{1}{4k_c^2}\delta_l^{\langle 4\rangle}\right)\left(\frac{U_{k,l}^{(m+1)} + U_{k,l}^{(m-1)}}{2}\right). \quad (79)$$

This scheme seems to be new.

The scheme dissipates the energy under the periodic boundary condition as follows:

THEOREM 6.4 (discrete energy dissipation). *Let* $\boldsymbol{U}^{(m)}$ *be a solution of* (79) *with the periodic boundary condition* (59). *Then the global energy* H_{d} (78) *dissipates*, *that is,*

$$H_{\mathrm{d}}\left(\boldsymbol{U}^{(m+1)}, \boldsymbol{U}^{(m)}\right) \le H_{\mathrm{d}}\left(\boldsymbol{U}^{(m)}, \boldsymbol{U}^{(m-1)}\right) \qquad (m = 1, 2, 3, \ldots). \quad (80)$$

We present a simple numerical example of the Scheme (79). We borrowed a problem from Sakaguchi [13]. There all numerical calculations are done by discretizing in x and y by finite-difference method and integrating in time by the fourth-order Runge–Kutta method. We call it simply the "Runge–Kutta scheme." The initial data $u_0(x, y)$ and the other parameters are chosen to be same as those given in [13] (i.e., $k_c = \sqrt{\pi/2}$, $\mu = 27\pi^2/800$, $L_x = 40$, $L_y = 20$, $N_x = 120$, $N_y = 60$, and the initial state $u(0, x, y) = \sqrt{\mu - 9\pi/400}e^{-3\mathrm{i}\pi x/20}(1 + \mathrm{i} \cdot 0.0105e^{3\mathrm{i}\pi/10} + \mathrm{i} \cdot 0.0095e^{-3\mathrm{i}\pi/10})$). With these parameters the Eckhaus instability phenomena should occur and the reconnection process of the roll pattern proceeds until finally a stable oblique roll pattern emerges. In our scheme $\boldsymbol{U}^{(1)}$ needed to start computation is obtained by the Runge–Kutta scheme.

Figure 1 shows (a) the initial state ($t = 0$), (b) the final state ($t = 100$) obtained by the our scheme (79) with $\Delta t = 5$, and (c) the final state ($t = 100$) by the Runge–Kutta scheme with $\Delta t = 1/120$ which is ascertained to be the maximum size allowed for the scheme. In the figure the real part of the pattern $u(t, x, y)$ is plotted. Our scheme successfully obtained the right final pattern in spite of the extraordinary coarse time step width (600 times larger than that of the Runge–Kutta scheme).

Figure 2 shows the evolution of the discrete energy. For the Runge–Kutta scheme, which is not strictly dissipative, we computed H_{d} defined in (55) for comparison (the dashed line). The scheme is so sensitive to Δt that the energy suddenly blows up within a few steps when Δt exceeds the limit (i.e., $\Delta t > 1/120$; not shown in the figure). In our scheme H_{d} defined in (78) is plotted for two different Δt, namely $\Delta t = 5$ and $5/6$. According to the result in the figure, $\Delta t = 5/6$ is enough in our scheme to obtain the same result as the one by the Runge–Kutta scheme, which is 100 times larger than that of the Runge–Kutta scheme. When Δt is chosen extraordinary large ($\Delta t = 5$), the evolution becomes quite slow. But the scheme strictly dissipates the energy until it reaches the same final pattern as above, where the final energy is also the same as the one by the Runge–Kutta scheme (or by our scheme with fine mesh). The experiment assures us that our scheme is insensitive to Δt, i.e., numerically stable.

Table I shows the computation time of the each scheme. We used the COMPAQ w AlphaStation XP1000 (CPU: Alpha 21264, 500 MHz) and DIGITAL Fortran 77 V5.2 compiler. Each scheme is tested several times and the mean time is listed in the table.

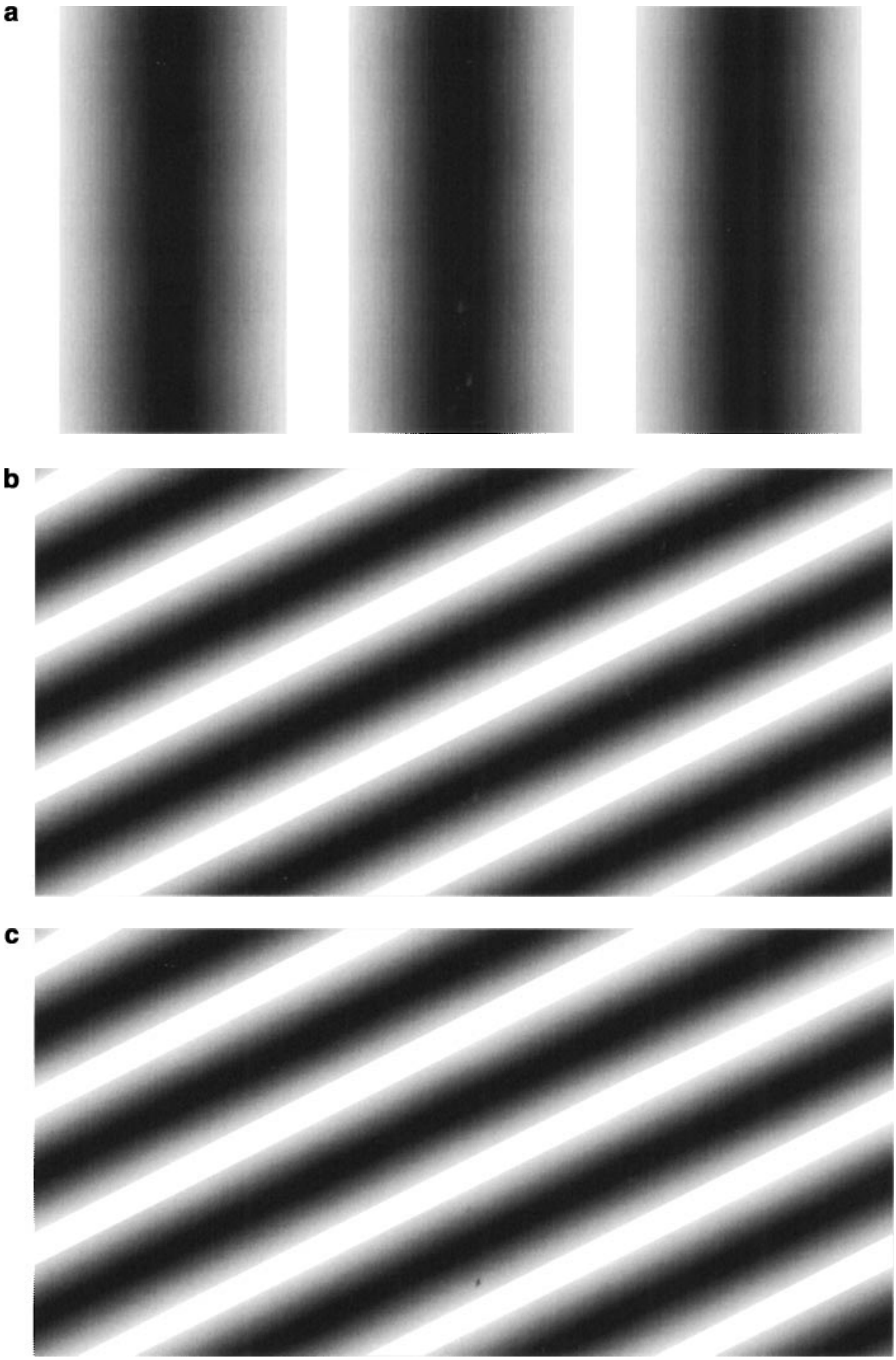

FIG. 1. Initial and final states for the NW problem. (a) Initial state; (b) final state by our scheme ($\Delta t = 5$); (c) final state by the Runge–Kutta scheme ($\Delta t = 1/120$).

According to the table our scheme is much faster than the Runge–Kutta scheme under the favor of the large Δt and the linearity of the scheme.

From the numerical experiment, we may conclude that the linearly implicit scheme is fast and stable.

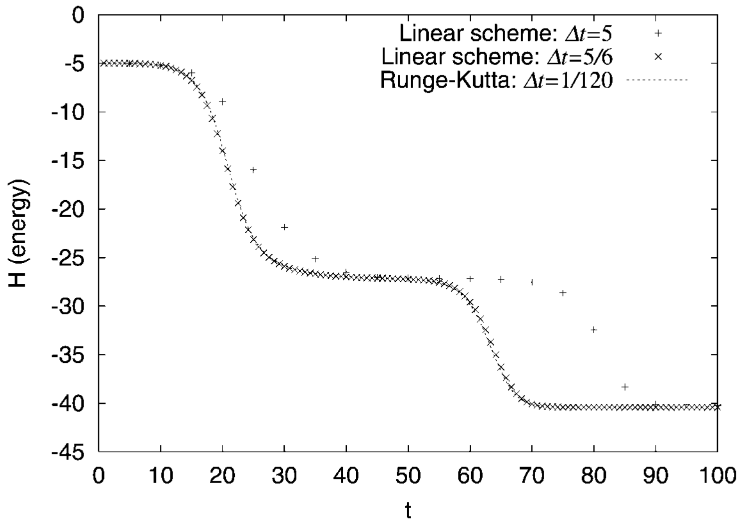

FIG. 2. Dissipation of the discrete energies.

6.4. *Remark—Linearly Implicit Schemes for the Real-Valued PDEs*

The modified procedure can also be applied to the real-valued PDEs with the nonlinearity of u^s $(s = 2, 3, \ldots)$, such as the real-valued Ginzburg–Landau equation (also known as the Kolmogorov–Fisher equation)

$$\frac{\partial}{\partial t}u(x,t) = pu_{xx} + qu^s + ru \quad (x \in [0, L], t > 0, s = 2, 3, \ldots, p > 0, q < 0, r \in \mathbf{R}), \tag{81}$$

the (real-valued) Swift–Hohenberg equation

$$\frac{\partial}{\partial t}u(x,t) = \varepsilon u - u^4 - u^6 - \left(\frac{\partial^2}{\partial x^2} + k_c^2\right)^2 u \qquad (x \in [0, L], t > 0, \varepsilon, k_c \in \mathbf{R}), \tag{82}$$

and the Cahn–Hilliard equation

$$\frac{\partial}{\partial t}u(x,t) = \frac{\partial^2}{\partial x^2}(pu + ru^3 + qu_{xx}) \qquad (x \in [0, L], t > 0, p < 0, q < 0, r > 0). \tag{83}$$

To design linearly implicit schemes for them, just decompose u^s to

$$\left(U_k^{(m+1)}\right)^2 \left(U_k^{(m)}\right)^2 \cdots \left(U_k^{(m-\frac{s}{2}+2)}\right)^2, \qquad \text{if } s \text{ is even}, \tag{84a}$$

$$U_k^{(m+1)} U_k^{(m)} \cdots U_k^{(m-s+2)}, \qquad \text{otherwise}, \tag{84b}$$

and consider the multiple points discrete variational derivatives accordingly.

TABLE I
Computation Time in Each Scheme (Unit: Second)

Runge–Kutta scheme	Our scheme ($\Delta t = 5$)	Our scheme ($\Delta t = 5/6$)
125	27.8	45.2

The detail of the derivation procedure and the proof of the dissipation properties are straightforward and hence omitted here. But it is worth mentioning that a linearly implicit scheme for the Cahn–Hilliard equation designed by the modified procedure is unconditionally stable and L_2-convergent [6]. This is a little surprising result, since the Cahn–Hilliard equation is known to be a hard problem for numerical methods, and even the *nonlinear* finite-difference scheme, which we formerly proposed in Furihata [5] and showed to be stable and convergent, was a big achievement.

Here we briefly comment on the derivation of the scheme (see [6] for the detailed analysis). The local energy G for the Cahn–Hilliard equation is

$$G(u, u_x) = \frac{1}{2}pu^2 + \frac{1}{4}ru^4 - \frac{1}{2}q(u_x)^2, \tag{85}$$

and Eq. (83) is defined as

$$\frac{\partial u}{\partial t} = \frac{\partial^2}{\partial x^2}\left(\frac{\delta G}{\delta u}\right). \tag{86}$$

To obtain a linearly implicit scheme we define the local energy as

$$\begin{aligned} G_{\mathrm{d}}\left(\boldsymbol{U}^{(m+1)}, \boldsymbol{U}^{(m)}\right)_k \stackrel{\mathrm{d}}{\equiv} &\frac{1}{2}pU_k^{(m+1)}U_k^{(m)} + \frac{1}{4}r\left(U_k^{(m+1)}\right)^2\left(U_k^{(m)}\right)^2 \\ &- \frac{1}{2}q\left(\frac{\left(\delta_k^+ U_k^{(m+1)}\right)^2 + \left(\delta_k^- U_k^{(m+1)}\right)^2 + \left(\delta_k^+ U_k^{(m)}\right)^2 + \left(\delta_k^- U_k^{(m)}\right)^2}{4}\right). \end{aligned} \tag{87}$$

Note that the nonlinear term $\frac{1}{4}ru^4$ is decomposed to $\frac{1}{4}r(U_k^{(m+1)})^2(U_k^{(m)})^2$ according to the rule (84a). The linear terms are also decomposed appropriately. The global energy is defined as

$$H_{\mathrm{d}}\left(\boldsymbol{U}^{(m+1)}, \boldsymbol{U}^{(m)}\right) \stackrel{\mathrm{d}}{\equiv} \sum_{k=0}^{N}{}'' G_{\mathrm{d}}\left(\boldsymbol{U}^{(m+1)}, \boldsymbol{U}^{(m)}\right)_k \Delta x. \tag{88}$$

The three points discrete variational derivative $\delta G_{\mathrm{d}}/\delta(\boldsymbol{U}^{(m+1)}, \boldsymbol{U}^{(m)}, \boldsymbol{U}^{(m-1)})$ is defined in like manner as the complex one. The scheme is defined with it as

$$\begin{aligned} \frac{U_k^{(m+1)} - U_k^{(m-1)}}{2\Delta t} &= \delta_k^{\langle 2\rangle}\left(\frac{\delta G_{\mathrm{d}}}{\delta\left(\boldsymbol{U}^{(m+1)}, \boldsymbol{U}^{(m)}, \boldsymbol{U}^{(m-1)}\right)_k}\right) \\ &= \delta_k^{\langle 2\rangle}\left\{pU_k^{(m)} + r\left(\frac{U_k^{(m+1)} + U_k^{(m-1)}}{2}\right)\left(U_k^{(m)}\right)^2 \right. \\ &\qquad \left. + q\delta_k^{\langle 2\rangle}\left(\frac{U_k^{(m+1)} + U_k^{(m-1)}}{2}\right)\right\}. \end{aligned} \tag{89}$$

7. CONCLUSIONS AND COMMENTS

We proposed a new procedure for designing finite-difference schemes that inherit energy conservation or dissipation property from complex-valued PDEs. The resulting schemes are generally nonlinear, but they can be solved adaptively in time. We also modified the procedure so that linearly implicit schemes can be designed without losing the properties. Some of the well-known finite-difference schemes for the NLS equation such as Delfour's and Fei's scheme can be regarded as particular results of the proposed procedures. The schemes for the CGL and NW are all new and the linearly implicit scheme for the NW is proven to be efficient by a numerical experiment.

A possible claim to the presented procedure, however, may be that it suffers from the restriction that it is limited to essentially one-dimensional problems on uniform spatial meshes, and more complex domains or the use of nonuniform meshes are out of its scope. But the techniques employed in this paper are basically also useful when we utilize finite elements instead of finite differences and that could solve the problem. We are now working on this issue and are going to present the result in the near future.

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