# Linearly Implicit Finite Difference Schemes Derived by the Discrete Variational Method 

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## 1 Introduction

In $[2,3]$ we devised a＂discrete＂variational method which can be regarded as a discrete version of the variational method and thereby gave a general procedure to design finite difference schemes that inherit the energy conservation or dissipation property from nonlinear partial differential equations，such as the K－dV equation，the Cahn－ Hilliard equation，and the nonlinear Schrödinger equation（NLS for short）．And we proved numerically that the derived schemes are stable and give good approximation of the exact solutions．However it also turned out that the derived schemes involve a drawback，that is，they require a huge number of iterative computations due to their nonlinearity．

We will here give a basic idea to design finite difference schemes without the draw－ $b a c k$ ，i．e．，linearly implicit finite difference schemes that inherit the energy conservation or dissipation property from the original equations．The key is to introduce a new concept＂multiple points discrete variational derivative＂into the discrete variational method．The idea is applicable to the nonlinear PDEs which have the nonlinearity of $|u|^{2 s} u \quad(s=1,2, \cdots)$（when the solution is complex－valued）such as the NLS，the Ginzburg－Landau equation and the Newell－Whitehead equation，or of $u^{s}$（when real－ valued）such as the Cahn－Hilliard equation．

In this note we first pick up the 1－dimensional cubic NLS for example to illustrate how a linearly implicit finite difference scheme can be derived．Then we briefly treat the

[^0]generalization to the other cases. The contents of this note is as follows : in the section 2 the cubic NLS problem is defined; in the section 3 symbols are defined and some discrete calculus is described; in the section 4 we shortly review the conventional (formerly proposed) discrete variational method and the nonlinear scheme for the NLS derived by the method; in the section 5, the "three points discrete variational derivative", which is a generalization of the conventional discrete variational derivative, is introduced and a linearly implicit finite difference scheme for the NLS is derived; in the section 6 , the discrete variational derivative is further generalized to "multiple points" ones and the general $|u|^{2 s} u$ (or $u^{s}$ ) case is discussed; the section 7 is for concluding remarks.

## 2 The 1-dimensional cubic NLS

Here we review the variational formulation of the 1-dimensional cubic NLS.
Let us consider the Cauchy problem of the 1-dimensional cubic NLS:

$$
\begin{align*}
\frac{\partial}{\partial t} u(x, t) & =\mathrm{i} \frac{\partial^{2}}{\partial x^{2}} u+\mathrm{i} \gamma|u|^{2} u,  \tag{1}\\
u(x, 0) & =u_{0}(x) \tag{2}
\end{align*} \quad t>0, x \in[-L, L], \quad \gamma \in \mathbf{R},
$$

under the periodic boundary condition

$$
\left\{\begin{array}{ccc}
u(x, t) & =u(x+2 L, t)  \tag{3}\\
\frac{\partial}{\partial x} u(x, t) & =\frac{\partial}{\partial x} u(x+2 L, t) .
\end{array}\right.
$$

It is well known that the NLS has the following two conserved quantities:
[energy]

$$
\begin{equation*}
H=\int_{-L}^{L}\left|u_{x}\right|^{2}-\frac{\gamma}{2}|u|^{4} \mathrm{~d} x=\text { const. } \tag{4}
\end{equation*}
$$

[probability]

$$
\begin{equation*}
P=\int_{-L}^{L}|u|^{2} \mathrm{~d} x=\text { const. } \tag{5}
\end{equation*}
$$

Taking the variation of the energy H we have:

$$
\begin{align*}
H(u+\delta u)-H(u) & =\int_{-L}^{L}\left(\left(-\overline{u_{x x}}-\gamma|u|^{2} \bar{u}\right) \delta u+\left(-u_{x x}-\gamma|u|^{2} u\right) \delta \bar{u}\right) \mathrm{d} x+O\left((\delta u)^{2}\right) \\
& \stackrel{\mathrm{d}}{\equiv} \int_{-L}^{L}\left(\frac{\delta H}{\delta u} \delta u+\frac{\delta H}{\delta \bar{u}} \delta \bar{u}\right) \mathrm{d} x+O\left((\delta u)^{2}\right) \tag{6}
\end{align*}
$$

where $\delta H / \delta \bar{u}, \delta H / \delta u$ are the variational derivatives. With the variational derivatives we can obtain the NLS:

$$
\begin{equation*}
\mathrm{i} u_{t}=\frac{\delta H}{\delta \bar{u}}=-u_{x x}-\gamma|u|^{2} u \tag{7}
\end{equation*}
$$

## 3 Notations and discrete calculus

Throughout this note we use the following notations and the discrete calculus.
[Numerical solution]

$$
\begin{equation*}
U_{k}^{(m)} \simeq u(k \Delta x, m \Delta t), \quad(0 \leq k \leq N-1, m=0,1,2, \cdots), \tag{8}
\end{equation*}
$$

where $\Delta x \stackrel{\mathrm{~d}}{\equiv} 2 L / N, \Delta t>0$ is the mesh size in $x, t$, respectively. The time step ( $m$ ) may be omitted where it can be. The periodic boundary condition (3) is treated as:

$$
\begin{equation*}
U_{k}^{(m)}=U_{k+N}^{(m)}, \quad(0 \leq k \leq N-1, m=0,1,2, \cdots) \tag{9}
\end{equation*}
$$

[Difference operator]

$$
\begin{array}{rll}
\delta^{+} U_{k} & \stackrel{\mathrm{~d}}{\equiv} \quad \frac{U_{k+1}-U_{k}}{\Delta x} \\
\delta^{-} U_{k} & \stackrel{\mathrm{~d}}{\equiv} & \frac{U_{k}-U_{k-1}}{\Delta x} \\
\delta^{(2)} U_{k} & \stackrel{\mathrm{~d}}{\equiv} & \frac{U_{k+1}-2 U_{k}+U_{k-1}}{\Delta x^{2}} \tag{12}
\end{array}
$$

The following equality is analogous to the integration-by-part equality in usual calculus, and holds for any two sequences $U_{k}, V_{k}$ (for the proof, see [2]). It may be instructive to point out that the remainder term [.] at the right hand side vanishes when the (discrete) periodic boundary condition $U_{k}=U_{k+N}$ or $V_{k}=V_{k+N}$ is applied.
[Summation by part]

$$
\begin{equation*}
\sum_{k=0}^{N-1} \delta^{+} U_{k} \delta^{+} V_{k} \Delta x=-\sum_{k=0}^{N-1}\left(\delta^{(2)} U_{k}\right) V_{k} \Delta x+\left[\left(\delta^{+} U_{N-1}\right) V_{N}-\left(\delta^{+} U_{-1}\right) V_{0}\right] \tag{13}
\end{equation*}
$$

## 4 Derivation of the nonlinear scheme for the NLS - the conventional discrete variational method[3]

In this section we briefly review the conventional discrete variational method and the resulting nonlinear finite difference scheme for the NLS.

In the discrete variational method, first we define some discrete energy analogous to the continuous one (4), and next take its (discrete) variation to obtain a finite difference scheme.

The most straightforward definition of the discrete energy, $H_{d}$, may be the following which only uses the numerical solution at one time step:

$$
\begin{equation*}
H_{\mathrm{d}}\left(\boldsymbol{U}^{(m)}\right) \equiv \sum_{k=0}^{N-1}\left\{\left|\delta^{+} U_{k}^{(m)}\right|^{2}-\frac{\gamma}{2}\left|U_{k}^{(m)}\right|^{4}\right\} \Delta x \tag{14}
\end{equation*}
$$

And consider the difference between energies at two consecutive time steps:

$$
\begin{align*}
& H_{\mathrm{d}}\left(\boldsymbol{U}^{(m+1)}\right)-H_{\mathrm{d}}\left(\boldsymbol{U}^{(m)}\right) \\
& =\sum_{k=0}^{N-1}\left\{\left(\left|\delta^{+} U_{k}^{(m+1)}\right|^{2}-\left|\delta^{+} U_{k}^{(m)}\right|^{2}\right)-\frac{\gamma}{2}\left(\left|U_{k}^{(m+1)}\right|^{4}-\left|U_{k}^{(m)}\right|^{4}\right)\right\} \Delta x \\
& =\sum_{k=0}^{N-1}\left[\left\{\frac{1}{2} \delta^{+} \overline{\left(U_{k}^{(m+1)}+U_{k}^{(m)}\right)} \delta^{+}\left(U_{k}^{(m+1)}-U_{k}^{(m)}\right)\right.\right. \\
& \left.-\frac{\gamma}{4}\left(\overline{U_{k}^{(m+1)}+U_{k}^{(m)}}\right)\left(\left|U_{k}^{(m+1)}\right|^{2}+\left|U_{k}^{(m)}\right|^{2}\right)\left(U_{k}^{(m+1)}-U_{k}^{(m)}\right)\right\} \\
& +\left\{\frac{1}{2} \delta^{+}\left(U_{k}^{(m+1)}+U_{k}^{(m)}\right) \delta^{+}\left(\overline{U_{k}^{(m+1)}-U_{k}^{(m)}}\right)\right. \\
& \left.-\frac{\gamma}{4}\left(U_{k}^{(m+1)}+U_{k}^{(m)}\right)\left(\left|U_{k}^{(m+1)}\right|^{2}+\left|U_{k}^{(m)}\right|^{2}\right)\left(\overline{\left.U_{k}^{(m+1)}-U_{k}^{(m)}\right)}\right\}\right] \Delta x \\
& =\sum_{k=0}^{N-1}\left[\left\{-\frac{1}{2} \delta^{(2)} \overline{\left(U_{k}^{(m+1)}+U_{k}^{(m)}\right.}\right)-\frac{\gamma}{4}\left(\overline{U_{k}^{(m+1)}+U_{k}^{(m)}}\right)\left(\left|U_{k}^{(m+1)}\right|^{2}+\left|U_{k}^{(m)}\right|^{2}\right)\right\}\left(U_{k}^{(m+1)}-U_{k}^{(m)}\right) \\
& \left.\left.+\left\{-\frac{1}{2} \delta^{(2)}\left(U_{k}^{(m+1)}+U_{k}^{(m)}\right)-\frac{\gamma}{4}\left(U_{k}^{(m+1)}+U_{k}^{(m)}\right)\left(\left|U_{k}^{(m+1)}\right|^{2}+\left|U_{k}^{(m)}\right|^{2}\right)\right\} \overline{\left(U_{k}^{(m+1)}-U_{k}^{(m)}\right.}\right)\right] \Delta x \\
& \stackrel{\mathrm{~d}}{\equiv} \sum_{k=0}^{N-1}\left\{\frac{\delta H_{\mathrm{d}}}{\delta\left(U_{k}^{(m)}, U_{k}^{(m+1)}\right)}\left(U_{k}^{(m+1)}-U_{k}^{(m)}\right)+\frac{\delta H_{\mathrm{d}}}{\delta\left(\overline{U_{k}^{(m)}}, \overline{U_{k}^{(m+1)}}\right)}\left(\overline{\left.U_{k}^{(m+1)}-U_{k}^{(m)}\right)}\right\} \Delta x\right. \text {. } \tag{15}
\end{align*}
$$

The above calculation is completely analogous to the continuous case (6), and the summation-by-part equality (13) is used in the third equality. The last equality is not a transformation, but a definition, which defines the "discrete variational derivative" $\delta H_{\mathrm{d}} / \delta\left(U_{k}^{(m)}, U_{k}^{(m+1)}\right)$, which is analogous to the variational derivative $\delta H / \delta u$.

Once we have the discrete variational derivative, we obtain the discrete NLS equation, i.e., the finite difference scheme for the NLS, as follows:

## Nonlinear finite difference scheme

For $m=0,1,2, \cdots$,

$$
\begin{align*}
\mathrm{i} \frac{U_{k}^{(m+1)}-U_{k}^{(m)}}{\Delta t} & =\frac{\delta H_{\mathrm{d}}}{\delta\left(\overline{U_{k}^{(m)}}, \overline{U_{k}^{(m+1)}}\right)}  \tag{16}\\
& =-\frac{1}{2} \delta^{(2)}\left(U_{k}^{(m+1)}+U_{k}^{(m)}\right)-\frac{\gamma}{4}\left(U_{k}^{(m+1)}+U_{k}^{(m)}\right)\left(\left|U_{k}^{(m+1)}\right|^{2}+\left|U_{k}^{(m)}\right|^{2}\right)
\end{align*}
$$

where $U_{k}^{(m)}=U_{k+N}^{(m)}(0 \leq k \leq N-1)$.
Because this scheme is nonlinear with regard to $U_{k}^{(m+1)}$ this is not trivial whether $U_{k}^{(m+1)}$ exists or not. If $\Delta t$ is chosen to be small enough, however, it is guaranteed that there exists an unique solution. And moreover, the solution conserves the discrete versions of the energy and the probability.

Theorem 1 (Discrete energy conservation[3]) The solution of the nonlinear scheme (17) conserves the discrete energy. That is,

$$
\begin{equation*}
H_{d}\left(\boldsymbol{U}^{(m)}\right)=\sum_{k=0}^{N-1}\left\{\left|\delta^{+} U_{k}^{(m)}\right|^{2}-\frac{\gamma}{2}\left|U_{k}^{(m)}\right|^{4}\right\} \Delta x=\text { const. }, \quad(m=0,1,2, \cdots) \tag{17}
\end{equation*}
$$

Theorem 2 (Discrete probability conservation[3]) The solution of the nonlinear scheme (17) conserves the discrete probability, in the sense that

$$
\begin{equation*}
\sum_{k=0}^{N-1}\left|U_{k}^{(m)}\right|^{2} \Delta x=\text { const., } \quad(m=0,1,2, \cdots) \tag{18}
\end{equation*}
$$

With the discrete conservation laws we can establish the convergence result for the numerical solution (i.e., for any fixed $T=m \Delta t>0, U_{k}^{(m)} \rightarrow u(x, T)$ as $\left.\Delta t, \Delta x \rightarrow 0\right)[3]$.

## 5 Derivation of the linearly implicit scheme for the NLS- the discrete variational method with linearization technique

To obtain a linearly implicit scheme, it is essential to understand the reason why the resulting scheme becomes nonlinear, or more precisely, the mechanism how the nonlinearity in the energy is passed down to the equation through the variation calculation. In the case of the continuous cubic NLS, the $|u|^{4}$ term in the energy $H(u)$ is the source of the nonlinear term $|u|^{2} u$. In general, the power of the nonlinearity in the energy is always 1 higher than that of the resulting nonlinearity, and so we easily come to the conclusion that if we want the resulting scheme to be linear we must reduce the power of the nonlinearity in the energy to 2 , at most. In the above cubic NLS case $(s=1)$, for example, decomposing $\left|U_{k}^{(m)}\right|^{4}$ to $\left|U_{k}^{(m+1)}\right|^{2}\left|U_{k}^{(m)}\right|^{2}$ will do and the corresponding part of the discrete variation calculation becomes:

$$
\begin{align*}
& \left|U_{k}^{(m+1)}\right|^{2}\left|U_{k}^{(m)}\right|^{2}-\left|U_{k}^{(m)}\right|^{2}\left|U_{k}^{(m-1)}\right|^{2}=  \tag{19}\\
& \quad\left|U_{k}^{(m)}\right|^{2} \frac{U_{k}^{(m+1)}+U_{k}^{(m-1)}}{2}\left(\overline{U_{k}^{(m+1)}-U_{k}^{(m-1)}}\right)+\left|U_{k}^{(m)}\right|^{2} \frac{\overline{U_{k}^{(m+1)}+U_{k}^{(m-1)}}}{2}\left(U_{k}^{(m+1)}-U_{k}^{(m-1)}\right) .
\end{align*}
$$

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

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

$$
\begin{equation*}
H_{\mathrm{d}}\left(\boldsymbol{U}^{(m)}, \boldsymbol{U}^{(m+1)}\right) \stackrel{\mathrm{d}}{\equiv} \sum_{k=0}^{N-1} \frac{1}{2}\left(\left|\delta^{+} U_{k}^{(m+1)}\right|^{2}+\left|\delta^{+} U_{k}^{(m)}\right|^{2}\right) \Delta x-\frac{\gamma}{2} \sum_{k=0}^{N-1}\left|U_{k}^{(m+1)}\right|^{2}\left|U_{k}^{(m)}\right|^{2} \Delta x . \tag{20}
\end{equation*}
$$

Taking its variation:

$$
\begin{align*}
& H_{\mathrm{d}}\left(\boldsymbol{U}^{(m+1)}, \boldsymbol{U}^{(m)}\right)-H_{\mathrm{d}}\left(\boldsymbol{U}^{(m)}, \boldsymbol{U}^{(m-1)}\right)=  \tag{21}\\
& \quad \frac{\delta H_{\mathrm{d}}}{\delta\left(U_{k}^{(m+1)}, U_{k}^{(m)}, U_{k}^{(m-1)}\right)} \frac{U_{k}^{(m+1)}-U_{k}^{(m-1)}}{2}+\frac{(21)}{\delta\left(\overline{U_{k}^{(m+1)}}, \overline{U_{\mathrm{d}}^{(m)}}, \overline{U_{k}^{(m-1)}}\right)} \frac{\overline{U_{k}^{(m+1)}-U_{k}^{(m-1)}}}{2}
\end{align*}
$$

where

$$
\begin{align*}
& \frac{\delta H_{\mathrm{d}}}{\delta\left(U_{k}^{(m+1)}, U_{k}^{(m)}, U_{k}^{(m-1)}\right)}=-\frac{1}{2} \delta^{(2)}\left(\overline{U_{k}^{(m+1)}+U_{k}^{(m-1)}}\right)-\frac{\gamma}{2}\left|U_{k}^{(m)}\right|^{2}\left(\overline{U_{k}^{(m+1)}+U_{k}^{(m-1)}}\right)  \tag{22}\\
& \frac{\delta \overline{U_{\mathrm{d}}}}{\delta\left(\overline{U_{k}^{(m+1)}}, \overline{U_{k}^{(m)}}, \overline{U_{k}^{(m-1)}}\right)}=\frac{\delta H_{\mathrm{d}}}{\delta\left(U_{k}^{(m+1)}, U_{k}^{(m)}, U_{k}^{(m-1)}\right)}, \tag{23}
\end{align*}
$$

are "three points discrete variational derivatives", which can be regarded as a generalization of the conventional (or "two points") discrete variational derivatives.

With them we can now define a linearly implicit finite difference scheme as:

## Linearly implicit finite difference scheme

For $m=1,2, \cdots$,

$$
\begin{align*}
\mathrm{i} \frac{U_{k}^{(m+1)}-U_{k}^{(m-1)}}{2 \Delta t} & =\frac{\delta H}{\delta\left(\overline{U_{k}^{(m+1)}}, \overline{U_{k}^{(m)}}, \overline{U_{k}^{(m-1)}}\right)}  \tag{24}\\
& =-\frac{1}{2} \delta^{(2)}\left(U_{k}^{(m+1)}+U_{k}^{(m-1)}\right)-\frac{\gamma}{2}\left|U_{k}^{(m)}\right|^{2}\left(U_{k}^{(m+1)}+U_{k}^{(m-1)}\right)
\end{align*}
$$

where $U_{k}^{(m)}=U_{k+N}^{(m)}(0 \leq k \leq N-1)$.
This is the same scheme as Fei[1] proposed. Fei also proved that the following two quantities are conserved by the scheme (24), but he did not mention the derivation of the scheme and the reason why the energy is conserved. Now it can be interpreted as one special example of the discrete variational method (with linearization technique) and therefore the conservation of the discrete energy is a quite natural result.

Theorem 3 (Discrete energy conservation[1]) The solution of the linearly implicit scheme (24) conserves the discrete energy. That is,

$$
\begin{equation*}
H_{\mathrm{d}}\left(\boldsymbol{U}^{(m)}, \boldsymbol{U}^{(m+1)}\right)=\text { const., } \quad(m=0,1,2, \cdots) \tag{25}
\end{equation*}
$$

The conservation of the probability which is defined as follows is not that trivial, however.

Theorem 4 (Discrete probability conservation[1]) The solution of the linearly implicit scheme (24) conserves the discrete probability, in the sense that

$$
\begin{equation*}
\sum_{k=0}^{N-1} \frac{\left|U_{k}^{(m+1)}\right|^{2}+\left|U_{k}^{(m)}\right|^{2}}{2} \Delta x=\text { const., } \quad(m=0,1,2, \cdots) \tag{26}
\end{equation*}
$$

With these conservation laws Fei also proved that the solution of the scheme (24) converges to the exact solution $u(x, T)$, like as the case of the nonlinear scheme. And the numerical solution is bounded $\left(\sup _{k, m}\left|U_{k}^{(m)}\right|<\infty\right)$ aside from the rounding errors. This does not necessarily imply that the numerical solution should remain stable practically, but according to our numerical experiments there was no problem as regards the stability.

Because the scheme (24) is linear with regard to $U_{k}^{(m)}$, we only need to solve a linear system at each time step, and therefore it is much faster than the nonlinear scheme (17) which needs quite a number of iterative calculations. But here arises a new minor drawback that we need not only $\boldsymbol{U}^{(0)}$ which is given by the initial data $u_{0}(x)$ but also $\boldsymbol{U}^{(1)}$ to start calculation, and which should be calculated by other integrating schemes such as the Runge-Kutta method. Yet again this seems not serious problem according to our numerical experiments.

## 6 Further generalizations and applications

In this section, we briefly mention the treatment of the higher order nonlinearities with several examples of applicable nonlinear PDEs.

The key of the above linearization is the three points discrete variational derivatives. That can be further generalized to the multiple points discrete variational derivatives ${ }^{1}$ so that higher order nonlinearities can be resolved. In this note we discuss the following two kinds of nonlinearities: (a) $|u|^{2 s} u$ (when $u$ is complex-valued), and (b) $u^{s}$ (when real-valued).

## $6.1|u|^{2 s} u(s=1,2, \cdots)$ (complex-valued case)

Not only the above cubic NLS $(s=1)$ but the following equations have the nonlinearity of this kind, and linearly implicit finite difference schemes can be derived by decomposing $\left|U_{k}^{(m)}\right|^{2 s+2}$ (in the energy) into $\left|U_{k}^{(m+1)}\right|^{2}\left|U_{k}^{(m)}\right|^{2} \cdots\left|U_{k}^{(m-s+1)}\right|^{2}$.
[The higher order NLS] (including cubic case)

$$
\begin{equation*}
\frac{\partial}{\partial t} u(x, t)=\mathrm{i} \frac{\partial^{2}}{\partial x^{2}} u+\mathrm{i} \gamma|u|^{2 s} u, \quad(s=1,2,3, \cdots) \tag{27}
\end{equation*}
$$

The discrete energy should be defined as:

$$
\begin{align*}
& H_{\mathrm{d}}\left(\boldsymbol{U}^{(m+1)}, \boldsymbol{U}^{(m)}, \cdots, \boldsymbol{U}^{(m-s+1)} \stackrel{\mathrm{d}}{\equiv}\right.  \tag{28}\\
& \quad \sum_{k=0}^{N-1}\left\{\frac{\left|\delta^{+} U_{k}^{(m+1)}\right|^{2}+\left|\delta^{+} U_{k}^{(m)}\right|^{2}+\cdots+\left|\delta^{+} U_{k}^{(m-s+1)}\right|^{2}}{s+1}+\left|U_{k}^{(m+1)}\right|^{2}\left|U_{k}^{(m)}\right|^{2} \cdots\left|U_{k}^{(m-s+1)}\right|^{2}\right\} \Delta x .
\end{align*}
$$

Through the discrete variation calculation we have:

$$
\begin{align*}
& \mathrm{i} \frac{U_{k}^{(m+1)}-U_{k}^{(m-s)}}{(s+1) \Delta t} \\
& =\frac{\delta H}{\delta\left(\overline{U_{k}^{(m+1)}}, \overline{U_{k}^{(m)}}, \cdots, \overline{U_{k}^{(m-s)}}\right)}  \tag{29}\\
& \quad=-\frac{1}{2} \delta^{(2)}\left(U_{k}^{(m+1)}+U_{k}^{(m-s)}\right)-\frac{\gamma}{2}\left|U_{k}^{(m)}\right|^{2}\left|U_{k}^{(m-1)}\right|^{2} \cdots\left|U_{k}^{(m-s+1)}\right|^{2}\left(U_{k}^{(m+1)}+U_{k}^{(m-s)}\right)
\end{align*}
$$

The resulting scheme depends on the solutions at $s+2$ time steps and linear as to $U_{k}^{(m+1)}$. This scheme conserves the discrete energy, and the probability as follows.

Theorem 5 (Discrete energy conservation) The solution of the linearly implicit scheme (29) conserves the discrete energy. That is,

$$
\begin{equation*}
H_{\mathrm{d}}\left(\boldsymbol{U}^{(m+1)}, \boldsymbol{U}^{(m)}, \cdots, \boldsymbol{U}^{(m-s+1)}\right)=\text { const., } \quad(m=s-1, s, s+1, \cdots) \tag{30}
\end{equation*}
$$

[^1]Theorem 6 (Discrete probability conservation) The solution of the linearly implicit scheme (29) conserves the discrete probability, in the sense that:

$$
\sum_{k=0}^{N-1} \frac{\left|U_{k}^{(m+1)}\right|^{2}+\left|U_{k}^{(m-s)}\right|^{2}}{2} \Delta x=\text { const., } \quad(m=s, s+1, s+2, \cdots)
$$

## [Ginzburg-Landau type equations]

Some of the Ginzburg-Landau type equations such as the real-coefficient complexvalued Ginzburg-Landau equation:

$$
\begin{equation*}
\frac{\partial}{\partial t} u(x, t)=p \frac{\partial^{2}}{\partial x^{2}} u+q|u|^{2 s} u+r u, \quad(s=1,2,3, \cdots, p>0, q<0, r \in \mathbf{R}) \tag{31}
\end{equation*}
$$

and the 2-dimensional Newell-Whitehead equation:

$$
\begin{equation*}
\frac{\partial}{\partial t} u(x, y, t)=\mu u-|u|^{2} u+\left(\frac{\partial}{\partial x}-\frac{\mathrm{i}}{2 k_{c}} \frac{\partial^{2}}{\partial y^{2}}\right)^{2} u, \quad\left(\mu, k_{c} \in \mathbf{R}\right) \tag{32}
\end{equation*}
$$

can be written with their variational derivatives as:

$$
\begin{equation*}
\frac{\partial}{\partial t} u=-\frac{\delta H}{\delta \bar{u}} \tag{33}
\end{equation*}
$$

where

$$
H(u) \stackrel{\mathrm{d}}{\equiv}\left\{\begin{array}{cc}
\int_{-L}^{L} p\left|u_{x}\right|^{2}-\frac{q}{2}|u|^{4}-r|u|^{2} \mathrm{~d} x, & \text { for (31) }  \tag{34}\\
\int_{-L}^{L} L_{-L}^{L}\left(-\mu|u|^{2}+\frac{1}{2}|u|^{4}+\left|u_{x}-\frac{i}{2 k_{c}} u_{y y}\right|^{2}\right) \mathrm{d} x \mathrm{~d} y, & \text { for (32). }
\end{array}\right.
$$

It is very straightforward to see that they are dissipative, that is:

$$
\begin{equation*}
\frac{\mathrm{d}}{\mathrm{~d} t} H(u) \leq 0 . \tag{35}
\end{equation*}
$$

The nonlinear or the linearly implicit finite difference schemes for the equations can be derived by the conventional or the linearizing discrete variational methods in like manner, and the resulting schemes dissipate the corresponding discrete energies. It is very straightforward so the details are omitted here.

## $6.2 u^{s}(s=2,3, \cdots)$ (real-valued case)

For example, the real-valued Ginzburg-Landau equation (also known as the KolmogorovFisher equation):

$$
\begin{equation*}
\frac{\partial}{\partial t} u(x, t)=p \frac{\partial^{2}}{\partial x^{2}} u+q u^{s}+r u, \quad(s=2,3, \cdots, p>0, q<0, r \in \mathbf{R}) \tag{36}
\end{equation*}
$$

the (real-valued) Swift-Hohenberg equation:

$$
\begin{equation*}
\frac{\partial}{\partial t} u(x, t)=\varepsilon u-u^{4}-u^{6}-\left(\frac{\partial^{2}}{\partial x^{2}}+k_{c}^{2}\right) u, \quad\left(\varepsilon, k_{c} \in \mathbf{R}\right) \tag{37}
\end{equation*}
$$

and the Cahn-Hilliard equation:

$$
\begin{equation*}
\frac{\partial}{\partial t} u(x, t)=\frac{\partial^{2}}{\partial x^{2}}\left(p u+r u^{3}+q \frac{\partial u}{\partial x^{2}}\right), \quad(p<0, q<0, r>0) . \tag{38}
\end{equation*}
$$

belong to this class of equations, and all dissipative. To derive linearly implicit schemes, just decompose $u^{s}$ to:

$$
\begin{align*}
\left(U_{k}^{(m+1)}\right)^{2}\left(U_{k}^{(m)}\right)^{2} \cdots\left(U_{k}^{\left(m-\frac{s}{2}+2\right)}\right)^{2}, & \text { if } s \text { is even }  \tag{39}\\
U_{k}^{(m+1)} U_{k}^{(m)} \cdots U_{k}^{(m-s+2)}, & \text { otherwise } \tag{40}
\end{align*}
$$

The details of the derivation and the proof of the dissipation property are again straightforward and therefore omitted here.

But it is worth mentioning that in the case of the Cahn-Hilliard equation, a linearly implicit scheme that is derived by the linearizing discrete variational method is unconditionally stable, and the solution of the scheme converge to the exact solution. 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[2] and showed it to be stable and convergent, was a big achievement. We are now preparing for the publication of the newly developed linearly implicit scheme. It will be available in the near future.

## 7 Concluding remarks

A linearization technique with multiple points discrete variational derivatives is built into the discrete variational method, and that gave an unified procedure to design linearly implicit finite difference schemes that inherit energy conservation or dissipation property from the original nonlinear PDEs.

Many similar linearizations by multi-stage technique are known in literature, but it is also known that careless linearization make numerical solution unstable. We hope the conservation or dissipation property that is inherited from the original equation helps stabilizing numerical solutions, still unfortunately it seems not enough in general. We are intensively working on this problem.

## References

[1] Fei,Z., Pérez-García,V.M., and Vázquez,L., Numerical Simulation of Nonlinear Schrödinger Systems: A New Conservative Scheme, Appl. Math. Comput., 71(1995), 165-177.
[2] Furihata, D., Finite Difference Schemes for $\frac{\partial u}{\partial t}=\left(\frac{\partial}{\partial x}\right)^{\alpha} \frac{\delta G}{\delta u}$ That Inherit Energy Conservation or Dissipation Property, J. Comput. Phys., 156(1999), 181-205.
[3] Matsuo, T., Sugihara, M., and Mori, M., A Derivation of a Finite Difference Scheme for the Nonlinear Schrödinger Equation, Proceedings of the Fourth JapanChina Joint Seminar on Numerical Mathematics, 1998.


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[^1]:    1 "multiple points discrete variational derivative" is a general term which denotes the 3 or more points ones. The two points (i.e. conventional) one is excluded from this definition, though "multiple" includes two in English and the definition is a little confusing. This is a matter of terminology.

