Dissipative Schemes for the Ginzburg–Landau Equations Takayasu Matsuo and Eitaro Torii¹

Abstract

Two existing and one new Galerkin schemes for the Time-Dependent Ginzburg-Landau (TDGL) equations are presented. The schemes have an welcome feature in common that each keeps a discrete counterpart of the original energy dissipation property of the TDGL. Based on the Lyapunov theory, asymptotic behavior of the solutions of the schemes are discussed, which is then confirmed by numerical experiments.

1 Introduction

The phenomelogical behavior of superconductivity is governed by the so-called Ginzburg– Landau model. The model in the so-called "zero electric potential gauge" is described as the following time-dependent Ginzburg–Landau (TDGL) equations:

$$\eta \frac{\partial \psi}{\partial t} + \frac{1}{2} \left\{ \left(\frac{\mathrm{i}}{\kappa} \nabla + \mathbf{A} \right)^2 \psi + \left(|\psi|^2 - 1 \right) \psi \right\} = 0 \quad \text{in } \Omega, \tag{1a}$$

$$\frac{\partial \boldsymbol{A}}{\partial t} + \operatorname{Re}\left[\overline{\psi}\left(\frac{\mathrm{i}}{\kappa}\nabla + \boldsymbol{A}\right)\psi\right] + \nabla \times (\nabla \times \boldsymbol{A} - \boldsymbol{H}) = 0 \quad \text{in } \Omega, \quad (1b)$$

where $\Omega \subset \mathbb{R}^d$ is a bounded subdomain with smooth boundary, $\kappa > 0$ is the material constant called the Ginzburg-Landau parameter, $\eta > 0$ is the friction coefficient, $\mathbf{H} \in \mathbb{R}^d$ is the applied magnetic field, $\psi : \Omega \times [0,T] \to \mathbb{C}$ is the complex-valued order parameter which denotes the conducting state of the material, and $\mathbf{A} : \Omega \times [0,T] \to \mathbb{R}^d$ is the magnetic potential. By $\overline{\psi}$ we mean the complex conjugate of ψ . The associated boundary conditions are:

$$\nabla \psi \cdot \boldsymbol{n} = 0, \quad \boldsymbol{A} \cdot \boldsymbol{n} = 0, \quad \boldsymbol{n} \times (\nabla \times \boldsymbol{A} - \boldsymbol{H}) = 0 \quad \text{on } \partial \Omega.$$
 (1c)

where n is the exterior unit normal of the boundary $\partial \Omega$. For this gauge choice and the well-posedness of the associated Cauchy problem, see [2].

The advantage of this particular gauge choice is that the problem can be viewed as a gradient-flow of the Ginzburg–Landau energy functional:

$$E(\psi, \boldsymbol{A}) = \int_{\Omega} \left\{ \frac{1}{2} \left| \left(\frac{\mathrm{i}}{\kappa} \nabla + \boldsymbol{A} \right) \psi \right|^2 + \frac{1}{4} (1 - |\psi|^2)^2 + \frac{1}{2} |\nabla \times \boldsymbol{A} - \boldsymbol{H}|^2 \right\} \mathrm{d}\boldsymbol{x}, \qquad (2)$$

$$\eta \frac{\partial \psi}{\partial t} = -\frac{\delta E}{\delta \overline{\psi}}, \qquad \frac{\partial A}{\partial t} = -\frac{\delta E}{\delta A}, \tag{3}$$

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where $\delta E/\delta \overline{\psi}$ and $\delta E/\delta A$ denote variational derivatives. This energy in other words serves as a Lyapunov functional of the system, and this suggests us to employ numerical schemes having some discrete counterpart of this property for stability and correct asymptotic behavior. So far several fully-implicit schemes having discrete Lyapunov functional have been proposed [3, 10], but due to their nonlinearity some iterative solver was necessarily required, and thus they were relatively expensive. A remedy to overcome this difficulty is to introduce some linearization technique, such as the one proposed in [9], which enables us to design a linearly-implicit scheme that still keeps discrete dissipation property in some sense. As its price, however, the resulting scheme can be unstable, since the discrete energy function in this case does not necessarily serve as Lyapunov functional.

In the present paper, after briefly reviewing the existing fully-implicit schemes [3, 10], we present a linearly-implicit scheme with the linearization technique [9]. Then the qualitative behavior of discrete solutions for each scheme is discussed based on the Lyapunov theory. In order to simplify the discussion, in what follows we limit ourselves to the simplified model ignoring all the magnetic effects:

$$\eta \frac{\partial \psi}{\partial t} = \frac{1}{2} \left\{ \frac{\Delta \psi}{\kappa^2} + (1 - |\psi|^2) \psi \right\} \quad \text{in } \Omega, \qquad \nabla \psi \cdot \boldsymbol{n} = 0 \quad \text{on } \partial \Omega.$$
(4)

This still deserves investigation since it still keeps interesting physical solutions such as vortices, and a Lyapunov functional:

$$E(\psi) = \int_{\Omega} \left\{ \frac{1}{2} \left| \frac{\nabla \psi}{\kappa} \right|^2 + \frac{1}{4} (1 - |\psi|^2)^2 \right\} \mathrm{d}\boldsymbol{x}.$$
 (5)

The simplified equation (4) is formally a gradient flow with respect to the energy:

$$\eta \frac{\partial \psi}{\partial t} = -\frac{\delta E}{\delta \overline{\psi}}.$$
(6)

We also assume d = 2 for brevity (we consider, say, a unit disk). Let $H_c^1(\Omega)$ be the standard Sobolev space of complex-valued functions and (\cdot, \cdot) be its associated inner product. Let S_d and W_d be the finite-dimensional subspaces in $H_c^1(\Omega)$ for trial and test functions satisfying $S_d \subseteq W_d$ (in most cases we simply take $S_d = W_d$, in particular to the standard piecewise linear function space).

2 Fully-implicit Schemes for the simplified GL equation

A method for designing Galerkin schemes preserving energy dissipation property has been proposed in [8]. By applying the method, we reach the following fully-implicit scheme as below. We denote the numerical solution by $\psi^{(m)}(\boldsymbol{x}) \simeq \psi(m\Delta t, \boldsymbol{x})$.

Scheme 1 (Fully-implicit scheme 1 [10]). Suppose an initial data $\psi^{(0)} \in S_d$ is given. Find $\psi^{(m)} \in S_d$ (m = 1, 2, ...) such that for any $\phi \in W_d$

$$\eta\left(\frac{\psi^{(m+1)}-\psi^{(m)}}{\Delta t},\phi\right) = -\left(\frac{\partial E_{\mathbf{d}}}{\partial(\nabla\overline{\psi}^{(m+1)},\nabla\overline{\psi}^{(m)})},\nabla\phi\right) - \left(\frac{\partial E_{\mathbf{d}}}{\partial(\overline{\psi}^{(m+1)},\overline{\psi}^{(m)})},\phi\right),$$

where

$$\begin{aligned} \frac{\partial E_{\mathrm{d}}}{\partial (\nabla \overline{\psi}^{(m+1)}, \nabla \overline{\psi}^{(m)})} &= \frac{1}{2\kappa^2} \left(\frac{\nabla \psi^{(m+1)} + \nabla \psi^{(m)}}{2} \right), \\ \frac{\partial E_{\mathrm{d}}}{\partial (\overline{\psi}^{(m+1)}, \overline{\psi}^{(m)})} &= -\frac{1}{2} \left(1 - \frac{|\psi^{(m+1)}|^2 + |\psi^{(m)}|^2}{2} \right) \left(\frac{\psi^{(m+1)} + \psi^{(m)}}{2} \right). \end{aligned}$$

This scheme has a desired dissipation property.

Proposition 1 (Dissipation property of Scheme 1 [10]). Let $\psi^{(m)}$ (m = 1, 2, ...) be the solutions of Scheme 1. Then the following discrete dissipation property holds:

$$\frac{1}{\Delta t} \int_{\Omega} E(\psi^{(m+1)}) - E(\psi^{(m)}) \mathrm{d}\boldsymbol{x} = -2\eta \int_{\Omega} \left| \frac{\psi^{(m+1)} - \psi^{(m)}}{\Delta t} \right|^2 \mathrm{d}\boldsymbol{x} \le 0.$$

That is, in Scheme 1 the original energy E dissipates as in the continuous case. This implies that the asymptotic behavior of the approximate solutions must be quite similar to that of the original TDGL (strictly speaking, to that of the corresponding ODE derived by discretizing the space variable).

In [3], an implicit Euler type scheme is derived from the energy functional based on minimization theory. Here only the resulting scheme is shown.

Scheme 2 (Fully-implicit scheme 2 [3]). Suppose an initial data $\psi^{(0)} \in S_d$ is given. Find $\psi^{(m)} \in S_d \ (m = 1, 2, ...)$ such that for any $\phi \in W_d$

$$\eta\left(\frac{\psi^{(m+1)} - \psi^{(m)}}{\Delta t}, \phi\right) = -\frac{1}{2\kappa^2} \left(\nabla\psi^{(m+1)}, \nabla\phi\right) - \frac{1}{2} \left((|\psi^{(m+1)}|^2 - 1)\psi^{(m+1)}, \phi\right)$$

Proposition 2 (Dissipation property of Scheme 2 [3]). Let $\psi^{(m)}$ (m = 1, 2, ...) be the solutions of Scheme 2. Then the following discrete dissipation property holds:

$$\frac{1}{\Delta t} \int_{\Omega} E(\psi^{(m+1)}) - E(\psi^{(m)}) \mathrm{d}\boldsymbol{x} \le -2\eta \int_{\Omega} \left| \frac{\psi^{(m+1)} - \psi^{(m)}}{\Delta t} \right|^2 \mathrm{d}\boldsymbol{x} \le 0$$

Thus the scheme should have similar asymptotic behavior as above; in fact, in [3], a detailed discussion on the asymptotic behavior is given for the full TDGL (1).

In these two similar schemes, however, we find several essential differences. First, notice that the first equality in Prop. 1 is replaced with an inequality in Prop. 2, whose equality does not holds in general (this can be understood by carefully inspecting its proof; interested readers may refer to [3]). Since in the continuous case, the equality holds: $(d/dt) \int E d\mathbf{x} = -2\eta \int |\psi_t|^2 d\mathbf{x}$, we can say that Scheme 1 is closer to the original TDGL.

Although the implicit Euler scheme happily keeps the Lyapunov functional, the dissipation (how the energy is dissipated) is slightly stronger there than it should be. Second, Scheme 1 should be second order with respect to Δt due to its temporal symmetry, while Scheme 2 is only first order.

Both schemes have an unwelcome feature in common: they are fully-implicit, and necessarily require time-consuming iterative solver. This disadvantage becomes even more crucial, if we consider the full TDGL, or like to proceed to the d = 3 cases. In the next section, we consider a linearly-implicit scheme in order to overcome this disadvantage.

3 A Linearly-Implicit Scheme for the simplified GL equation

By combining the method [8] and the linearization technique [9], we can derive the following linearly-implicit scheme.

Scheme 3 (Linearly-implicit scheme). Suppose an initial data $\psi^{(0)} \in S_d$ and a starting value $\psi^{(1)}$ are given. Find $\psi^{(m)} \in S_d$ (m = 2, 3, ...) such that for any $\phi \in W_d$

$$\eta\left(\frac{\psi^{(m+1)} - \psi^{(m-1)}}{2\Delta t}, \phi\right) = -\left(\frac{\partial E_{\mathrm{d}}}{\partial(\nabla\overline{\psi}^{(m+1)}, \nabla\overline{\psi}^{(m)}, \nabla\overline{\psi}^{(m-1)})}, \nabla\phi\right) - \left(\frac{\partial E_{\mathrm{d}}}{\partial(\overline{\psi}^{(m+1)}, \overline{\psi}^{(m)}, \overline{\psi}^{(m-1)})}, \phi\right)$$

where

$$\frac{\partial E_{d}}{\partial (\nabla \overline{\psi}^{(m+1)}, \nabla \overline{\psi}^{(m)}, \nabla \overline{\psi}^{(m-1)})} = \frac{1}{2\kappa^{2}} \left\{ b \nabla \psi^{(m)} + (1-b) \frac{\nabla \psi^{(m+1)} + \nabla \psi^{(m-1)}}{2} \right\},$$

$$\frac{\partial E_{d}}{\partial (\overline{\psi}^{(m+1)}, \overline{\psi}^{(m)}, \overline{\psi}^{(m-1)})} = \frac{a}{2} \left(-1 + \frac{\psi^{(m+1)} + \psi^{(m-1)}}{2} \overline{\psi}^{(m)} \right) \psi^{(m)} + \frac{1-a}{2} (-1 + |\psi^{(m)}|^{2}) \left(\frac{\psi^{(m+1)} + \psi^{(m-1)}}{2} \right),$$

and $a, b \in \mathbb{R}$ are scheme parameters.

The scheme parameters a, b should be chosen carefully, since they severely affect the stability of the resulting scheme as will be shown below. Observe that the scheme is linear with respect to the latest value $\psi^{(m+1)}$. This scheme enjoys the following dissipation property.

Theorem 1 (Dissipation property of Scheme 3). Let $\psi^{(m)}$ (m = 2, 3, ...) be the solutions of Scheme 1. Then the following discrete dissipation property holds:

$$\int_{\Omega} E_{\rm d}(\psi^{(m+1)},\psi^{(m)}) - E_{\rm d}(\psi^{(m)},\psi^{(m-1)}) \mathrm{d}\boldsymbol{x} = -2\eta \int_{\Omega} \left| \frac{\psi^{(m+1)} - \psi^{(m-1)}}{2\Delta t} \right|^2 \mathrm{d}\boldsymbol{x} \le 0,$$

where

$$E_{d}(\psi^{(m+1)},\psi^{(m)}) = \frac{1}{4} \left\{ a(1-\psi^{(m+1)}\overline{\psi}^{(m)})(1-\overline{\psi}^{(m+1)}\psi^{(m)}) + (1-a)(1-|\psi^{(m+1)}|^{2})(1-|\psi^{(m)}|^{2}) \right\} + \frac{1}{2\kappa^{2}} \left\{ b\left(\frac{\nabla\psi^{(m)}\cdot\nabla\overline{\psi}^{(m+1)}+\nabla\overline{\psi}^{(m)}\cdot\nabla\psi^{(m)}}{2} \right) + (1-b)\left(\frac{|\nabla\psi^{(m+1)}|^{2}+|\nabla\psi^{(m)}|^{2}}{2} \right) \right\}.$$
(7)

Note that now the discrete energy function (7) depends on two consecutive numerical solutions (i.e. it is "multistep"), and quadratic with respect to the latest value $\psi^{(m+1)}$; this is the key for the linearization. The scheme parameters a, b appear as the coefficients of the linear combination of the quadratic approximations. The theorem states that for any choice of a, b, the discrete dissipation property holds in the above sense. The discrete energy function (7) is, however, totally different from the original one (5), and as a consequence the discrete dissipation property does not immediately imply the correct asymptotic behavior, as was the case in the fully-implicit schemes.

Still, the discrete energy function gives us useful information for designing good (stable) schemes; more specifically, for the choice of appropriate scheme parameters a, b. Below we demonstrate this. The first step is to rewrite the energy function as follows.

$$E_{d}(\psi^{(m+1)},\psi^{(m)}) = \frac{1}{4} \left\{ |1-\psi^{(m+1)}\overline{\psi}^{(m)}|^{2} + (a-1)|\psi^{(m+1)}-\psi^{(m)}|^{2} \right\} \\ \frac{1}{2\kappa^{2}} \left\{ \left| \frac{\nabla\psi^{(m+1)}+\nabla\psi^{(m)}}{2} \right|^{2} + (1-2b) \left| \frac{\nabla\psi^{(m+1)}-\nabla\psi^{(m)}}{2} \right|^{2} \right\}.(8)$$

Let us then consider a "doubled" phase space $(\psi^{(m+1)}, \psi^{(m)})$, and regard that Scheme 3 defines a discrete map on the doubled space: $(\psi^{(m-1)}, \psi^{(m-2)}) \mapsto (\psi^{(m+1)}, \psi^{(m)})$. We then observe that depending on the parameters a, b the dynamical system can behave in the following three ways.

- 1. When a < 1 or b > 1/2, $E_d(\psi^{(m+1)}, \psi^{(m)})$ obviously is not bounded from below, and thus it can never serve as Lyapunov functional. In this case, by losing the Lyapunov property the system can be unstable.
- 2. When a = 1 and b = 1/2, which here we call the "critical" case, the energy function is bounded and can serve as Lyapunov functional. By the Lyapunov theory, the dynamical system it governs asymptotically tends to the minimizers. But by a careful glance we notice that the dynamics is a bit different from the original one. Let us consider the global minimizers ∫ E_d(ψ^(m+1), ψ^(m))d**x** = 0. In view of (8), we see that the global minimizers are such points that ψ^(m+1)ψ^(m) = 1 and ∇(ψ^(m+1) + ψ^(m)) = 0. This allows an oscillatory "steady state" solution ψ^(m) = c, ψ^(m+1) = 1/c̄ where c ∈ C is an arbitrary constant. This is in fact "steady state" in that in the doubled phase space, it corresponds to a fixed point (c, 1/c̄) of the dynamical system; in the

original undoubled space, however, it represents an oscillatory solution $c \to 1/\overline{c} \to c \to 1/\overline{c} \to \cdots$. Thus we conclude that in the critical case, the system is equipped with a Lyapunov functional, but the dynamics is different such that it allows spurious fixed points (in the doubled space).

3. When a > 1 and $b \le 1/2$, the spurious fixed points vanish, and the Lyapunov functional allows only original steady state solutions as its fixed points.

In the last case, the dynamical system is expected to behave the same way as the fully-implicit cases, although the corresponding linearly-implicit scheme is far cheaper. We like to generalize the above observation as follows: as an unavoidable consequence of the linearization, the resulting scheme should be necessarily multistep, and the associated dynamical system should be understood in the doubled (or more higher) phase space. There are often degrees of freedom in the definition of multistep energy functions, and it crucially determines the dynamics, which is then observed as its (numerical) stability. In some happy cases, such as the above, by carefully choosing the free (scheme) parameters we can enforce the scheme (the dynamical system) to behave the same as the original system. A question, however, still remains that in which circumstances we can find such "happy" cases. In particular, whether or not we can do that for any PDEs is an important open problem to be answered.

4 Numerical Examples

In this section we present numerical examples that illustrate the discussion in the previous section. We here test Scheme 3, with two parameter sets (a, b) = (0.9, 0.5) and (2, -0.5), each of which corresponds to the first and third patterns described above. For comparison, we also test the standard semi-implicit scheme, where the diffusion term is discretized in time by the implicit Euler, and the nonlinear term by the explicit Euler. We set the TDGL parameters to be $\eta = 1$, $\kappa = 15$, and solved the simplified TDGL on the unit disk with a triangulation of 9,375 elements by FreeFEM. As the initial data, we set the two vortices of indices +1 and -1. With this setting, it is known that the annihilation (disappearing by merging) of vortices should occur.

First we show a result with a fine time mesh $\Delta t = 0.1$. We tested the semi-implicit scheme and Scheme 3 with (a, b) = (2, -0.5), and found no difference; both schemes run quite happily in this case. We show the result in Fig. 1.

The corresponding energy profiles are shown in Fig. 2. For Scheme 3, we calculated E_d (the multistep energy function (7)) and E (the original energy function (5)). For the semi-implicit scheme, we calculated only the latter. In this setting, all the three lines well agree.

The semi-implicit scheme, however, becomes unstable as Δt increases. We demonstrate it by setting $\Delta t = 1.1$ in Fig. 3; they are the snapshots of four consecutive time steps around t = 50. We can observe severe numerical oscillation there. In contrast, Scheme 3 holds



Figure 1: Evolution of the solution with $\Delta t = 0.1$: the semi-implicit scheme and Scheme 3 with (a, b) = (2, -0.5)



Figure 2: Evolution of the energies with $\Delta t = 0.1$: the semi-implicit scheme and Scheme 3 with (a, b) = (2, -0.5)

out with the same coarse time step as shown in Fig. 4. The energy profiles are shown in Fig. 5, where we can observe oscillation in the semi-implicit scheme.



Figure 3: Evolution of the solution with $\Delta t = 1.1$: the semi-implicit scheme



Figure 4: Evolution of the solution with $\Delta t = 1.1$: Scheme 3

Finally we test Scheme 3 with the parameters (a, b) = (0, 9, 0.5) with $\Delta t = 0.5$. As shown in Fig. 6, the result is catastrophic. This agrees with the discussion in the previous section.

5 Concluding Remarks

In this paper, we presented a new linearly-implicit dissipative scheme for the time-dependent Ginzburg-Landau (TDGL) equations without magnetic effects, and discussed its asymp-



Figure 5: Evolution of the energies with $\Delta t = 1.1$: the semi-implicit scheme and Scheme 3 with (a, b) = (2, -0.5)



Figure 6: Evolution of the solution with $\Delta t = 0.5$: Scheme 3 with (a, b) = (0.9, 0.5)

totic behavior from the perspective of the Lyapunov theory. Two existing fully-implicit schemes were also shown and discussed.

It is possible to construct linearly-implicit dissipative scheme for the full TDGL (with magnetic effects) based on the same idea employed in this paper. That will be reported elsewhere soon.

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