GENERALIZED SAV-EXPONENTIAL INTEGRATOR SCHEMES FOR ALLEN–CAHN TYPE GRADIENT FLOWS[*]

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Abstract. The energy dissipation law and the maximum bound principle (MBP) are two important physical features of the well-known Allen–Cahn equation. While some commonly used first-order time stepping schemes have turned out to preserve unconditionally both the energy dissipation law and the MBP for the equation, restrictions on the time step size are still needed for existing second-order or even higher order schemes in order to have such simultaneous preservation. In this paper, we develop and analyze novel first- and second-order linear numerical schemes for a class of Allen–Cahn type gradient flows. Our schemes combine the generalized scalar auxiliary variable (SAV) approach and the exponential time integrator with a stabilization term, while the standard central difference stencil is used for discretization of the spatial differential operator. We not only prove their unconditional preservation of the energy dissipation law and the MBP in the discrete setting, but we also derive their optimal temporal error estimates under fixed spatial mesh. Numerical experiments are also carried out to demonstrate the properties and performance of the proposed schemes.

Key words. second-order linear scheme, energy dissipation law, maximum bound principle, exponential integrator, scalar auxiliary variable

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1. Introduction. The classic Allen–Cahn equation, originally introduced in [2] to model the motion of the antiphase boundaries in crystalline solids, takes the following form:

$$(1.1) \qquad u_t = \varepsilon^2 \Delta u + f(u), \quad t > 0, \ \boldsymbol{x} \in \Omega,$$

where the spatial domain $\Omega \subset \mathbb{R}^d$, $u(t, \boldsymbol{x}) : [0, \infty) \times \overline{\Omega} \to \mathbb{R}$ is the unknown function, $\varepsilon > 0$ is an interfacial parameter, and $f(u) = u - u^3$ is the nonlinear reaction. Equipped with the periodic or homogeneous Neumann boundary condition, (1.1) can be viewed as the L^2 gradient flow with respect to the energy functional

$$(1.2) \qquad E(u) = \int_\Omega \left(\frac{\varepsilon^2}{2} |\nabla u(\boldsymbol{x})|^2 + F(u(\boldsymbol{x})) \right) \mathrm{d}\boldsymbol{x},$$

where $F(u) = \frac{1}{4}(u^2 - 1)^2$ (i.e., $-F' = f$) is the double-well potential function, and thus satisfies the so-called *energy dissipation law* in the sense that the solution to (1.1)

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decreases the energy (1.2) along with the time, i.e., $\frac{\mathrm{d}}{\mathrm{d}t}E(u(t)) \leq 0$. The solution u usually represents the difference between the concentrations of two components of the alloy, and thus should be evaluated between -1 and 1 naturally, which corresponds to another important feature, the *maximum bound principle* (MBP); i.e., if the initial value falls pointwise between -1 and 1, then so is the solution for all time. Recently, some variants of the Allen–Cahn equation (1.1) have been developed to model various processes of phase transition, such as the nonlocal Allen–Cahn equation for phase separations within long-range interactions [3] and the fractional Allen–Cahn equation for anomalous diffusion processes [23], and they also satisfy the energy dissipation law with respect to their respective energy and the MBP. Since the analytic solutions to these models are usually not available, numerical solutions play a key role in their study and applications. In order to obtain efficient and stable numerical simulations and avoid nonphysical results, it is highly desirable to design accurate numerical methods in space and time which also preserve important physical features of the models, such as the energy dissipation law and the MBP.

In recent years, numerical schemes preserving the energy dissipation law have attracted a lot of attention for time integration of the Allen–Cahn type equations and other gradient flows, including convex splitting schemes [22, 42, 50], stabilized implicit-explicit (IMEX) schemes [18, 46, 51], discrete gradient schemes [15, 19, 38], exponential time differencing (ETD) schemes [14, 32, 56], invariant energy quadratization (IEQ) schemes [52, 54], scalar auxiliary variable (SAV) schemes [9, 43, 44, 45], and some variants of the SAV method [7, 8, 26, 28, 37]. By combining the SAV approach with the Runge–Kutta (RK) method, arbitrarily high order linear schemes preserving the energy dissipation law were developed in [1, 20]. In addition, there is also a large amount of literature denoted to MBP-preserving numerical schemes for the Allen–Cahn type gradient flow problems, such as the stabilized IMEX schemes [41, 48] and the exponential integrator methods [14, 34]. Borrowing the idea of strong stability-preserving methods [21], MBP-preserving RK-type schemes with high-order accuracy were studied theoretically and up to fourth-order schemes were provided for practical computations in [31, 35, 55]. However, among all schemes we have just mentioned, only a few first-order schemes can preserve simultaneously the energy dissipation law and the MBP *unconditionally* [14, 16, 41] (i.e., without any restriction on the time step size), while the second-order schemes always require certain restrictions on the time step size [27, 36]. It is an interesting and important question whether there exist second-order or even higher order time stepping schemes preserving both the energy dissipation law and the MBP unconditionally. An initial improvement was made in [53] by considering the high-order SAV-RK method [1] to guarantee the energy dissipation, and the maximum bound is enforced by the cut-off postprocessing but not by the scheme itself.

The H^{-1} gradient flow with respect to the energy (1.2) gives the classic Cahn–Hilliard equation $u_t = -\Delta(\varepsilon^2 \Delta u + f(u))$, which fails to satisfy the MBP due to the existence of the fourth-order dissipation term. It is also worth noting that if the nonlinear reaction function f is changed to the logarithmic one defined by (4.2) (i.e., corresponding to the Flory–Huggins potential) tested in our numerical experiments, the solution of the Cahn–Hilliard equation still remains in the open interval $(-1, 1)$ for all time under some appropriate boundary conditions [10, 17], where ± 1 are the points near which the singularities occur. Implicit or IMEX numerical schemes preserving such uniform boundedness have also been developed, where the singularity of the nonlinear term plays a crucial role [5, 13] in their construction.

In this paper, our main purpose is to systematically develop first- and second-

order (in time) linear numerical schemes preserving both the energy dissipation law and the MBP unconditionally for a family of Allen–Cahn type gradient flows. More precisely, we will consider (1.1) with a more general reaction term $f : \mathbb{R} \to \mathbb{R}$ given by a continuously differentiable function satisfying

(1.3)   there exists a constant $\beta > 0$ such that $f(\beta) \leq 0 \leq f(-\beta)$.

The periodic or homogeneous Neumann boundary condition is equipped, and the initial condition is given as $u(0, \cdot) = u_{\text{init}}$ on $\overline{\Omega}$. Then the MBP holds [14] in the sense that if the absolute value of the initial value is bounded pointwise by β, then the absolute value of the solution is also bounded pointwise by β for all time, i.e.,

(1.4) $\displaystyle\max_{\boldsymbol{x} \in \overline{\Omega}} |u_{\text{init}}(\boldsymbol{x})| \leq \beta \qquad \Longrightarrow \qquad \max_{\boldsymbol{x} \in \overline{\Omega}} |u(t, \boldsymbol{x})| \leq \beta \quad \forall t > 0.$

Furthermore, the energy dissipation law is also satisfied with respect to the energy (1.2) with F now being a smooth potential function satisfying $F' = -f$. The key ingredient is the appropriate combination of the SAV approach and the exponential integrator method [11, 25]. Note that similar ideas have been applied to some nonlinear hyperbolic-type equations [12, 29]. We first reformulate the model equation (1.1) in an equivalent form by defining an auxiliary variable, similar to the idea of the generalized SAV approach [8]. Then we introduce a stabilization term to the system and apply exponential integrators to develop first- and second-order linear schemes in time. We show that both schemes simultaneously preserve the energy dissipation law and the MBP unconditionally under an appropriate stabilizing constant. In the error analysis, one of the major difficulties is caused by the variable coefficients from the nonlinear reaction and the stabilization terms. By using the energy dissipation law and the MBP, these variable coefficients are shown to be bounded from above and below by certain generic positive constants, which helps us to successfully prove the optimal temporal convergence under fixed spatial mesh. To the best of our knowledge, this is the first work providing a second-order linear numerical scheme for time integration of the model Allen–Cahn type gradient flows, with provable unconditional preservation of both the energy dissipation law and the MBP.

The rest of this paper is organized as follows. In section 2, we present the spatial discretization with the central finite difference and some useful lemmas. In section 3, we propose the first- and second-order generalized SAV-exponential integrator (GSAV-EI) schemes and then prove their unconditional preservation of both the energy dissipation law and the MBP, followed by their temporal convergence analysis. Numerical experiments are carried out to validate the theoretical results and demonstrate the performance of the proposed schemes in section 4. Finally, some concluding remarks are given in section 5.

2. Spatial discretization and some preliminaries. Throughout this paper, we consider the two-dimensional square domain $\Omega = (0, L) \times (0, L)$ for the model equation (1.1) with f satisfying the assumption (1.3). Without loss of generality, we impose the periodic boundary condition. Extensions to the three-dimensional case and homogeneous Neumann boundary condition do not have any difficulties. In this section, we will present some notations related to the spatial discretization and a few preliminary lemmas for the analysis of the time integration schemes proposed later.

Given a positive integer M, let $h = L/M$ be the size of the uniform mesh partitioning $\overline{\Omega}$, and denote by $\Omega_h = \{(x_i, y_j) = (ih, jh) \,|\, 1 \leq i, j \leq M\}$ the set of mesh points. For a grid function v defined on Ω_h, we denote $v_{ij} = v(x_i, y_j)$. Let $\mathcal{M}_h$ be the

set of all M-periodic grid functions on Ω_h, i.e., $\mathcal{M}_h = \{v : \Omega_h \to \mathbb{R} \,|\, v_{i+kM,j+lM} = v_{ij}, \ k,l \in \mathbb{Z}, \ 1 \leq i,j \leq M\}$. Let us apply the central finite difference method to approximate the spatial differential operators. For any $v \in \mathcal{M}_h$, the discrete Laplace operator Δ_h is defined by

$$\Delta_h v_{ij} = \frac{1}{h^2}(v_{i+1,j} + v_{i-1,j} + v_{i,j+1} + v_{i,j-1} - 4v_{ij}), \quad 1 \leq i,j \leq M,$$

and the discrete gradient operator ∇_h is defined by

$$\nabla_h v_{ij} = \left(\frac{v_{i+1,j} - v_{ij}}{h}, \frac{v_{i,j+1} - v_{ij}}{h}\right)^T, \quad 1 \leq i,j \leq M.$$

The eigenvalues of Δ_h are given by [33]

$$(2.1) \qquad \lambda_{kl} = -\frac{4}{h^2}\left(\sin^2 \frac{k\pi}{M} + \sin^2 \frac{l\pi}{M}\right) \leq 0, \quad 0 \leq k,l \leq M-1.$$

As usual, the discrete inner product $\langle \cdot, \cdot \rangle$, the discrete L^2 norm $\|\cdot\|$, and the discrete L^∞ norm $\|\cdot\|_\infty$ can be defined, respectively, by

$$\langle v, w \rangle = h^2 \sum_{i,j=1}^{M} v_{ij} w_{ij}, \qquad \|v\| = \sqrt{\langle v, v \rangle}, \qquad \|v\|_\infty = \max_{1 \leq i,j \leq M} |v_{ij}|$$

for any $v, w \in \mathcal{M}_h$ and

$$\langle \boldsymbol{v}, \boldsymbol{w} \rangle = \langle v^1, w^1 \rangle + \langle v^2, w^2 \rangle, \qquad \|\boldsymbol{v}\| = \sqrt{\langle \boldsymbol{v}, \boldsymbol{v} \rangle}$$

for any $\boldsymbol{v} = (v^1, v^2)^T, \boldsymbol{w} = (w^1, w^2)^T \in \mathcal{M}_h \times \mathcal{M}_h$. By the periodicity, the summation-by-parts formula obviously holds:

$$\langle v, \Delta_h w \rangle = -\langle \nabla_h v, \nabla_h w \rangle = \langle \Delta_h v, w \rangle \quad \forall\, v, w \in \mathcal{M}_h.$$

The space-discrete problem corresponding to (1.1) is then to find a function $u_h : [0, \infty) \to \mathcal{M}_h$ that satisfies

$$(2.2) \qquad \frac{\mathrm{d}u_h}{\mathrm{d}t} = \varepsilon^2 \Delta_h u_h + f(u_h), \quad t > 0,$$

with $u_h(0) = \hat{u}_{\text{init}}$, where $\hat{u}_{\text{init}}$ is the pointwise projection of u_{init} onto $\mathcal{M}_h$. Throughout the paper, we do not differ $\hat{u}_{\text{init}}$ and u_{init} anymore since there is no ambiguity. It is easy to verify the energy dissipation law for the space-discrete problem (2.2), i.e., $\frac{\mathrm{d}}{\mathrm{d}t} E_h(u_h(t)) \leq 0$, where E_h is the spatially discretized energy functional defined as

$$(2.3) \qquad E_h(v) := \frac{\varepsilon^2}{2} \|\nabla_h v\|^2 + \langle F(v), 1 \rangle \quad \forall\, v \in \mathcal{M}_h.$$

As shown in [14], the MBP is also valid for the space-discrete problem (2.2), i.e.,

$$(2.4) \qquad \|u_{\text{init}}\|_\infty \leq \beta \quad \implies \quad \|u_h(t)\|_\infty \leq \beta \quad \forall\, t > 0.$$

We have assumed that f is continuously differentiable, so $\|f'\|_{C[-\beta,\beta]}$ is finite. Then the following result is valid [14].

LEMMA 2.1. *Under the assumption* (1.3), *if* $\kappa \geq \|f'\|_{C[-\beta,\beta]}$ *holds for some positive constant* κ, *then we have* $|f(\xi) + \kappa\xi| \leq \kappa\beta$ *for any* $\xi \in [-\beta, \beta]$.

Since $\mathcal{M}_h$ is a finite-dimensional linear space, any grid function in $\mathcal{M}_h$ and any linear operator from $\mathcal{M}_h$ to $\mathcal{M}_h$ can be treated as a vector in $\mathbb{R}^{M^2}$ and a matrix in $\mathbb{R}^{M^2 \times M^2}$, respectively. For functions of matrix/operator, we have the following lemma (see [24]).

LEMMA 2.2. *Let* ϕ *be defined on the spectrum of a diagonalizable matrix* $A \in \mathbb{R}^{m \times m}$, *i.e., the values* $\{\phi(\lambda_i)\}_{i=1}^m$ *exist, where* $\{\lambda_i\}_{i=1}^m$ *are the eigenvalues of* A. *Then the following hold:*
  (i) $\phi(A)$ *commutes with* A *and* $\phi(A^T) = \phi(A)^T$;
  (ii) *the eigenvalues of* $\phi(A)$ *are* $\{\phi(\lambda_i) \,|\, 1 \leq i \leq m\}$;
  (iii) $\phi(P^{-1}AP) = P^{-1}\phi(A)P$ *for any nonsingular matrix* $P \in \mathbb{R}^{m \times m}$.

We still use the notations $\|\cdot\|$ and $\|\cdot\|_\infty$ to denote the matrix-induced norms consistent with $\|\cdot\|$ and $\|\cdot\|_\infty$ defined before, respectively. By viewing Δ_h as a matrix, we know that Δ_h is symmetric, negative semidefinite, and weakly diagonally dominant with all diagonal entries negative. Moreover, we have the following useful estimate, which comes from the fact that Δ_h is the generator of a contraction semigroup [14], and the proof can be found in [14, 31].

LEMMA 2.3. *For any real numbers* $a \geq 0$ *and* $b \geq 0$, *we have* $\|e^{a\Delta_h - bI}\|_\infty \leq e^{-b}$, *where* $I \in \mathbb{R}^{M^2 \times M^2}$ *is the identity matrix.*

REMARK 2.1. *Apart from the central difference discretization discussed above, the lumped mass finite element method with piecewise linear basis functions can also be adopted and Lemma* 2.3 *still holds correspondingly* [14]. *In addition, there have been some initial explorations on the MBP-preserving methods using the fourth-order accurate spatial discretization, such as the compact difference approximation* [49] *and the finite difference formulation of the* Q^2 *spectral element method* [47], *combined with the Euler-type time-stepping approaches. However, it is not obvious whether these fourth-order discrete Laplace operators satisfy Lemma* 2.3, *and thus it is worthy of further investigations on the combination of higher-order spatial discretizations with the exponential integrator methods studied in this paper.*

3. Generalized SAV-exponential integrator schemes. From now on, we always assume the initial value u_{init} has enough regularity as needed. Let us define the bulk energy term $E_{1h}(v) := \langle F(v), 1 \rangle$ for any $v \in \mathcal{M}_h$. The continuity of F implies that F is bounded from below on $[-\beta, \beta]$. Therefore, according to the MBP (2.4), there exist two constants $C_* \geq 0$ and $C^* \geq 0$ such that

$$(3.1) \qquad\qquad -C_* \leq E_{1h}(u_h) \leq C^*.$$

Motivated by the idea of the generalized SAV approach [8], we define the auxiliary variable $s_h(t) = E_{1h}(u_h(t))$ and rewrite the space-discrete equation (2.2) in an alternate but equivalent form as

$$(3.2\text{a}) \qquad\qquad \frac{\mathrm{d}u_h}{\mathrm{d}t} = \varepsilon^2 \Delta_h u_h + \frac{\sigma(s_h)}{\sigma(E_{1h}(u_h))} f(u_h),$$

$$(3.2\text{b}) \qquad\qquad \frac{\mathrm{d}s_h}{\mathrm{d}t} = -\frac{\sigma(s_h)}{\sigma(E_{1h}(u_h))} \Big\langle f(u_h), \frac{\mathrm{d}u_h}{\mathrm{d}t} \Big\rangle,$$

where $\sigma : \mathbb{R} \to \mathbb{R}$ is a one-variable function satisfying the following two conditions:

(Σ_1) $\sigma > 0$ on $\mathbb{R}$;

(Σ_2) σ is continuously differentiable and $\sigma' \geq 0$ on $\mathbb{R}$.

These conditions are crucial to the MBP preservation and error analysis of the proposed time integration schemes in this paper. For any $v \in \mathcal{M}_h$ and $r \in \mathbb{R}$, define

$$(3.3) \qquad g(v, r) := \frac{\sigma(r)}{\sigma(E_{1h}(v))}$$

(clearly, $g(v, r) > 0$ due to the condition (Σ_1)) and the modified energy

$$(3.4) \qquad \mathcal{E}_h(v, r) := \frac{\varepsilon^2}{2} \|\nabla_h v\|^2 + r.$$

Obviously, $g(u_h, s_h) \equiv 1$ and $\mathcal{E}_h(u_h, s_h) \equiv E_h(u_h)$ without time discretization.

REMARK 3.1. *The form (3.2) and the conditions (Σ_1) and (Σ_2) differ from those given in [8], where σ may not be defined on the whole real line $\mathbb{R}$ and the constructed schemes may be nonlinear, while our schemes developed later are all linear. A trivial choice for the function σ satisfying (Σ_1) and (Σ_2) is the positive constant mapping, e.g., $\sigma \equiv 1$. This gives a degenerate case since we still have exactly $g(u_h, s_h) \equiv 1$ with whatever time discretization, and consequently s_h does not provide any feedback to the update of u_h at each time step, which is similar to the idea adopted in [39]. Some nontrivial choices [8] include elementary functions such as $\sigma(x) = e^x$, $\sigma(x) = \frac{\pi}{2} + \arctan(x)$, $\sigma(x) = 1 + \tanh(x)$, or even special functions constructed by the integration such as $\sigma(x) = \int_{-\infty}^{x} \eta(y)\, dy$ for some continuous function $\eta \geq 0$ on $\mathbb{R}$.*

Next, we develop exponential integrators for the space-discrete system (3.2), instead of the original one (2.2). Let us partition the time interval using the nodes $\{t_n = n\tau\}_{n \geq 0}$ with a uniform time step size $\tau > 0$, and set u^n and s^n as the approximations of $u_{h,e}(t_n)$ and $s_{h,e}(t_n) = E_{1h}(u_{h,e}(t_n))$, respectively, where $u_{h,e}$ denotes the exact solution to the problem (2.2) (equivalently (3.2)).

3.1. First-order GSAV-EI scheme. Set $u^0 = u_{\text{init}}$ and $s^0 = E_{1h}(u^0)$. Suppose the numerical solution (u^n, s^n) is known for some $n \geq 0$. Introducing a positive stabilizing constant $\kappa > 0$, (3.2a) is equivalent to

$$\frac{du_h}{dt} = \varepsilon^2 \Delta_h u_h + g(u_h, s_h)f(u_h) + \kappa g(u^n, s^n)(u_h - u_h)$$
$$= -L_\kappa^n u_h + N_\kappa^n(u_h, s_h),$$

where the linear operator $L_\kappa^n = \kappa g(u^n, s^n)I - \varepsilon^2 \Delta_h$ and the nonlinear operator

$$N_\kappa^n(v, r) = g(v, r)f(v) + \kappa g(u^n, s^n)v \quad \forall v \in \mathcal{M}_h, \ \forall r \in \mathbb{R}.$$

We know that L_κ^n is self-adjoint and positive definite since $g(u^n, s^n) > 0$ and $\kappa > 0$. Using the variation-of-constants formula on $[t_n, t_{n+1}]$, we have

$$u_h(t_{n+1}) = e^{-\tau L_\kappa^n} u_h(t_n) + \int_0^\tau e^{-(\tau-\theta)L_\kappa^n} N_\kappa^n(u_h(t_n + \theta), s_h(t_n + \theta))\, d\theta.$$

By approximating the term N_κ^n by its value at $\theta = 0$, i.e., $N_\kappa^n(u_h(t_n + \theta), s_h(t_n + \theta)) \approx N_\kappa^n(u_h(t_n), s_h(t_n))$, we obtain the first-order exponential integrator scheme for computing u^{n+1} as

$$(3.5a) \qquad u^{n+1} = e^{-\tau L_\kappa^n} u^n + \left(\int_0^\tau e^{-(\tau-\theta)L_\kappa^n}\, d\theta \right) N_\kappa^n(u^n, s^n)$$

$$= \mathrm{e}^{-\tau L_\kappa^n} u^n + \tau \phi_1(-\tau L_\kappa^n) N_\kappa^n(u^n, s^n),$$

where $\phi_1(a) = a^{-1}(\mathrm{e}^a - 1)$ for $a \neq 0$. Integrating (3.2b) from t_n to t_{n+1} and using the approximation $g(u_h(t_n + t), s_h(t_n + t)) f(u_h(t_n + t)) \approx g(u_h(t_n), s_h(t_n)) f(u_h(t_n))$, we obtain the first-order formula for computing s^{n+1} as

$$(3.5b) \qquad s^{n+1} = s^n - g(u^n, s^n) \langle f(u^n), u^{n+1} - u^n \rangle.$$

The combination of (3.5a) and (3.5b) defines the first-order generalized SAV-exponential integrator (GSAV-EI1) scheme, which is uniquely solvable for any $\tau > 0$ due to its explicit formulation.

3.1.1. Energy dissipation and MBP. We first show the unconditional preservation of the energy dissipation law with respect to the modified energy $\mathcal{E}_h$ defined by (3.4) and the MBP of the GSAV-EI1 scheme (3.5). As a consequence, we then prove the uniform boundedness of $g(u^n, s^n)$, which is crucial to the convergence analysis.

THEOREM 3.1 (energy dissipation of GSAV-EI1). *The GSAV-EI1 scheme (3.5) is unconditionally energy dissipative in the time-discrete sense that $\mathcal{E}_h(u^{n+1}, s^{n+1}) \leq \mathcal{E}_h(u^n, s^n)$ holds for any $\tau > 0$ and $n \geq 0$.*

Proof. Using (3.5b), some simple calculations yield

$$
\begin{aligned}
(3.6) \quad \mathcal{E}_h(u^{n+1}, s^{n+1}) - \mathcal{E}_h(u^n, s^n) &= \frac{\varepsilon^2}{2} \|\nabla_h u^{n+1}\|^2 - \frac{\varepsilon^2}{2} \|\nabla_h u^n\|^2 + s^{n+1} - s^n \\
&= \varepsilon^2 \langle \nabla_h u^{n+1}, \nabla_h u^{n+1} - \nabla_h u^n \rangle - \frac{\varepsilon^2}{2} \|\nabla_h u^{n+1} - \nabla_h u^n\|^2 \\
&\quad - g(u^n, s^n) \langle f(u^n), u^{n+1} - u^n \rangle \\
&= -\langle \varepsilon^2 \Delta_h u^{n+1} + g(u^n, s^n) f(u^n), u^{n+1} - u^n \rangle - \frac{\varepsilon^2}{2} \|\nabla_h u^{n+1} - \nabla_h u^n\|^2 \\
&= \langle L_\kappa^n u^{n+1} - N_\kappa^n(u^n, s^n), u^{n+1} - u^n \rangle \\
&\quad - \kappa g(u^n, s^n) \|u^{n+1} - u^n\|^2 - \frac{\varepsilon^2}{2} \|\nabla_h u^{n+1} - \nabla_h u^n\|^2.
\end{aligned}
$$

It can also be derived from (3.5a) that

$$u^{n+1} - u^n = (\mathrm{e}^{-\tau L_\kappa^n} - I) u^n + \tau \phi_1(-\tau L_\kappa^n) N_\kappa^n(u^n, s^n).$$

Multiplying $[\tau \phi_1(-\tau L_\kappa^n)]^{-1} = (I - \mathrm{e}^{-\tau L_\kappa^n})^{-1} L_\kappa^n$ on both sides of the above equation leads to

$$
\begin{aligned}
[\tau \phi_1(-\tau L_\kappa^n)]^{-1}(u^{n+1} - u^n) &= -L_\kappa^n u^n + N_\kappa^n(u^n, s^n) \\
&= L_\kappa^n(u^{n+1} - u^n) - L_\kappa^n u^{n+1} + N_\kappa^n(u^n, s^n),
\end{aligned}
$$

and thus

$$(3.7) \qquad L_\kappa^n u^{n+1} - N_\kappa^n(u^n, s^n) = [L_\kappa^n - (I - \mathrm{e}^{-\tau L_\kappa^n})^{-1} L_\kappa^n](u^{n+1} - u^n).$$

Note that L_κ^n is positive definite and $a - (1 - \mathrm{e}^{-a})^{-1} a < 0$ for any $a > 0$, which means, by Lemma 2.2, that $L_\kappa^n - (I - \mathrm{e}^{-\tau L_\kappa^n})^{-1} L_\kappa^n$ is negative definite. Combining (3.6) and (3.7), we obtain the energy dissipation $\mathcal{E}_h(u^{n+1}, s^{n+1}) \leq \mathcal{E}_h(u^n, s^n)$. $\qquad \square$

REMARK 3.2. *Theorem 3.1 states that the GSAV-EI1 scheme* (3.5) *is energy dissipative with respect to the modified energy* $\mathcal{E}_h(u^n, s^n)$ *rather than the original energy* $E_h(u^n)$. *Note that* $\mathcal{E}_h(u^n, s^n)$ *is only an approximation of* $E_h(u^n)$ *after time discretization since usually* $s^n \neq E_{1h}(u^n)$ *for* $n > 0$.

COROLLARY 3.2. *For any* $\tau > 0$ *and* $n \geq 0$, *it holds that* $s^n \leq E_h(u_{\text{init}})$.

Proof. Since $s^0 = E_{1h}(u_{\text{init}})$, we have by Theorem 3.1 that

$$\frac{\varepsilon^2}{2}\|\nabla_h u^n\|^2 + s^n = \mathcal{E}_h(u^n, s^n) \leq \mathcal{E}_h(u^{n-1}, s^{n-1}) \leq \cdots \leq \mathcal{E}_h(u^0, s^0) = E_h(u_{\text{init}}).$$

Dropping off the nonnegative term $\frac{\varepsilon^2}{2}\|\nabla_h u^n\|^2$ leads to the expected result. $\square$

THEOREM 3.3 (MBP of GSAV-EI1). *If* $\kappa \geq \|f'\|_{C[-\beta,\beta]}$, *then the GSAV-EI1 scheme* (3.5) *preserves the MBP unconditionally; i.e., for any* $\tau > 0$, *the time-discrete version of* (2.4) *is valid as follows:*

$$(3.8) \qquad \|u_{\text{init}}\|_\infty \leq \beta \qquad \Longrightarrow \qquad \|u^n\|_\infty \leq \beta \quad \forall n \geq 0.$$

Proof. Suppose (u^n, s^n) is given and $\|u^n\|_\infty \leq \beta$ for some $n \geq 0$. By Lemma 2.3, we get $\|e^{-\tau L_\kappa^n}\|_\infty \leq e^{-\tau \kappa g(u^n, s^n)}$. Since $\kappa \geq \|f'\|_{C[-\beta,\beta]}$ and $g(u^n, s^n) > 0$, by Lemma 2.1 we have

$$\|N_\kappa^n(u^n, s^n)\|_\infty = g(u^n, s^n)\|f(u^n) + \kappa u^n\|_\infty \leq \kappa \beta g(u^n, s^n).$$

Therefore, we obtain from (3.5a) that

$$\|u^{n+1}\|_\infty \leq e^{-\tau \kappa g(u^n, s^n)}\beta + \left(\int_0^\tau e^{-(\tau-\theta)\kappa g(u^n, s^n)}\, d\theta\right) \cdot \kappa \beta g(u^n, s^n)$$

$$= e^{-\tau \kappa g(u^n, s^n)}\beta + \frac{1 - e^{-\tau \kappa g(u^n, s^n)}}{\kappa g(u^n, s^n)} \cdot \kappa \beta g(u^n, s^n) = \beta.$$

By induction, we have $\|u^n\|_\infty \leq \beta$ for any $n \geq 0$. $\square$

REMARK 3.3. *By applying* $e^{-\tau L_\kappa^n} \approx (I + \tau L_\kappa^n)^{-1}$ *to* (3.5a), *we can obtain*

$$(3.9) \qquad \frac{u^{n+1} - u^n}{\tau} = \varepsilon^2 \Delta_h u^{n+1} + g(u^n, s^n)f(u^n) + \kappa g(u^n, s^n)(u^{n+1} - u^n).$$

The scheme formed by (3.9) *and* (3.5b) *can be regarded as the stabilizing version of the generalized-SAV scheme* [8], *which also satisfies the energy dissipation law (Theorem 3.1) and the MBP (Theorem 3.3). In particular, by setting* $\sigma(x) = e^x$, *it recovers exactly the first-order stabilized exponential-SAV scheme* [30].

Unlike the time-continuous case in which $g(u_h, s_h) \equiv 1$, the coefficient $g(u^n, s^n)$ may vary at each time step unless σ is chosen as a constant function, which leads to some difficulties for the error analysis. Fortunately, by the energy dissipation law and the MBP, we can show that $g(u^n, s^n)$ is bounded uniformly in n. The following lemma (without proof) is useful to estimate some exponential-related functions of matrices.

LEMMA 3.4. *For any* $a > 0$, *the following inequalities hold:*

$$0 < 1 - e^{-a} < a, \qquad 0 < \phi_1(-a) < 1, \qquad 1 < (1+a)\phi_1(-a) < 2.$$

COROLLARY 3.5. *Given any fixed $h > 0$ and $T > 0$, if $\kappa \geq \|f'\|_{C[-\beta,\beta]}$ and $\|u_{\mathrm{init}}\|_\infty \leq \beta$, then there are two constants $G_* > 0$ and $G^* > 0$ such that*

$$G_* \leq g(u^n, s^n) \leq G^*, \quad 0 \leq n \leq \lfloor T/\tau \rfloor,$$

where G_* and G^* depend on C_*, C^*, $|\Omega|$, T, u_{init}, κ, ε, and $\|f\|_{C[-\beta,\beta]}$ but are independent of τ.

Proof. Since $\|u^n\|_\infty \leq \beta$ (by Theorem 3.3), according to (3.1) and the conditions (Σ_1) and (Σ_2), it holds that $0 < \sigma(-C_*) \leq \sigma(E_{1h}(u^n)) \leq \sigma(C^*)$. According to Corollary 3.2, we have

$$g(u^n, s^n) = \frac{\sigma(s^n)}{\sigma(E_{1h}(u^n))} \leq \frac{\sigma(E_h(u_{\mathrm{init}}))}{\sigma(-C_*)} := G^*.$$

Using (2.1), we then obtain the uniform bound of the spectral radius of L_κ^n, $\rho(L_\kappa^n)$, as

$$(3.10) \qquad \rho(L_\kappa^n) \leq \kappa g(u^n, s^n) + \varepsilon^2 \rho(\Delta_h) \leq G^* \kappa + \frac{8\varepsilon^2}{h^2} := M_h.$$

Next, we show the existence of the lower bound of $\{s^n\}$. By making use of the MBP and the first inequality in Lemma 3.4, we derive from (3.5a) that

$$\|u^{n+1} - u^n\| \leq \|I - \mathrm{e}^{-\tau L_\kappa^n}\| \|u^n\| + \tau \|\phi_1(-\tau L_\kappa^n)\| \|N_\kappa(u^n, s^n)\|$$
$$\leq \tau \rho(L_\kappa^n) \cdot \beta |\Omega|^{\frac{1}{2}} + \tau \cdot \kappa \beta g(u^n, s^n) |\Omega|^{\frac{1}{2}} \leq \tau \beta |\Omega|^{\frac{1}{2}} (M_h + G^* \kappa).$$

Since $\|f(u^n)\| \leq F_0 |\Omega|^{\frac{1}{2}}$ with $F_0 := \|f\|_{C[-\beta,\beta]}$, we then obtain from (3.5b) that

$$(3.11) \quad s^{n+1} \geq s^n - g(u^n, s^n) \|f(u^n)\| \|u^{n+1} - u^n\| \geq s^n - G^* F_0 \beta |\Omega| (M_h + G^* \kappa) \tau.$$

By recursion, noting that $s^0 = E_{1h}(u_{\mathrm{init}}) \geq -C_*$, we obtain

$$(3.12) \quad s^n \geq s^0 - G^* F_0 \beta |\Omega| (M_h + G^* \kappa) n\tau \geq -C_* - G^* F_0 \beta |\Omega| (M_h + G^* \kappa) T := S_*.$$

Thus, $g(u^n, s^n) \geq \sigma(S_*)/\sigma(C^*) := G_*$, which completes the proof. $\qquad\square$

3.1.2. Temporal error analysis. Note that (3.5a) is equivalent to finding $u^{n+1} = w(\tau)$ with $w(\theta)$ satisfying

$$(3.13) \qquad \begin{cases} \dfrac{\mathrm{d}w(\theta)}{\mathrm{d}\theta} + L_\kappa^n w(\theta) = N_\kappa^n(u^n, s^n), & \theta \in (0, \tau], \\ w(0) = u^n. \end{cases}$$

Let $s_{h,e}(t) = E_{1h}(u_{h,e}(t))$. Define $w_{h,e}(\theta) = u_{h,e}(t_n + \theta)$ for $\theta \in [0, \tau]$. It holds that

$$(3.14) \qquad \begin{cases} \dfrac{\mathrm{d}w_{h,e}(\theta)}{\mathrm{d}\theta} + L_\kappa^n w_{h,e}(\theta) = N_\kappa^n(u_{h,e}(t_n), s_{h,e}(t_n)) + R_{1u}^n(\theta), & \theta \in (0, \tau], \\ w_{h,e}(0) = u_{h,e}(t_n), \end{cases}$$

where the truncation error

$$R_{1u}^n(\theta) = g(u_{h,e}(t_n + \theta), s_{h,e}(t_n + \theta)) f(u_{h,e}(t_n + \theta)) - g(u_{h,e}(t_n), s_{h,e}(t_n)) f(u_{h,e}(t_n))$$
$$+ \kappa g(u^n, s^n)(u_{h,e}(t_n + \theta) - u_{h,e}(t_n)).$$

For $s_{h,e}(t)$, we have

$$(3.15) \quad s_{h,e}(t_{n+1}) - s_{h,e}(t_n)$$
$$= -g(u_{h,e}(t_n), s_{h,e}(t_n)) \langle f(u_{h,e}(t_n)), u_{h,e}(t_{n+1}) - u_{h,e}(t_n) \rangle + \tau R_{1s}^n$$

for some truncation residual R_{1s}^n. Furthermore, it is easy to verify that

$$(3.16) \qquad \sup_{\theta \in (0,\tau)} \|R_{1u}^n(\theta)\| \le C_{e,h}\tau, \qquad |R_{1s}^n| \le C_{e,h}\tau,$$

where the constant $C_{e,h} > 0$ depends on $u_{h,e}$, κ, ε, and $\|f\|_{C^1[-\beta,\beta]}$. Now we define the error functions as

$$(3.17) \qquad e_u^n = u^n - u_{h,e}(t_n), \qquad e_s^n = s^n - s_{h,e}(t_n).$$

LEMMA 3.6. *Given any fixed $h > 0$ and $T > 0$, if $\kappa \ge \|f'\|_{C[-\beta,\beta]}$ and $\|u_{\mathrm{init}}\|_\infty \le \beta$, then we have*

$$\|g(u^n, s^n)f(u^n) - g(u_{h,e}(t_n), s_{h,e}(t_n))f(u_{h,e}(t_n))\| \le C_g(\|e_u^n\| + |e_s^n|), \quad 0 \le n \le \lfloor T/\tau \rfloor,$$

where $C_g > 0$ is a constant depending on C_*, $|\Omega|$, u_{init}, and $\|f\|_{C^1[-\beta,\beta]}$.

A special case of this lemma with $\sigma(x) = e^x$ has been proved in [30]. Using (3.1) and the conditions (Σ_1) and (Σ_2), there is no essential difficulty to obtain the general result, so we omit the proof.

THEOREM 3.7 (temporal error estimate of GSAV-EI1). *Given any fixed $h > 0$ and $T > 0$ and letting $\kappa \ge \|f'\|_{C[-\beta,\beta]}$, assume that the exact solution $u_{h,e}$ is smooth enough on $[0,T]$ and $\|u_{\mathrm{init}}\|_\infty \le \beta$. If $\tau > 0$ is sufficiently small, then we have the following error estimate for the GSAV-EI1 scheme* (3.5):

$$(3.18) \qquad \|u^n - u_{h,e}(t_n)\| + |s^n - s_{h,e}(t_n)| \le C_{h,1}\tau, \quad 0 \le n \le \lfloor T/\tau \rfloor,$$

where the constant $C_{h,1} > 0$ is independent of τ.

Proof. Define $e(\theta) = w(\theta) - w_{h,e}(\theta)$. The difference between (3.13) and (3.14) leads to

$$\begin{cases} \dfrac{\mathrm{d}e(\theta)}{\mathrm{d}\theta} + L_\kappa^n e(\theta) = N_\kappa^n(u^n, s^n) - N_\kappa^n(u_{h,e}(t_n), s_{h,e}(t_n)) - R_{1u}^n(\theta), \quad \theta \in (0,\tau], \\ e(0) = e_u^n, \end{cases}$$

whose solution $e(\tau) = u^{n+1} - u_{h,e}(t_{n+1}) = e_u^{n+1}$ can be expressed as

$$(3.19) \qquad e_u^{n+1} = e^{-\tau L_\kappa^n} e_u^n + \tau \phi_1(-\tau L_\kappa^n)[N_\kappa^n(u^n, s^n) - N_\kappa^n(u_{h,e}(t_n), s_{h,e}(t_n))]$$
$$- \int_0^\tau e^{-(\tau - \theta)L_\kappa^n} R_{1u}^n(\theta) \, \mathrm{d}\theta.$$

Acting $I + \tau L_\kappa^n$ on both sides of (3.19), we obtain

$$(3.20) \qquad (1 + \tau \kappa g(u^n, s^n))(e_u^{n+1} - e_u^n) - \tau \varepsilon^2 (\Delta_h e_u^{n+1} - \Delta_h e_u^n)$$
$$= \tau(I + \tau L_\kappa^n)\phi_1(-\tau L_\kappa^n)[N_\kappa^n(u^n, s^n) - N_\kappa^n(u_{h,e}(t_n), s_{h,e}(t_n))]$$
$$+ (I + \tau L_\kappa^n)(e^{-\tau L_\kappa^n} - I)e_u^n - \int_0^\tau (I + \tau L_\kappa^n)e^{-(\tau - \theta)L_\kappa^n} R_{1u}^n(\theta) \, \mathrm{d}\theta.$$

Taking the discrete inner product of (3.20) with $\delta_t e_u^{n+1} := (e_u^{n+1} - e_u^n)/\tau$, we get the reformulation of the left-hand side (LHS) of (3.20) as

$$\text{LHS} = \tau\|\delta_t e_u^{n+1}\|^2 + \kappa g(u^n, s^n)\|e_u^{n+1} - e_u^n\|^2 + \varepsilon^2\|\nabla_h e_u^{n+1} - \nabla_h e_u^n\|^2$$

and the reformulation of the right-hand side (RHS) of (3.20) as

$$\text{RHS} = \tau\langle(I + \tau L_\kappa^n)\phi_1(-\tau L_\kappa^n)[N_\kappa^n(u^n, s^n) - N_\kappa^n(u_{h,e}(t_n), s_{h,e}(t_n))], \delta_t e_u^{n+1}\rangle$$
$$+ \langle(I + \tau L_\kappa^n)(\mathrm{e}^{-\tau L_\kappa^n} - I)e_u^n, \delta_t e_u^{n+1}\rangle - \int_0^\tau \langle(I + \tau L_\kappa^n)\mathrm{e}^{-(\tau-\theta)L_\kappa^n}R_{1u}^n(\theta), \delta_t e_u^{n+1}\rangle \, \mathrm{d}\theta.$$

By using Corollary 3.5, the identity $\|e_u^{n+1} - e_u^n\|^2 = \|e_u^{n+1}\|^2 - \|e_u^n\|^2 - 2\tau\langle e_u^n, \delta_t e_u^{n+1}\rangle$, and Young's inequality, we obtain

$$(3.21) \qquad \text{LHS} \geq \tau\|\delta_t e_u^{n+1}\|^2 + G_*\kappa\|e_u^{n+1}\|^2 - G_*\kappa\|e_u^n\|^2 - 2G_*\kappa\tau\langle e_u^n, \delta_t e_u^{n+1}\rangle$$
$$\geq \frac{7\tau}{8}\|\delta_t e_u^{n+1}\|^2 + G_*\kappa\|e_u^{n+1}\|^2 - G_*\kappa\|e_u^n\|^2 - 8G_*^2\kappa^2\tau\|e_u^n\|^2.$$

According to (3.10), when $\tau \leq M_h^{-1}$, we have $\|I + \tau L_\kappa^n\| \leq 1 + \tau\rho(L_\kappa^n) \leq 2$. By Lemma 3.4, we have $\|\mathrm{e}^{-\tau L_\kappa^n} - I\| \leq \|\tau L_\kappa^n\| \leq M_h\tau$. Thus, for $\tau \leq M_h^{-1}$, we have

$$(3.22) \qquad \text{RHS} \leq 2\tau\|N_\kappa^n(u^n, s^n) - N_\kappa^n(u_{h,e}(t_n), s_{h,e}(t_n))\|\|\delta_t e_u^{n+1}\|$$
$$+ 2M_h\tau\|e_u^n\|\|\delta_t e_u^{n+1}\| + 2\tau \sup_{\theta\in(0,\tau)}\|R_{1u}^n(\theta)\|\|\delta_t e_u^{n+1}\|$$
$$\leq 8\tau\|N_\kappa^n(u^n, s^n) - N_\kappa^n(u_{h,e}(t_n), s_{h,e}(t_n))\|^2$$
$$+ 8M_h^2\tau\|e_u^n\|^2 + 8\tau \sup_{\theta\in(0,\tau)}\|R_{1u}^n(\theta)\|^2 + \frac{3\tau}{8}\|\delta_t e_u^{n+1}\|^2.$$

Using Lemma 3.6, we have

$$(3.23) \quad \|N_\kappa^n(u^n, s^n) - N_\kappa^n(u_{h,e}(t_n), s_{h,e}(t_n))\|$$
$$\leq \|g(u^n, s^n)f(u^n) - g(u_{h,e}(t_n), s_{h,e}(t_n))f(u_{h,e}(t_n))\| + \kappa g(u^n, s^n)\|e_u^n\|$$
$$\leq (C_g + G^*\kappa)\|e_u^n\| + C_g|e_s^n|,$$

and thus we obtain from (3.22) and (3.23) that

$$(3.24) \qquad \text{RHS} \leq [16(C_g + G^*\kappa)^2 + 8M_h^2]\tau\|e_u^n\|^2 + 16C_g^2\tau|e_s^n|^2$$
$$+ 8\tau \sup_{\theta\in(0,\tau)}\|R_{1u}^n(\theta)\|^2 + \frac{3\tau}{8}\|\delta_t e_u^{n+1}\|^2.$$

Combining (3.24) with (3.21), we obtain

$$(3.25) \qquad G_*\kappa\|e_u^{n+1}\|^2 - G_*\kappa\|e_u^n\|^2 + \frac{\tau}{2}\|\delta_t e_u^{n+1}\|^2$$
$$\leq [16(C_g + G^*\kappa)^2 + 8M_h^2 + 8G_*^2\kappa^2]\tau\|e_u^n\|^2 + 16C_g^2\tau|e_s^n|^2$$
$$+ 8\tau \sup_{\theta\in(0,\tau)}\|R_{1u}^n(\theta)\|^2.$$

The difference between (3.5b) and (3.15) leads to

$$e_s^{n+1} - e_s^n = \langle g(u_{h,e}(t_n), s_{h,e}(t_n))f(u_{h,e}(t_n)) - g(u^n, s^n)f(u^n), u_{h,e}(t_{n+1}) - u_{h,e}(t_n)\rangle$$

$$- g(u^n, s^n)\langle f(u^n), e_u^{n+1} - e_u^n\rangle - \tau R_{1s}^n.$$

Multiplying the above equation by $2e_s^{n+1}$ yields

$$(3.26) \quad |e_s^{n+1}|^2 - |e_s^n|^2 + |e_s^{n+1} - e_s^n|^2$$
$$= 2e_s^{n+1}\langle g(u_{h,e}(t_n), s_{h,e}(t_n))f(u_{h,e}(t_n)) - g(u^n, s^n)f(u^n),$$
$$u_{h,e}(t_{n+1}) - u_{h,e}(t_n)\rangle - 2\tau g(u^n, s^n)e_s^{n+1}\langle f(u^n), \delta_t e_u^{n+1}\rangle - 2\tau R_{1s}^n e_s^{n+1}.$$

For the first term on the RHS of (3.26), using Lemma 3.6, we have

$$(3.27)$$
$$2e_s^{n+1}\langle g(u_{h,e}(t_n), s_{h,e}(t_n))f(u_{h,e}(t_n)) - g(u^n, s^n)f(u^n), u_{h,e}(t_{n+1}) - u_{h,e}(t_n)\rangle$$
$$\leq 2|e_s^{n+1}|\|g(u_{h,e}(t_n), s_{h,e}(t_n))f(u_{h,e}(t_n)) - g(u^n, s^n)f(u^n)\|\|u_{h,e}(t_{n+1}) - u_{h,e}(t_n)\|$$
$$\leq 2C_g\tau|e_s^{n+1}|(\|e_u^n\| + |e_s^n|)\|(u_{h,e})_t(\theta_n)\| \qquad (t_n < \theta_n < t_{n+1})$$
$$\leq C_1\tau(\|e_u^n\|^2 + |e_s^n|^2 + |e_s^{n+1}|^2),$$

where $C_1 > 0$ depends on C_*, $|\Omega|$, $u_{h,e}$, and $\|f\|_{C^1[-\beta,\beta]}$. For the second term on the RHS of (3.26), we have

$$(3.28) \qquad -2\tau g(u^n, s^n)e_s^{n+1}\langle f(u^n), \delta_t e_u^{n+1}\rangle \leq 2\tau G^*\|f(u^n)\||e_s^{n+1}|\|\delta_t e_u^{n+1}\|$$
$$\leq C_2\tau|e_s^{n+1}|^2 + \frac{\tau}{2}\|\delta_t e_u^{n+1}\|^2,$$

where $C_2 > 0$ depends on C_*, $|\Omega|$, u_{init}, and $\|f\|_{C[-\beta,\beta]}$. For the third term on the RHS of (3.26), we have

$$(3.29) \qquad -2\tau R_{1s}^n e_s^{n+1} \leq \tau|R_{1s}^n|^2 + \tau|e_s^{n+1}|^2.$$

Substituting (3.27)–(3.29) into (3.26) leads to
$$(3.30)$$
$$|e_s^{n+1}|^2 - |e_s^n|^2 \leq C_1\tau\|e_u^n\|^2 + C_1\tau|e_s^n|^2 + (1 + C_1 + C_2)\tau|e_s^{n+1}|^2 + \frac{\tau}{2}\|\delta_t e_u^{n+1}\|^2 + \tau|R_{1s}^n|^2.$$

Adding (3.25) and (3.30) and using (3.16), we reach

$$G_*\kappa(\|e_u^{n+1}\|^2 - \|e_u^n\|^2) + (|e_s^{n+1}|^2 - |e_s^n|^2) \leq C_3\tau(\|e_u^n\|^2 + |e_s^n|^2 + |e_s^{n+1}|^2) + 9C_{e,h}^2\tau^3,$$

where $C_3 > 0$ depends on C_*, $|\Omega|$, T, $u_{h,e}$, κ, ε, and $\|f\|_{C^1[-\beta,\beta]}$. Finally, by applying the discrete Gronwall inequality, we obtain

$$G_*\kappa\|e_u^n\|^2 + |e_s^n|^2 \leq \tilde{C}_{h,1}\tau^2,$$

where $\tilde{C}_{h,1} > 0$ is a constant independent of τ, which finally gives us (3.18) by taking $C_{h,1} = \sqrt{\tilde{C}_{h,1}/\min\{1, \widehat{G}_*\kappa\}}$. $\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\Box$

3.2. Second-order GSAV-EI scheme. Now we present the second-order generalized SAV-exponential integrator (GSAV-EI2) scheme, which is developed in the prediction-correction fashion. Let $\kappa > 0$ again be the stabilizing constant. First, we adopt the GSAV-EI1 scheme (3.5) to generate a solution $(\widetilde{u}^{n+1}, \widetilde{s}^{n+1})$ as the prediction and define $\widetilde{u}^{n+\frac{1}{2}} = (u^n + \widetilde{u}^{n+1})/2$ and $\widetilde{s}^{n+\frac{1}{2}} = (s^n + \widetilde{s}^{n+1})/2$. Then we rewrite the space-discrete system (3.2a) in the equivalent form as

$$\frac{\mathrm{d}u_h}{\mathrm{d}t} = \varepsilon^2 \Delta_h u_h + g(u_h, s_h)f(u_h) + \kappa g(\widetilde{u}^{n+\frac{1}{2}}, \widetilde{s}^{n+\frac{1}{2}})(u_h - u_h)$$

$$= -L_\kappa^{n+\frac{1}{2}} u_h + N_\kappa^{n+\frac{1}{2}}(u_h, s_h),$$

where the linear operator $L_\kappa^{n+\frac{1}{2}} = \kappa g(\widetilde{u}^{n+\frac{1}{2}}, \widetilde{s}^{n+\frac{1}{2}})I - \varepsilon^2 \Delta_h$ is self-adjoint and positive definite since $g(\widetilde{u}^{n+\frac{1}{2}}, \widetilde{s}^{n+\frac{1}{2}}) > 0$ and $\kappa > 0$, and the nonlinear operator

$$(3.31) \qquad N_\kappa^{n+\frac{1}{2}}(v, r) = g(v, r) f(v) + \kappa g(\widetilde{u}^{n+\frac{1}{2}}, \widetilde{s}^{n+\frac{1}{2}}) v \quad \forall v \in \mathcal{M}_h, \ \forall r \in \mathbb{R}.$$

Applying the variation-of-constants formula gives us

$$(3.32) \quad u_h(t_{n+1}) = \mathrm{e}^{-\tau L_\kappa^{n+\frac{1}{2}}} u_h(t_n) + \int_0^\tau \mathrm{e}^{-(\tau - \theta) L_\kappa^{n+\frac{1}{2}}} N_\kappa^{n+\frac{1}{2}}(u_h(t_n + \theta), s_h(t_n + \theta)) \, \mathrm{d}\theta.$$

Approximating the term $N_\kappa^{n+\frac{1}{2}}$ by its value at $\theta = \frac{\tau}{2}$ in the above equation, i.e.,

$$(3.33) \qquad N_\kappa^{n+\frac{1}{2}}(u_h(t_n + \theta), s_h(t_n + \theta)) \approx N_\kappa^{n+\frac{1}{2}}(u_h(t_{n+\frac{1}{2}}), s_h(t_{n+\frac{1}{2}})),$$

we obtain the GSAV-EI2 scheme for computing u^{n+1} as

$$(3.34\mathrm{a}) \qquad u^{n+1} = \mathrm{e}^{-\tau L_\kappa^{n+\frac{1}{2}}} u^n + \left(\int_0^\tau \mathrm{e}^{-(\tau - \theta) L_\kappa^{n+\frac{1}{2}}} \, \mathrm{d}\theta \right) N_\kappa^{n+\frac{1}{2}}(\widetilde{u}^{n+\frac{1}{2}}, \widetilde{s}^{n+\frac{1}{2}})$$

$$= \mathrm{e}^{-\tau L_\kappa^{n+\frac{1}{2}}} u^n + \tau \phi_1(-\tau L_\kappa^{n+\frac{1}{2}}) N_\kappa^{n+\frac{1}{2}}(\widetilde{u}^{n+\frac{1}{2}}, \widetilde{s}^{n+\frac{1}{2}}).$$

To update s^{n+1}, we discretize (3.2b) at $t = t_{n+\frac{1}{2}}$ to give

$$(3.34\mathrm{b}) \qquad s^{n+1} = s^n - g(\widetilde{u}^{n+\frac{1}{2}}, \widetilde{s}^{n+\frac{1}{2}}) \langle f(\widetilde{u}^{n+\frac{1}{2}}), u^{n+1} - u^n \rangle$$

$$+ \frac{\kappa}{2} g(\widetilde{u}^{n+\frac{1}{2}}, \widetilde{s}^{n+\frac{1}{2}}) \langle u^{n+1} - \widetilde{u}^{n+1}, u^{n+1} - u^n \rangle.$$

The second term on the RHS of (3.34b) is based on the Crank–Nicolson discretization, and the third term is an artificial stabilization term of high order.

3.2.1. Energy dissipation and MBP. Similar to the analysis of the GSAV-EI1 scheme, we first prove the unconditional preservation of the energy dissipation law and the MBP of the GSAV-EI2 scheme (3.34); then we show the uniform boundedness of $g(u^n, s^n)$ and $g(\widetilde{u}^{n+\frac{1}{2}}, \widetilde{s}^{n+\frac{1}{2}})$, which is important to the error analysis.

THEOREM 3.8 (energy dissipation of GSAV-EI2). *The GSAV-EI2 scheme* (3.34) *is unconditionally energy dissipative in the time-discrete sense that* $\mathcal{E}_h(u^{n+1}, s^{n+1}) \leq \mathcal{E}_h(u^n, s^n)$ *holds for any* $\tau > 0$ *and* $n \geq 0$.

Proof. Similar to the proof of Theorem 3.1, some simple calculations give us

$$\mathcal{E}_h(u^{n+1}, s^{n+1}) - \mathcal{E}_h(u^n, s^n) = \langle L_\kappa^{n+\frac{1}{2}} u^{n+1} - N_\kappa^{n+\frac{1}{2}}(\widetilde{u}^{n+\frac{1}{2}}, \widetilde{s}^{n+\frac{1}{2}}), u^{n+1} - u^n \rangle$$

$$- \kappa g(\widetilde{u}^{n+\frac{1}{2}}, \widetilde{s}^{n+\frac{1}{2}}) \langle u^{n+1} - \widetilde{u}^{n+\frac{1}{2}}, u^{n+1} - u^n \rangle$$

$$- \frac{\varepsilon^2}{2} \|\nabla_h u^{n+1} - \nabla_h u^n\|^2 + \frac{\kappa}{2} g(\widetilde{u}^{n+\frac{1}{2}}, \widetilde{s}^{n+\frac{1}{2}}) \langle u^{n+1} - \widetilde{u}^{n+1}, u^{n+1} - u^n \rangle$$

$$= \langle (L_\kappa^{n+\frac{1}{2}} - (I - \mathrm{e}^{-\tau L_\kappa^{n+\frac{1}{2}}})^{-1} L_\kappa^{n+\frac{1}{2}})(u^{n+1} - u^n), u^{n+1} - u^n \rangle$$

$$- \frac{\varepsilon^2}{2} \|\nabla_h u^{n+1} - \nabla_h u^n\|^2 - \frac{\kappa}{2} g(\widetilde{u}^{n+\frac{1}{2}}, \widetilde{s}^{n+\frac{1}{2}}) \|u^{n+1} - u^n\|^2.$$

Then the energy dissipation comes from the negative definiteness of the operator $L_\kappa^{n+\frac{1}{2}} - (I - \mathrm{e}^{-\tau L_\kappa^{n+\frac{1}{2}}})^{-1} L_\kappa^{n+\frac{1}{2}}$. $\square$

COROLLARY 3.9. *For any $\tau > 0$ and $n \geq 0$, it holds that $s^n \leq E_h(u_{\mathrm{init}})$ and $\widetilde{s}^{n+1} \leq E_h(u_{\mathrm{init}})$ for the GSAV-EI2 scheme* (3.34).

Proof. Similar to the proof of Corollary 3.2, the uniform boundedness of $\{s^n\}$ is a direct consequence of Theorem 3.8. Since $\widetilde{s}^{n+1}$ is generated by the GSAV-EI1 scheme (3.5), we have $\widetilde{s}^{n+1} \leq \mathcal{E}_h(\widetilde{u}^{n+1}, \widetilde{s}^{n+1}) \leq \mathcal{E}_h(u^n, s^n)$ according to Theorem 3.1, and thus $\widetilde{s}^{n+1} \leq E_h(u_{\mathrm{init}})$. □

THEOREM 3.10 (MBP of GSAV-EI2). *If $\kappa \geq \|f'\|_{C[-\beta,\beta]}$, then the GSAV-EI2 scheme* (3.34) *preserves the MBP unconditionally; i.e., for any $\tau > 0$, the time-discrete version of MBP* (3.8) *is valid.*

Proof. Suppose (u^n, s^n) is given and $\|u^n\|_\infty \leq \beta$ for some n. According to Theorem 3.3, we know that $\|\widetilde{u}^{n+1}\|_\infty \leq \beta$, and thus $\|\widetilde{u}^{n+\frac{1}{2}}\|_\infty \leq \beta$. We also have from Theorem 3.8 that $\widetilde{s}^{n+\frac{1}{2}} \leq E_h(u_{\mathrm{init}})$. Noting that (3.34a) has the same form as (3.5a), the proof can be completed in a way similar to that of Theorem 3.3. □

COROLLARY 3.11. *Given any fixed $h > 0$ and $T > 0$, if $\kappa \geq \|f'\|_{C[-\beta,\beta]}$ and $\|u_{\mathrm{init}}\|_\infty \leq \beta$, then there are two constants $\widehat{G}_* > 0$ and $G^* > 0$ such that*

$$\widehat{G}_* \leq g(u^n, s^n) \leq G^*, \quad \widehat{G}_* \leq g(\widetilde{u}^{n+\frac{1}{2}}, \widetilde{s}^{n+\frac{1}{2}}) \leq G^*, \quad 0 \leq n \leq \lfloor T/\tau \rfloor - 1,$$

where G^* is the same constant defined in Corollary 3.5, and $\widehat{G}_*$ depends on C_*, C^*, $|\Omega|$, T, u_{init}, κ, ε, and $\|f\|_{C[-\beta,\beta]}$ but is independent of τ.

Proof. As done in the proof of Corollary 3.5, the upper bound G^* of $\{g(u^n, s^n)\}$ and $\{g(\widetilde{u}^{n+\frac{1}{2}}, \widetilde{s}^{n+\frac{1}{2}})\}$ is the direct result of the monotonicity of σ and Theorems 3.8 and 3.10, and thus $\rho(L_\kappa^n) \leq M_h$ and $\rho(L_\kappa^{n+\frac{1}{2}}) \leq M_h$ with $M_h > 0$ the same constant defined in (3.10). For the existence of the lower bound $\widehat{G}_*$, it suffices to show the existence of the lower bounds of $\{s^n\}$ and $\{\widetilde{s}^{n+\frac{1}{2}}\}$. Similar to the derivations in the proof of Corollary 3.5, we have

$$\|u^{n+1} - u^n\| \leq \tau\beta|\Omega|^{\frac{1}{2}}(M_h + G^*\kappa), \qquad \|\widetilde{u}^{n+1} - u^n\| \leq \tau\beta|\Omega|^{\frac{1}{2}}(M_h + G^*\kappa),$$

and thus $\|u^{n+1} - \widetilde{u}^{n+1}\| \leq 2T\beta|\Omega|^{\frac{1}{2}}(M_h + G^*\kappa)$. Then we derive from (3.34b) that

$$\begin{aligned} s^{n+1} &\geq s^n - g(\widetilde{u}^{n+\frac{1}{2}}, \widetilde{s}^{n+\frac{1}{2}})\|f(\widetilde{u}^{n+\frac{1}{2}})\|\|u^{n+1} - u^n\| \\ &\quad - \frac{\kappa}{2}g(\widetilde{u}^{n+\frac{1}{2}}, \widetilde{s}^{n+\frac{1}{2}})\|u^{n+1} - \widetilde{u}^{n+1}\|\|u^{n+1} - u^n\| \\ &\geq s^n - G^*F_0\beta|\Omega|(M_h + G^*\kappa)\tau - G^*\kappa T\beta^2|\Omega|(M_h + G^*\kappa)^2\tau. \end{aligned}$$

By recursion, we obtain

$$s^n \geq -C_* - G^*F_0\beta|\Omega|(M_h + G^*\kappa)T - G^*\kappa\beta^2|\Omega|(M_h + G^*\kappa)^2T^2.$$

Finally, according to (3.11), we also have

$$\widetilde{s}^{n+1} \geq s^n - G^*F_0\beta|\Omega|(M_h + G^*\kappa)T,$$

which completes the proof. □

3.2.2. Temporal error analysis. The following lemma claims that the temporal truncation error of (3.34) is of second order. The proof involves some careful computations in calculus, and we present it in Appendix A.

LEMMA 3.12. *Given any fixed $h > 0$ and $T > 0$, assume that the exact solution $u_{h,e}$ is smooth enough on $[0, T]$. Define $\widetilde{u}_{h,e}^{n+\frac{1}{2}} = (u_{h,e}(t_n) + u_{h,e}(t_{n+1}))/2$ and $\widetilde{s}_{h,e}^{n+\frac{1}{2}} = (s_{h,e}(t_n) + s_{h,e}(t_{n+1}))/2$. It holds that*

(3.35a)
$$u_{h,e}(t_{n+1}) = \mathrm{e}^{-\tau L_\kappa^{n+\frac{1}{2}}} u_{h,e}(t_n) + \tau \phi_1(-\tau L_\kappa^{n+\frac{1}{2}}) N_\kappa^{n+\frac{1}{2}}(\widetilde{u}_{h,e}^{n+\frac{1}{2}}, \widetilde{s}_{h,e}^{n+\frac{1}{2}}) + \tau R_{2u}^n,$$

(3.35b)
$$s_{h,e}(t_{n+1}) = s_{h,e}(t_n) - g(\widetilde{u}_{h,e}^{n+\frac{1}{2}}, \widetilde{s}_{h,e}^{n+\frac{1}{2}}) \langle f(\widetilde{u}_{h,e}^{n+\frac{1}{2}}), u_{h,e}(t_{n+1}) - u_{h,e}(t_n) \rangle + \tau R_{2s}^n,$$

with the truncation terms R_{2u}^n and R_{2s}^n satisfying

(3.36)
$$\|R_{2u}^n\| \le C_{e,h} \tau^2, \qquad |R_{2s}^n| \le C_{e,h} \tau^2,$$

where the constant $C_{e,h} > 0$ is independent of τ.

The error functions e_u^n and e_s^n are defined by (3.17). In addition, we define

$$\widetilde{e}_u^{n+1} = \widetilde{u}^{n+1} - u_{h,e}(t_{n+1}), \qquad \widetilde{e}_s^{n+1} = \widetilde{s}^{n+1} - s_{h,e}(t_{n+1}).$$

We first present a lemma on the estimates with respect to $\widetilde{e}_u^{n+1}$ and $\widetilde{e}_s^{n+1}$. The proof is similar to that of Theorem 3.7 and will be given in Appendix B.

LEMMA 3.13. *Given any fixed $h > 0$ and $T > 0$, let $\kappa \ge \|f'\|_{C[-\beta,\beta]}$. Assume that the exact solution $u_{h,e}$ is smooth enough on $[0, T]$ and $\|u_{\mathrm{init}}\|_\infty \le \beta$. If τ is sufficiently small, then it holds that*

(3.37)
$$\|\widetilde{e}_u^{n+1}\|^2 + |\widetilde{e}_s^{n+1}|^2 \le \widetilde{C}_h(\|e_u^n\|^2 + |e_s^n|^2) + \widetilde{C}_h C_{e,h}^2 \tau^4, \quad 0 \le n \le \lfloor T/\tau \rfloor,$$

where the constant $\widetilde{C}_h > 0$ is independent of τ.

THEOREM 3.14 (temporal error estimate of GSAV-EI2). *Given any fixed $h > 0$ and $T > 0$, let $\kappa \ge \|f'\|_{C[-\beta,\beta]}$. Assume that the exact solution $u_{h,e}$ is smooth enough on $[0, T]$ and $\|u_{\mathrm{init}}\|_\infty \le \beta$. If τ is sufficiently small, then we have the following error estimate for the GSAV-EI2 scheme (3.34):*

(3.38)
$$\|u^n - u_{h,e}(t_n)\| + |s^n - s_{h,e}(t_n)| \le C_{h,2} \tau^2, \quad 0 \le n \le \lfloor T/\tau \rfloor,$$

where the constant $C_{h,2} > 0$ is independent of τ.

Proof. The difference between (3.34a) and (3.35a) gives

$$e_u^{n+1} = \mathrm{e}^{-\tau L_\kappa^{n+\frac{1}{2}}} e_u^n + \tau \phi_1(-\tau L_\kappa^{n+\frac{1}{2}}) [N_\kappa^{n+\frac{1}{2}}(\widetilde{u}^{n+\frac{1}{2}}, \widetilde{s}^{n+\frac{1}{2}}) - N_\kappa^{n+\frac{1}{2}}(\widetilde{u}_{h,e}^{n+\frac{1}{2}}, \widetilde{s}_{h,e}^{n+\frac{1}{2}})] - \tau R_{2u}^n.$$

Acting $I + \tau L_\kappa^{n+\frac{1}{2}}$ on both sides of the above equation, we obtain

(3.39) $$(1 + \tau \kappa g(\widetilde{u}^{n+\frac{1}{2}}, \widetilde{s}^{n+\frac{1}{2}}))(e_u^{n+1} - e_u^n) - \tau \varepsilon^2 (\Delta_h e_u^{n+1} - \Delta_h e_u^n)$$
$$= \tau(I + \tau L_\kappa^{n+\frac{1}{2}}) \phi_1(-\tau L_\kappa^{n+\frac{1}{2}}) [N_\kappa^{n+\frac{1}{2}}(\widetilde{u}^{n+\frac{1}{2}}, \widetilde{s}^{n+\frac{1}{2}}) - N_\kappa^{n+\frac{1}{2}}(\widetilde{u}_{h,e}^{n+\frac{1}{2}}, \widetilde{s}_{h,e}^{n+\frac{1}{2}})]$$
$$+ (I + \tau L_\kappa^{n+\frac{1}{2}})(\mathrm{e}^{-\tau L_\kappa^{n+\frac{1}{2}}} - I)e_u^n - \tau(I + \tau L_\kappa^{n+\frac{1}{2}}) R_{2u}^n.$$

Taking the discrete inner product of (3.39) with $\delta_t e_u^{n+1}$, similarly to (3.21), we estimate the LHS of the above identity as

$$\mathrm{LHS} = \tau \|\delta_t e_u^{n+1}\|^2 + \kappa g(\widetilde{u}^{n+\frac{1}{2}}, \widetilde{s}^{n+\frac{1}{2}}) \|e_u^{n+1} - e_u^n\|^2 + \varepsilon^2 \|\nabla_h e_u^{n+1} - \nabla_h e_u^n\|^2$$

$$\geq \tau\|\delta_t e_u^{n+1}\|^2 + \kappa\widehat{G}_*\|e_u^{n+1} - e_u^n\|^2$$

$$= \tau\|\delta_t e_u^{n+1}\|^2 + \widehat{G}_*\kappa\|e_u^{n+1}\|^2 - \widehat{G}_*\kappa\|e_u^n\|^2 - 2\widehat{G}_*\kappa\tau\langle e_u^n, \delta_t e_u^{n+1}\rangle$$

$$\geq \frac{7\tau}{8}\|\delta_t e_u^{n+1}\|^2 + \widehat{G}_*\kappa\|e_u^{n+1}\|^2 - \widehat{G}_*\kappa\|e_u^n\|^2 - 8\widehat{G}_*^2\kappa^2\tau\|e_u^n\|^2,$$

and, when $\tau \leq M_h^{-1}$, we estimate the RHS of (3.39) as

$$\text{RHS} = \tau\langle(I + \tau L_\kappa^{n+\frac{1}{2}})\phi_1(-\tau L_\kappa^{n+\frac{1}{2}})[N_\kappa^{n+\frac{1}{2}}(\widetilde{u}^{n+\frac{1}{2}}, \widetilde{s}^{n+\frac{1}{2}}) - N_\kappa^{n+\frac{1}{2}}(\widetilde{u}_{h,e}^{n+\frac{1}{2}}, \widetilde{s}_{h,e}^{n+\frac{1}{2}})], \delta_t e_u^{n+1}\rangle$$

$$+ \langle(I + \tau L_\kappa^{n+\frac{1}{2}})(e^{-\tau L_\kappa^{n+\frac{1}{2}}} - I)e_u^n, \delta_t e_u^{n+1}\rangle - \tau\langle(I + \tau L_\kappa^{n+\frac{1}{2}})R_{2u}^n, \delta_t e_u^{n+1}\rangle$$

$$\leq 2\tau\|N_\kappa^{n+\frac{1}{2}}(\widetilde{u}^{n+\frac{1}{2}}, \widetilde{s}^{n+\frac{1}{2}}) - N_\kappa^{n+\frac{1}{2}}(\widetilde{u}_{h,e}^{n+\frac{1}{2}}, \widetilde{s}_{h,e}^{n+\frac{1}{2}})\|\|\delta_t e_u^{n+1}\|$$

$$+ 2M_h\tau\|e_u^n\|\|\delta_t e_u^{n+1}\| + 2\tau\|R_{2u}^n\|\|\delta_t e_u^{n+1}\|$$

$$\leq 8\tau\|N_\kappa^{n+\frac{1}{2}}(\widetilde{u}^{n+\frac{1}{2}}, \widetilde{s}^{n+\frac{1}{2}}) - N_\kappa^{n+\frac{1}{2}}(\widetilde{u}_{h,e}^{n+\frac{1}{2}}, \widetilde{s}_{h,e}^{n+\frac{1}{2}})\|^2$$

$$+ 8M_h^2\tau\|e_u^n\|^2 + 8\tau\|R_{2u}^n\|^2 + \frac{3\tau}{8}\|\delta_t e_u^{n+1}\|^2.$$

Note that

$$N_\kappa^{n+\frac{1}{2}}(\widetilde{u}^{n+\frac{1}{2}}, \widetilde{s}^{n+\frac{1}{2}}) - N_\kappa^{n+\frac{1}{2}}(\widetilde{u}_{h,e}^{n+\frac{1}{2}}, \widetilde{s}_{h,e}^{n+\frac{1}{2}})$$

$$= g(\widetilde{u}^{n+\frac{1}{2}}, \widetilde{s}^{n+\frac{1}{2}})f(\widetilde{u}^{n+\frac{1}{2}}) - g(\widetilde{u}_{h,e}^{n+\frac{1}{2}}, \widetilde{s}_{h,e}^{n+\frac{1}{2}})f(\widetilde{u}_{h,e}^{n+\frac{1}{2}}) + \kappa g(\widetilde{u}^{n+\frac{1}{2}}, \widetilde{s}^{n+\frac{1}{2}})\widetilde{e}_u^{n+\frac{1}{2}}$$

and $\widetilde{u}^{n+\frac{1}{2}}, \widetilde{u}_{h,e}^{n+\frac{1}{2}}, \widetilde{s}^{n+\frac{1}{2}}, \widetilde{s}_{h,e}^{n+\frac{1}{2}}$ are all bounded uniformly according to the energy dissipation law and the MBP. Similar to the proof of Lemma 3.6, we can obtain

$$(3.40) \qquad \|N_\kappa^{n+\frac{1}{2}}(\widetilde{u}^{n+\frac{1}{2}}, \widetilde{s}^{n+\frac{1}{2}}) - N_\kappa^{n+\frac{1}{2}}(\widetilde{u}_{h,e}^{n+\frac{1}{2}}, \widetilde{s}_{h,e}^{n+\frac{1}{2}})\|$$

$$\leq \frac{C_g + G^*\kappa}{2}(\|e_u^n\| + \|\widetilde{e}_u^{n+1}\|) + \frac{C_g}{2}(|e_s^n| + |\widetilde{e}_s^{n+1}|).$$

Combining (3.40) with estimates of the LHS and RHS of (3.39), we get

$$(3.41) \qquad \widehat{G}_*\kappa\|e_u^{n+1}\|^2 - \widehat{G}_*\kappa\|e_u^n\|^2 + \frac{\tau}{2}\|\delta_t e_u^{n+1}\|^2$$

$$\leq [8(C_g + G^*\kappa)^2 + 8M_h^2 + 8\widehat{G}_*^2\kappa^2]\tau\|e_u^n\|^2 + 8(C_g + G^*\kappa)^2\tau\|\widetilde{e}_u^{n+1}\|^2$$

$$+ 8C_g^2\tau(|e_s^n|^2 + |\widetilde{e}_s^{n+1}|^2) + 8\tau\|R_{2u}^n\|^2.$$

For the error equation (3.35b), we can add a zero-value term to the RHS to give

$$(3.42) \qquad s_{h,e}(t_{n+1}) - s_{h,e}(t_n)$$

$$= -g(\widetilde{u}_{h,e}^{n+\frac{1}{2}}, \widetilde{s}_{h,e}^{n+\frac{1}{2}})\langle f(\widetilde{u}_{h,e}^{n+\frac{1}{2}}), u_{h,e}(t_{n+1}) - u_{h,e}(t_n)\rangle + \frac{\kappa}{2}g(\widetilde{u}^{n+\frac{1}{2}}, \widetilde{s}^{n+\frac{1}{2}})$$

$$\cdot \langle u_{h,e}(t_{n+1}) - u_{h,e}(t_{n+1}), u_{h,e}(t_{n+1}) - u_{h,e}(t_n)\rangle + \tau R_{2s}^n.$$

The difference between (3.34b) and (3.42) leads to

$$e_s^{n+1} - e_s^n = \langle g(\widetilde{u}_{h,e}^{n+\frac{1}{2}}, \widetilde{s}_{h,e}^{n+\frac{1}{2}})f(\widetilde{u}_{h,e}^{n+\frac{1}{2}}) - g(\widetilde{u}^{n+\frac{1}{2}}, \widetilde{s}^{n+\frac{1}{2}})f(\widetilde{u}^{n+\frac{1}{2}}), u_{h,e}(t_{n+1}) - u_{h,e}(t_n)\rangle$$

$$+ \frac{\kappa}{2}g(\widetilde{u}^{n+\frac{1}{2}}, \widetilde{s}^{n+\frac{1}{2}})\langle u^{n+1} - \widetilde{u}^{n+1}, e_u^{n+1} - e_u^n\rangle$$

$$- g(\widetilde{u}^{n+\frac{1}{2}}, \widetilde{s}^{n+\frac{1}{2}})\langle f(\widetilde{u}^{n+\frac{1}{2}}), e_u^{n+1} - e_u^n\rangle$$

$$+ \frac{\kappa}{2}g(\widetilde{u}^{n+\frac{1}{2}},\widetilde{s}^{n+\frac{1}{2}})\langle e_u^{n+1} - \widetilde{e}_u^{n+1}, u_{h,e}(t_{n+1}) - u_{h,e}(t_n)\rangle - \tau R_{2s}^n.$$

Multiplying the above equation by $2e_s^{n+1}$ yields

$$|e_s^{n+1}|^2 - |e_s^n|^2 + |e_s^{n+1} - e_s^n|^2$$
$$= 2e_s^{n+1}\langle g(\widetilde{u}_{h,e}^{n+\frac{1}{2}},\widetilde{s}_{h,e}^{n+\frac{1}{2}})f(\widetilde{u}_{h,e}^{n+\frac{1}{2}}) - g(\widetilde{u}^{n+\frac{1}{2}},\widetilde{s}^{n+\frac{1}{2}})f(\widetilde{u}^{n+\frac{1}{2}}), u_{h,e}(t_{n+1}) - u_{h,e}(t_n)\rangle$$
$$+ \tau\kappa g(\widetilde{u}^{n+\frac{1}{2}},\widetilde{s}^{n+\frac{1}{2}})e_s^{n+1}\langle u^{n+1} - \widetilde{u}^{n+1}, \delta_t e_u^{n+1}\rangle$$
$$- 2\tau e_s^{n+1}g(\widetilde{u}^{n+\frac{1}{2}},\widetilde{s}^{n+\frac{1}{2}})\langle f(\widetilde{u}^{n+\frac{1}{2}}), \delta_t e_u^{n+1}\rangle$$
$$+ \kappa g(\widetilde{u}^{n+\frac{1}{2}},\widetilde{s}^{n+\frac{1}{2}})e_s^{n+1}\langle e_u^{n+1} - \widetilde{e}_u^{n+1}, u_{h,e}(t_{n+1}) - u_{h,e}(t_n)\rangle - 2\tau e_s^{n+1}R_{2s}^n.$$

Similar to the deduction from (3.26) to (3.30), we then obtain

(3.43) $\quad |e_s^{n+1}|^2 - |e_s^n|^2 \le C_5\tau(\|e_u^n\|^2 + \|e_u^{n+1}\|^2 + \|\widetilde{e}_u^{n+1}\|^2$
$$+ |e_s^n|^2 + |e_s^{n+1}|^2 + |\widetilde{e}_s^{n+1}|^2) + \frac{\tau}{2}\|\delta_t e_u^{n+1}\|^2 + \tau|R_{2s}^n|^2$$

with C_5 depending on C_*, $|\Omega|$, $u_{h,e}$, κ, and $\|f\|_{C^1[-\beta,\beta]}$.

Adding (3.41) and (3.43), we obtain

(3.44) $\quad \widehat{G}_*\kappa(\|e_u^{n+1}\|^2 - \|e_u^n\|^2) + (|e_s^{n+1}|^2 - |e_s^n|^2)$
$$\le C_6\tau(\|e_u^n\|^2 + \|e_u^{n+1}\|^2 + \|\widetilde{e}_u^{n+1}\|^2 + |e_s^n|^2 + |e_s^{n+1}|^2 + |\widetilde{e}_s^{n+1}|^2)$$
$$+ 8\tau\|R_{2u}^n\|^2 + \tau|R_{2s}^n|^2,$$

where $C_6 > 0$ depends on C_*, $|\Omega|$, $u_{h,e}$, and $\|f\|_{C^1[-\beta,\beta]}$. Substituting (3.37) into (3.44) and using the estimate (3.36), we obtain

(3.45) $\widehat{G}_*\kappa(\|e_u^{n+1}\|^2 - \|e_u^n\|^2) + (|e_s^{n+1}|^2 - |e_s^n|^2)$
$$\le C_6(\widetilde{C}_h + 1)\tau(\|e_u^n\|^2 + \|e_u^{n+1}\|^2 + |e_s^n|^2 + |e_s^{n+1}|^2) + (C_6\widetilde{C}_h + 9)C_{e,h}^2\tau^5.$$

When τ is sufficiently small, similar to the last paragraph in the proof of Theorem 3.7, applying the discrete Gronwall inequality to (3.45) leads to

$$\widehat{G}_*\kappa\|e_u^n\|^2 + |e_s^n|^2 \le \tilde{C}_{h,2}\tau^4,$$

where $\tilde{C}_{h,2} > 0$ is a constant independent of τ, which gives us (3.38) by taking $C_{h,2} = \sqrt{\tilde{C}_{h,2}/\min\{1,\widehat{G}_*\kappa\}}$. $\qquad\square$

REMARK 3.4. *In addition to the periodic or homogeneous Neumann boundary condition considered above, one can also equip (1.1) with the Dirichlet boundary condition $u(t,\boldsymbol{x}) = \psi(t,\boldsymbol{x})$ for $t > 0$ and $\boldsymbol{x} \in \partial\Omega$. Then it is shown in [14] that the solution satisfies the MBP (1.4) if $|\psi(t,\boldsymbol{x})| \le \beta$ for any $t > 0$ and $\boldsymbol{x} \in \partial\Omega$, and the energy dissipation law is also valid if $\psi(t,\boldsymbol{x}) = \psi(\boldsymbol{x})$ is independent of t. In particular, for (1.1) with a time-independent boundary value $\|\psi\|_{C(\partial\Omega)} \le \beta$, we are still able to develop the GSAV-EI schemes simultaneously preserving the MBP and the energy dissipation law, based on a slight modification of the space-discrete system (3.2). The main idea is to add an extra term B_h to (3.2a), where B_h depends only on the ratio ε^2/h^2 and the boundary value ψ; see [14] for details of the form of B_h. For example, the GSAV-EI2 scheme can be established by combining (3.34a) with $N_\kappa^{n+\frac{1}{2}}$ replaced by $N_\kappa^{n+\frac{1}{2}} + B_h$ and (3.34b) with $-\langle B_h, u^{n+1} - u^n\rangle$ added to its RHS. Since B_h is time-independent, the B_h-related terms do not affect the order of the truncation error in time. The first-order scheme can be developed in a similar spirit. We omit the details due to the limited space.*

4. Numerical experiments. Let us consider the model equation (1.1) for Allen–Cahn type gradient flows in two-dimensional square domain $\Omega = (0,1) \times (0,1)$ equipped with a periodic boundary condition or a homogeneous Neumann boundary condition. In either case, the product of a matrix exponential with a vector can be efficiently implemented by using the fast transform based on Lemma 2.2(iii). We also set the interfacial parameter $\varepsilon = 0.01$. There are two commonly used forms of the nonlinear function $f(u)$. One is given by the cubic function

$$(4.1) \qquad\qquad f(u) = -F'(u) = u - u^3,$$

where $F(u) = \frac{1}{4}(1 - u^2)^2$ is the double-well potential. In this case, one can set $\beta = 1$ and $\|f'\|_{C[-1,1]} = 2$. The other one is determined by the Flory–Huggins potential $F(u) = \frac{\theta}{2}[(1+u)\ln(1+u) + (1-u)\ln(1-u)] - \frac{\theta_c}{2}u^2$, and

$$(4.2) \qquad\qquad f(u) = -F'(u) = \frac{\theta}{2}\ln\frac{1-u}{1+u} + \theta_c u,$$

where $\theta_c > \theta > 0$. In the following numerical experiments, we set $\theta = 0.8$ and $\theta_c = 1.6$; then the positive root of $f(u) = 0$ is $\beta \approx 0.9575$ and $\|f'\|_{C[-\beta,\beta]} \approx 8.02$. We always set $\kappa = \|f'\|_{C[-\beta,\beta]}$ for both cases in the following experiments. In addition, we always adopt the exponential function with a constant parameter $a > 0$ as

$$(4.3) \qquad\qquad \sigma(x) = \mathrm{e}^{ax}, \quad x \in \mathbb{R}.$$

Clearly, $\sigma(0) = 1$ and $\sigma'(0) = a$.

REMARK 4.1. *For the double-well potential* (4.1) *and the Flory–Huggins potential* (4.2)*, it is easy to see that the value of the bulk energy part $E_{1h}(u^n)$ is close to 0 due to the MBP of $\{u^n\}$. Since s^n is also an approximation of $E_{1h}(u^n)$, only the behavior of σ near 0 has a relatively large effect on the performance of the proposed GSAV-EI schemes. By the Taylor expansion, these typical elementary functions for σ given in Remark 3.1 perform like a linear function near 0 with the y-intercept being 1 and the slope $a = \sigma'(0)$ if parameterized as* (4.3)*. Thus, there is no essential difference on all these choices for the above test problems.*

4.1. Convergence in time. To verify the temporal convergence rates of the GSAV-EI schemes, let us consider the problem (1.1) with a smooth initial value

$$u_{\mathrm{init}}(x,y) = 0.1\sin(2\pi x)\sin(2\pi y).$$

By fixing the uniform spatial mesh size $h = 1/2048$, we compute the numerical solutions at $t = 2$ using the GSAV-EI1 and GSAV-EI2 schemes with various time step sizes $\tau = 2^{-k}$, $k = 4, 5, \ldots, 12$. To compute the numerical errors, the benchmark solution is generated by using the fourth-order integrating factor Runge–Kutta (IFRK4) scheme [31] with the time step size $\tau = 0.1 \times 2^{-12}$. Figure 1 plots the L^2 norms of the numerical errors versus the time step sizes, produced by GSAV-EI1 and GSAV-EI2 with σ given by (4.3) with $a = 1$, $a = 10$, and $a = 100$, where the left graph shows the results for the double-well potential case (4.1) and the right one corresponds to the Flory–Huggins potential case (4.2). The expected convergence rates in time, first order for GSAV-EI1 and second order for GSAV-EI2, are clearly observed for all cases. In addition, we find that the larger a leads to smaller numerical errors for the GSAV-EI2 scheme, but such an effect is not obvious for the GSAV-EI1 scheme.

We also repeat all the above convergence tests on the spatial mesh with $h = 1/512$ and find that the results are almost identical to those with $h = 1/2048$ shown in Figure 1. This suggests that the temporal convergence constants in (3.18) and (3.38) could be independent of the spatial mesh size h, although we are not able to remove their dependence on h in the theoretical analysis.
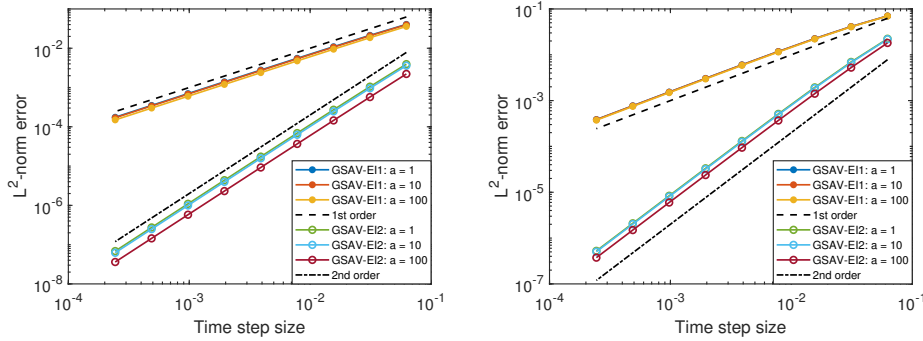

FIG. 1. *The L^2 norm errors vs. the time step sizes produced by the GSAV-EI1 and GSAV-EI2 schemes with the spatial mesh of $h = 1/2048$ for (1.1). Left: the double-well potential (4.1); right: the Flory–Huggins potential (4.2).*

4.2. Unconditional preservation of MBP and energy dissipation law. We numerically verify the MBP and the energy dissipation law of the proposed GSAV-EI1 and GSAV-EI2 schemes by simulating the phase transition process beginning with a random state. Though the discrete energy dissipation law is proved with respect to the slightly modified energy (3.4), we are more concerned about the original energy defined by (2.3) since it reflects the real physical mechanism of the dynamic process. We consider (1.1) on the uniform spatial mesh with $h = 1/512$. Different from the previous convergence tests, the initial state is generated by random numbers ranging from -0.8 to 0.8 on each mesh point, and thus it has highly oscillated values.

We compute the numerical solutions by the GSAV-EI1 and GSAV-EI2 schemes with $\tau = 0.01$ and various values of a ($a = 1, 5, 10$, respectively) and treat the results obtained by the IFRK4 scheme with the time step size $\tau = 10^{-4}$ as the benchmark. First, we adopt the double-well potential (4.1), and the evolutions of the supremum norms and the energies of the numerical solutions are shown in Figure 2. Obviously, the MBP and the energy dissipation law are preserved perfectly. In addition, we observe that the smaller a produces slightly more accurate numerical solutions in this case. This behavior is opposite to that with a smooth initial value shown in the convergence tests. Then we consider the Flory–Huggins potential (4.2) and Figure 3 presents the evolutions of the supremum norms and the energies of the numerical solutions. Similar to the double-well potential case, the preservation of the MBP and the energy dissipation law are obvious, and the smaller value of a in (4.3) yields slightly more accurate numerical solution.

Next, we repeat the above experiments by choosing the (10 times) larger time step size $\tau = 0.1$. We can observe the similar results that the MBP and the energy dissipation law are still preserved well, although the large time step size leads to a little less accurate numerical solutions.

4.3. Adaptive time-stepping and long-time simulation. Since the two proposed GSAV-EI schemes (3.5) and (3.34) are both one-step approaches, without sac-
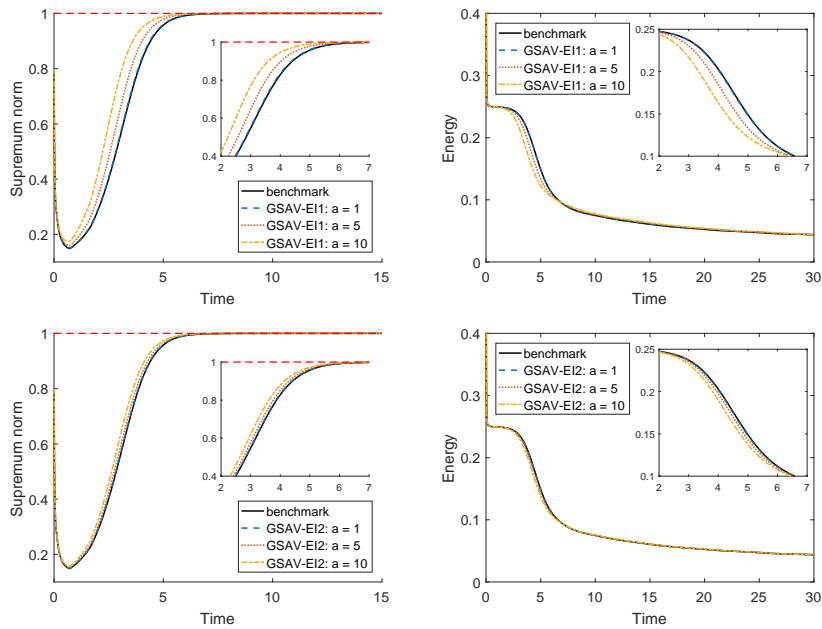
FIG. 2. *Evolutions of the supremum norms and the energies of simulated solutions computed by the GSAV-EI1 (top row) and GSAV-EI2 (bottom row) schemes with $\tau = 0.01$ for (1.1) with the double-well potential* (4.1).
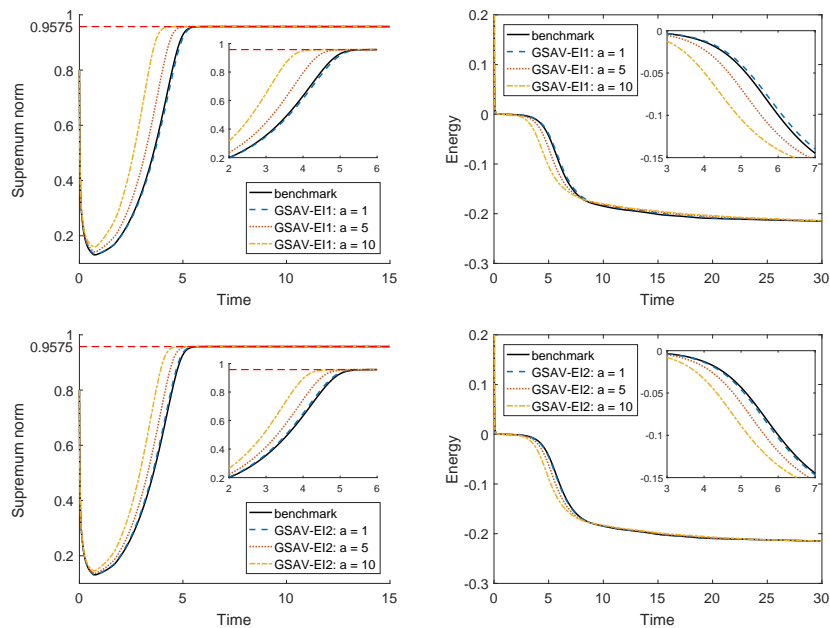

FIG. 3. *Evolutions of the supremum norms and the energies of simulated solutions computed by the GSAV-EI1 (top row) and GSAV-EI2 (bottom row) schemes with $\tau = 0.01$ for (1.1) with the Flory–Huggins potential* (4.2).

rificing the energy dissipation law and the MBP, they can also be applied on a set of nonuniform temporal nodes $\{t_n\}_{n\geq 0}$ with $t_0 = 0$ and $t_{n+1} = t_n + \tau_{n+1}$, where the time step size τ_{n+1} varies in n. Let us consider (1.1) with $\varepsilon = 0.01$ and the Flory–Huggins potential (4.2) again but with the homogeneous Neumann boundary condition. The spatial mesh and the random initial value are the same as aforementioned. We adopt the GSAV-EI2 scheme (3.34) with $\sigma(x) = e^x$ and variable time step sizes τ_{n+1} updated by using the approach from [40]:

$$\tau_{n+1} = \max\left\{\tau_{\min}, \frac{\tau_{\max}}{\sqrt{1 + \alpha|\mathrm{d}_t E_h(u^n)|^2}}\right\},$$

where $\mathrm{d}_t E_h(u^n) = (E_h(u^n) - E_h(u^{n-1}))/\tau_n$ and $\alpha > 0$ is a constant parameter. Here we choose the minimal and maximal time step sizes as $\tau_{\min} = 0.0001$ and $\tau_{\max} = 0.1$, respectively, and set $\alpha = 10^5$ as done in [40]. For comparison, we also conduct the simulation by the GSAV-EI2 scheme with the uniform time step size $\tau = 0.01$.

The coarsening dynamics reach the steady state at around $t = 3000$. We find that the CPU time for the whole simulation with adaptive time stepping is only about 10% of that with uniform time step size. One can observe from the left and middle graphs in Figure 4 that the energy dissipation law and the MBP are preserved perfectly. The right graph in Figure 4 plots the evolution of the adaptive time step sizes. In the time interval $[0, 20]$, the time step size varies significantly and sometimes is very small since the energy decreases rapidly most of the time. Then, after $t = 20$, the energy changes more and more slowly and the time step size is magnified gradually. When $t > 200$, the time step size remains around 0.1 (not shown in the graph), and we find that, although the large step size is used for this period, the relative error of the energy is only about 1% in comparison with the case of uniform time step size. One can also observe from Figure 5 that the configurations at some moments simulated by the adaptive time stepping match those generated with the uniform time step size very well. These results show that the adaptive time-stepping strategy can greatly help accelerate the computation without sacrificing the desired properties and the accuracy.
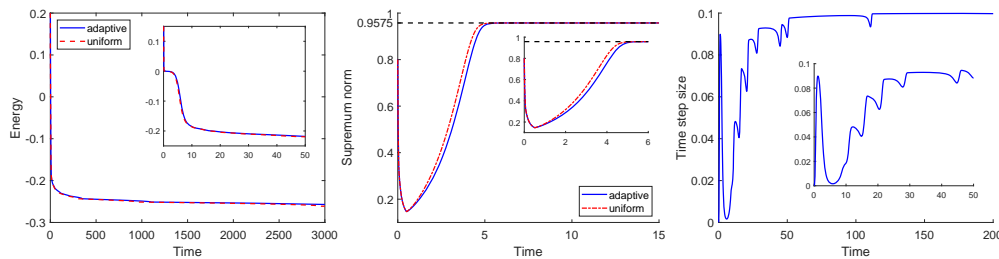

FIG. 4. *Evolutions of the energies (left), the supremum norms (middle), and the time step sizes (right) of simulated solutions computed by the GSAV-EI2 schemes for (1.1) with the homogeneous Neumann boundary condition and the Flory–Huggins potential (4.2).*

5. Concluding remarks. In this paper, we study the numerical schemes preserving both the energy dissipation law and the MBP unconditionally for a class of Allen–Cahn type gradient flows by combining the exponential integrator method and the generalized SAV approach. With the appropriate stabilization terms, we develop first- and second-order GSAV-EI schemes and prove their unconditional preservation
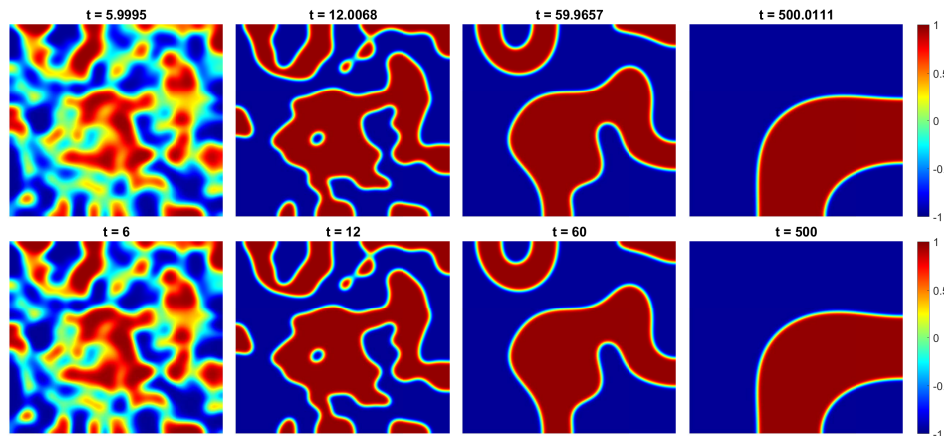
FIG. 5. *Snapshots of the phase transition generated by the GSAV-EI2 schemes with adaptive time step (top) and uniform time step (bottom) for* (1.1) *with the homogeneous Neumann boundary condition and the Flory–Huggins potential* (4.2).

of the energy dissipation law and the MBP in the time discrete sense, as well as their optimal temporal error estimates under fixed spatial mesh. Different from most existing numerical schemes, the energy dissipation law and the MBP of the proposed GSAV-EI schemes can be established in parallel, which provides more flexibility to apply the proposed schemes to other types of gradient flow equations to preserve some important physical properties. We also note that the fully discrete error estimate for the case that the spatial mesh size and the time step size change simultaneously is still an open question for the proposed GSAV-EI schemes and surely worthy of further study. A major difficulty comes from the issue that the matrix exponential $\mathrm{e}^{\tau L_\kappa^n}$, defined by a power series of the sparse matrix τL_κ^n, is dense and affects the solution globally. In particular, to estimate the temporal truncation error of the GSAV-EI2 scheme (Lemma 3.12), an h-dependent bound is inevitable, and thus we fix the spatial mesh size to regard such a bound as a constant in this paper.

When constructing the second-order GSAV-EI scheme (3.34), we approximate the term $N_\kappa^{n+\frac{1}{2}}(u_h(t_n + \theta), s_h(t_n + \theta))$ in (3.32) by its value at the midpoint $\theta = \frac{\tau}{2}$ rather than its linear interpolation in $[0, \tau]$. This allows the cancellation between the nonlinear terms in the analysis of the energy dissipation (Theorem 3.8). Instead, if we adopt the linear interpolation as usually done for the RK2 method, two terms involving the numerical solutions at t_n and t_{n+1} will be included with the ϕ-functions of $\tau L_\kappa^{n+\frac{1}{2}}$ as the coefficients, which makes the cancellation unavailable due to the different coefficients between the updating formula for u^{n+1} and that for s^{n+1}. For a similar reason, it is an open question whether higher-order GSAV-EI schemes exist in either RK or multistep form, although there have been third-order multistep schemes based on the standard ETD method for the epitaxial thin film model [4, 6].

It also remains interesting how to choose the function σ appropriately for the GSAV-EI schemes in practical applications. As we explain in Remark 4.1, we only use the exponential function (4.3) in section 4 since the differences can hardly be observed for the typical choices of σ given in Remark 3.1 for the specific problems we consider in the numerical experiments. However, their performance could be significantly different for some other situations and gradient flows, and more careful investigation is needed. In addition, the effect of the parameter a on the numerical errors seems completely

opposite for the smooth and nonsmooth initial data based on our observation from numerical experiments, and such a phenomenon also deserves deeper study.

Appendix A. Proof of Lemma 3.12.

Proof. From (3.32), we have

$$u_{h,e}(t_{n+1}) = \mathrm{e}^{-\tau L_\kappa^{n+\frac{1}{2}}} u_{h,e}(t_n) + \int_0^\tau \mathrm{e}^{-(\tau-\theta)L_\kappa^{n+\frac{1}{2}}} N_\kappa^{n+\frac{1}{2}}(u_{h,e}(t_n+\theta), s_{h,e}(t_n+\theta))\, \mathrm{d}\theta$$

$$= \mathrm{e}^{-\tau L_\kappa^{n+\frac{1}{2}}} u_{h,e}(t_n) + \left(\int_0^\tau \mathrm{e}^{-(\tau-\theta)L_\kappa^{n+\frac{1}{2}}}\, \mathrm{d}\theta\right) N_\kappa^{n+\frac{1}{2}}(\widetilde{u}_{h,e}^{n+\frac{1}{2}}, \widetilde{s}_{h,e}^{n+\frac{1}{2}}) + \tau R_{2u}^n,$$

which gives (3.35a) with

$$R_{2u}^n = \frac{1}{\tau}\int_0^\tau \mathrm{e}^{-(\tau-\theta)L_\kappa^{n+\frac{1}{2}}}[N_\kappa^{n+\frac{1}{2}}(u_{h,e}(t_n+\theta), s_{h,e}(t_n+\theta)) - N_\kappa^{n+\frac{1}{2}}(\widetilde{u}_{h,e}^{n+\frac{1}{2}}, \widetilde{s}_{h,e}^{n+\frac{1}{2}})]\, \mathrm{d}\theta$$

$$= \frac{1}{\tau}\left(\int_0^\tau [N_\kappa^{n+\frac{1}{2}}(u_{h,e}(t_n+\theta), s_{h,e}(t_n+\theta)) - N_\kappa^{n+\frac{1}{2}}(\widetilde{u}_{h,e}^{n+\frac{1}{2}}, \widetilde{s}_{h,e}^{n+\frac{1}{2}})]\, \mathrm{d}\theta\right.$$

$$\left. + \int_0^\tau (\mathrm{e}^{-(\tau-\theta)L_\kappa^{n+\frac{1}{2}}} - I)[N_\kappa^{n+\frac{1}{2}}(u_{h,e}(t_n+\theta), s_{h,e}(t_n+\theta)) - N_\kappa^{n+\frac{1}{2}}(\widetilde{u}_{h,e}^{n+\frac{1}{2}}, \widetilde{s}_{h,e}^{n+\frac{1}{2}})]\, \mathrm{d}\theta\right)$$

$$=: \frac{1}{\tau}(R_{2u}^{n,1} + R_{2u}^{n,2}).$$

For the function $N_\kappa^{n+\frac{1}{2}}(v,r)$ defined in (3.31), let us denote by $\nabla_v N_\kappa^{n+\frac{1}{2}}(v,r)$ and $\partial_r N_\kappa^{n+\frac{1}{2}}(v,r)$ the derivatives of $N_\kappa^{n+\frac{1}{2}}(v,r)$ with respect to v and r, respectively. By the Taylor expansion, we have

(A.1)

$$N_\kappa(u_{h,e}(t_n+\theta), s_{h,e}(t_n+\theta)) - N_\kappa(\widetilde{u}_{h,e}^{n+\frac{1}{2}}, \widetilde{s}_{h,e}^{n+\frac{1}{2}})$$

$$= \nabla_v N_\kappa(\widetilde{u}_{h,e}^{n+\frac{1}{2}}, \widetilde{s}_{h,e}^{n+\frac{1}{2}})(u_{h,e}(t_n+\theta) - \widetilde{u}_{h,e}^{n+\frac{1}{2}})$$

$$\quad + \partial_r N_\kappa(\widetilde{u}_{h,e}^{n+\frac{1}{2}}, \widetilde{s}_{h,e}^{n+\frac{1}{2}})(s_{h,e}(t_n+\theta) - \widetilde{s}_{h,e}^{n+\frac{1}{2}}) + r_e$$

$$= \frac{2\theta-\tau}{2}\left(\nabla_v N_\kappa(\widetilde{u}_{h,e}^{n+\frac{1}{2}}, \widetilde{s}_{h,e}^{n+\frac{1}{2}})(u_{h,e})'(t_{n+\frac{1}{2}}) + \partial_r N_\kappa(\widetilde{u}_{h,e}^{n+\frac{1}{2}}, \widetilde{s}_{h,e}^{n+\frac{1}{2}})(s_{h,e})'(t_{n+\frac{1}{2}})\right)$$

$$\quad + \nabla_v N_\kappa(\widetilde{u}_{h,e}^{n+\frac{1}{2}}, \widetilde{s}_{h,e}^{n+\frac{1}{2}})\left(\frac{(2\theta-\tau)^2}{4}(u_{h,e})''(t_{n+\frac{1}{2}}) - \frac{\theta^2+(\theta-\tau)^2}{4}(u_{h,e})''(t_{n+\frac{1}{2}})\right)$$

$$\quad + \partial_r N_\kappa(\widetilde{u}_{h,e}^{n+\frac{1}{2}}, \widetilde{s}_{h,e}^{n+\frac{1}{2}})\left(\frac{(2\theta-\tau)^2}{4}(s_{h,e})''(t_{n+\frac{1}{2}}) - \frac{\theta^2+(\theta-\tau)^2}{4}(s_{h,e})''(t_{n+\frac{1}{2}})\right) + r_e,$$

where r_e represents the higher-order remainder term.

If we integrate both sides of (A.1) with respect to θ from 0 to τ and notice that $\int_0^\tau (2\theta - \tau)\, \mathrm{d}\theta = 0$, then we obtain $\|R_{2u}^{n,1}\| \leq \widetilde{C}_h' \tau^3$, where $\widetilde{C}_h' > 0$ is a constant depending on $u_{h,e}$, T, h, and κ because we have $\|u_{h,e}(t)\|_\infty \leq \beta$ and $-C_* \leq s_{h,e}(t) \leq E_h(u_{\mathrm{init}})$ for all t, and $N_\kappa(u_{h,e}, s_{h,e})$ is smooth with respect to $u_{h,e}$ and $s_{h,e}$.

According to Lemma 3.4, we also know that

$$\|\mathrm{e}^{-(\tau-\theta)L_\kappa^{n+\frac{1}{2}}} - I\| \leq (\tau-\theta)\rho(L_\kappa^{n+\frac{1}{2}}) \leq M_h(\tau-\theta).$$

Combining it with (A.1), we obtain that the leading term of $\|R_{2u}^{n,2}\|$ is

$$\int_0^\tau (\tau-\theta)|2\theta-\tau|\, \mathrm{d}\theta = \frac{\tau^3}{4},$$

which implies $\|R_{2u}^{n,2}\| \leq \widetilde{C}_h'' \tau^3$ for some constant $\widetilde{C}_h'' > 0$ depending on $u_{h,e}$, T, h, and κ. Thus, we complete the proof of the first inequality in (3.36).

The second inequality in (3.36) can be viewed as a direct consequence of the Crank–Nicolson discretization. □

Appendix B. Proof of Lemma 3.13.

Proof. According to the proof of Theorem 3.7, the error equations with respect to $\widetilde{e}_u^{n+1}$ and $\widetilde{e}_s^{n+1}$ are given by

$$
\begin{aligned}
\text{(B.1a)} \quad \widetilde{e}_u^{n+1} - e_u^n &= (\mathrm{e}^{-\tau L_\kappa^n} - I)e_u^n + \tau \phi_1(-\tau L_\kappa^n)[N_\kappa^n(u^n, s^n) \\
&\quad - N_\kappa^n(u_{h,e}(t_n), s_{h,e}(t_n))] - \int_0^\tau \mathrm{e}^{-(\tau-\theta)L_\kappa^n} R_{1u}^n(\theta)\, \mathrm{d}\theta,
\end{aligned}
$$

$$
\begin{aligned}
\text{(B.1b)} \quad \widetilde{e}_s^{n+1} - e_s^n &= \langle g(u_{h,e}(t_n), s_{h,e}(t_n))f(u_{h,e}(t_n)) - g(u^n, s^n)f(u^n), \\
&\quad u_{h,e}(t_{n+1}) - u_{h,e}(t_n)\rangle - g(u^n, s^n)\langle f(u^n), \widetilde{e}_u^{n+1} - e_u^n\rangle - \tau R_{1s}^n,
\end{aligned}
$$

where the truncation errors R_{1u}^n and R_{1s}^n are identical to those in (3.14) and (3.15), respectively, and satisfy (3.16).

Taking the discrete inner product of (B.1a) with $2\widetilde{e}_u^{n+1}$ and using Lemma 3.4 and (3.23), we get

$$
\begin{aligned}
&\|\widetilde{e}_u^{n+1}\|^2 - \|e_u^n\|^2 + \|\widetilde{e}_u^{n+1} - e_u^n\|^2 \\
&\leq 4\|e_u^n\|\|\widetilde{e}_u^{n+1}\| + 2\tau\|N_\kappa^n(u^n, s^n) - N_\kappa^n(u_{h,e}(t_n), s_{h,e}(t_n))\|\|\widetilde{e}_u^{n+1}\| + 2\tau \sup_{\theta \in (0,\tau)} \|R_{1u}^n(\theta)\|\|\widetilde{e}_u^{n+1}\| \\
&\leq 16\|e_u^n\|^2 + \frac{1}{4}\|\widetilde{e}_u^{n+1}\|^2 + 8\tau^2[(C_g + G^*\kappa)^2\|e_u^n\|^2 + C_g^2|e_s^n|^2] + \frac{1}{4}\|\widetilde{e}_u^{n+1}\|^2 \\
&\quad + 4\tau^2 \sup_{\theta \in (0,\tau)} \|R_{1u}^n(\theta)\|^2 + \frac{1}{4}\|\widetilde{e}_u^{n+1}\|^2 \\
&= 16\|e_u^n\|^2 + 8(C_g + G^*\kappa)^2\tau^2\|e_u^n\|^2 + 8C_g^2\tau^2|e_s^n|^2 + \frac{3}{4}\|\widetilde{e}_u^{n+1}\|^2 + 4\tau^2 \sup_{\theta \in (0,\tau)} \|R_{1u}^n(\theta)\|^2,
\end{aligned}
$$

and then

$$
\begin{aligned}
\frac{1}{4}\|\widetilde{e}_u^{n+1}\|^2 + \|\widetilde{e}_u^{n+1} - e_u^n\|^2 &\leq 17\|e_u^n\|^2 + 8(C_g + G^*\kappa)^2\tau^2\|e_u^n\|^2 \\
&\quad + 8C_g^2\tau^2|e_s^n|^2 + 4\tau^2 \sup_{\theta \in (0,\tau)} \|R_{1u}^n(\theta)\|^2.
\end{aligned}
$$

When $\tau \leq 1$, by using (3.16), we get

$$
\text{(B.2)} \quad \|\widetilde{e}_u^{n+1}\|^2 + 4\|\widetilde{e}_u^{n+1} - e_u^n\|^2 \leq (68 + 32(C_g + G^*\kappa)^2)\|e_u^n\|^2 + 32C_g^2|e_s^n|^2 + 16C_{e,h}^2\tau^4.
$$

Multiplying (B.1b) by $2\widetilde{e}_s^{n+1}$ yields

$$
\begin{aligned}
&|\widetilde{e}_s^{n+1}|^2 - |e_s^n|^2 + |\widetilde{e}_s^{n+1} - e_s^n|^2 \\
&= 2\widetilde{e}_s^{n+1}\langle g(u_{h,e}(t_n), s_{h,e}(t_n))f(u_{h,e}(t_n)) - g(u^n, s^n)f(u^n), u_{h,e}(t_{n+1}) - u_{h,e}(t_n)\rangle \\
&\quad - 2\widetilde{e}_s^{n+1}g(u^n, s^n)\langle f(u^n), \widetilde{e}_u^{n+1} - e_u^n\rangle - 2\tau R_{1s}^n \widetilde{e}_s^{n+1}.
\end{aligned}
$$

The last two terms on the RHS of the above equality can be estimated as

$$
-2\tau R_{1s}^n \widetilde{e}_s^{n+1} \leq 4\tau^2|R_{1s}^n|^2 + \frac{1}{4}|\widetilde{e}_s^{n+1}|^2,
$$

$$
-2\widetilde{e}_s^{n+1}g(u^n, s^n)\langle f(u^n), \widetilde{e}_u^{n+1} - e_u^n\rangle \leq \frac{1}{4}|\widetilde{e}_s^{n+1}|^2 + C_4\|\widetilde{e}_u^{n+1} - e_u^n\|^2
$$

with $C_4 > 0$ depending on C_*, $|\Omega|$, u_{init}, and $\|f\|_{C[-\beta,\beta]}$. The first term can be estimated in a way similar to (3.27), and then we obtain

$$|\widetilde{e}_s^{n+1}|^2 - |e_s^n|^2 + |\widetilde{e}_s^{n+1} - e_s^n|^2 \leq C_1\tau(\|e_u^n\|^2 + |e_s^n|^2 + |\widetilde{e}_s^{n+1}|^2)$$
$$+ C_4\|\widetilde{e}_u^{n+1} - e_u^n\|^2 + \frac{1}{2}|\widetilde{e}_s^{n+1}|^2 + 4\tau^2|R_{1s}^n|^2,$$

and thus

$$(1 - 2C_1\tau)|\widetilde{e}_s^{n+1}|^2 \leq 2|e_s^n|^2 + 2C_1\tau(\|e_u^n\|^2 + |e_s^n|^2) + 2C_4\|\widetilde{e}_u^{n+1} - e_u^n\|^2 + 8\tau^2|R_{1s}^n|^2.$$

When $\tau \leq \frac{1}{4C_1}$, we can get, by using (3.16),

$$(B.3) \qquad |\widetilde{e}_s^{n+1}|^2 \leq \|e_u^n\|^2 + 5|e_s^n|^2 + 4C_4\|\widetilde{e}_u^{n+1} - e_u^n\|^2 + 16C_{e,h}^2\tau^4.$$

The sum of (B.2) multiplied by C_4 and (B.3) leads to (3.37). $\qquad\square$

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