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A GRADIENT FLOW MODEL FOR THE GROSS–PITAEVSKII PROBLEM: MATHEMATICAL AND NUMERICAL ANALYSIS

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Abstract. This paper concerns the mathematical and numerical analysis of the L^2 normalized gradient flow model for the Gross–Pitaevskii eigenvalue problem, which has been widely used to design the numerical schemes for the computation of the ground state of the Bose–Einstein condensate. We first provide the mathematical analysis for the model, including the well-posedness and the asymptotic behavior of the solution. Then we propose a normalized implicit-explicit fully discrete numerical scheme for the gradient flow model, and give some numerical analysis for the scheme, including the well-posedness and optimal convergence of the approximation. Some numerical experiments are provided to validate the theory.

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1. Introduction

Bose–Einstein condensate (BEC) is an exotic state of matter that occurs in a dilute gas of bosons cooled to temperature extremely close to absolute zero. This phenomenon was first theoretically predicted by Einstein in the 1920s [30], building upon the foundational work of Bose [14]. Experimental realization of BEC in ultracold bosonic gases was achieved in 1995, as documented in pioneering studies by Anderson *et al.* [5] and Davis *et al.* [27]. The theoretical framework for understanding BEC is largely based on the Gross–Pitaevskii (GP) theory, independently developed by Gross [36] and Pitaevskii [49] in the 1960s. The GP theory has been widely validated in predicting key properties of BECs and remains a cornerstone of the mathematical model for describing the BEC. In the GP theory, the quantum state of the BEC is given by the solution of the following nonlinear Schrödinger equation (also called the time-dependent GP equation):

$$i\psi_t = -\Delta\psi + V\psi + \beta|\psi|^2\psi, \qquad \text{in } \mathbb{R}^3, \quad t > 0, \tag{1.1}$$

with a given initial value $\psi(x,0) = \psi_0(x)$ satisfying $\|\psi_0\|_{L^2(\mathbb{R}^3)} = 1$. The stationary (standing-wave) wave solutions to (1.1) are of the form $\psi(x,t) = \varphi(x)e^{-i\mu t}$. In this sense, $\varphi(x)$ satisfies the following GP eigenvalue problem (also called the time-independent GP equation): find $(\varphi,\mu) \in H^1(\mathbb{R}^3) \times \mathbb{R}$ with $\|\varphi\|_{L^2(\mathbb{R}^3)} = 1$ such

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that in the weak sense

$$-\Delta\varphi + V\varphi + \beta|\varphi|^2\varphi = \mu\varphi. \tag{1.2}$$

The ground state of BEC is described as the normalized eigenfunction φ of (1.2) with minimum GP energy, which is given by

$$E(v) := \int_{\mathbb{R}^3}\left(\frac{1}{2}|\nabla v|^2 + \frac{1}{2}V|v|^2 + \frac{\beta}{4}|v|^4\right)\,\mathrm{d}x. \tag{1.3}$$

Meanwhile, note that (1.2) represents the Euler–Lagrange equation of the GP energy functional, therefore, the ground state of a BEC can also be described as the minimizer of the following problem:

$$\varphi \in \operatorname*{arg\,min}_{v\in S} E(v), \qquad S := \{v \in H^1(\mathbb{R}^3) : \|v\|_{L^2(\mathbb{R}^3)} = 1\}. \tag{1.4}$$

For more details about the background of the BEC and the mathematical theory of the GP theory, we refer readers to the review paper [12].

Nowadays, the computation of the ground state of BEC is one of the fundamental objects in numerical studies of BEC and there are mainly two approaches to obtain the ground state: solving the nonlinear eigenvalue problem (1.2) and solving the minimization problem (1.4). The first approach, *i.e.*, directly solving the nonlinear eigenvalue problem (1.2), usually contains two steps. The first step is the spatial discretization such as the finite difference method, the finite element method, the spectral method, etc. There are some existing works on the error estimates for the spatial discretization, including the priori error analysis [18,21,41,55] and the *a posteriori* analysis [21,29]. The second step is to solve the nonlinear algebraic problem of the form

$$A(\mathbf{v})\mathbf{v} = \lambda\mathbf{v} \qquad \mathbf{v} \in \mathbb{R}^N. \tag{1.5}$$

The most common iterative technique for solving (1.5) is the self-consistent field iteration (*cf.* [16,17,19,28,50]), where a linearized eigenvalue problem is solved in each iteration. A systematic and comprehensive introduction of this approach can be found in a recent review paper, Sections 3 and 4 in [40]. For the second approach, *i.e.*, solving the problem (1.4), there are many existing works such as directly minimizing the energy functional in the finite element space [9], the Riemannian optimization method [3,4,26], the preconditioned nonlinear conjugate gradient method [6], the regularized Newton method [52], the J-method [2,43], the gradient-flow based methods, etc.

In this paper, we study the so-called gradient flow based method, which is widely used to solve (1.2). The main idea of the gradient flow approach is to introduce an artificial notion of time t and a corresponding time-dependent state $\phi(t)$, then construct a continuous (projected) gradient flow model (an evolution equation with respect to $\phi(t)$), for which $\lim_{t\to\infty}\phi(t)$ is the solution of (1.2). After that, we can get several methods by discretizing the gradient flow model in time. Roughly speaking, there are mainly two types of the gradient flow model: the L^2 projected gradient flow and the H^1 projected gradient flow. The L^2 projected gradient flow was first introduced in [10], called continuous normalized gradient flow (CNGF), which was used as a mathematical justification for the imaginary time evolution method [1, 20, 24]. Due to the simplicity and efficiency of the gradient flow with discrete normalization (GFDN) and CNGF models [10], based on which lots of numerical methods have been applied to compute the ground state [10–13, 46, 51, 56]. Convergence of GFDN iteration (*cf.* [38], Def. 4.1) in 1D for focusing nonlinearities ($\beta < 0$) was considered in [32], and was considered in [38] for higher dimensions with defocusing nonlinearities ($\beta > 0$). Several H^1 gradient flows for the GP eigenvalue problem have been proposed in [25, 39, 45]. With these H^1 Sobolev gradient flow models, combining a forward Euler discretization, several semi-discrete methods have been proposed in [25, 39, 45] with numerical analysis in [22, 38, 39, 54]. Furthermore, combining with some spatial discretization, fully discrete methods have been proposed in [23, 37].

The L^2-normalized gradient flow, as a continuous model provided to design the numerical schemes, its mathematical properties such as well-posedness and asymptotic behaviors are of importance to guarantee the reasonability of the corresponding numerical schemes. Compared to the H^1-normalized gradient flow, there are few works on the mathematical analysis for the L^2 gradient flow. With the absence of the potential function, *i.e.*, $V \equiv 0$, for the case of 1D with $\beta < 0$, Faou and Jézéquel [32] proved the exponential convergence in L^2 space under the assumption that the initial value is sufficiently close to the ground state. Antonelli *et al.* [7] proved the well-posedness of the L^2 gradient flow with general nonlinearity, *i.e.*, $|\varphi|^{2\sigma}\varphi$, in higher dimensions. Different from the H^1 case, the mathematical analysis of the L^2 gradient flow, especially the well-posedness of the model, requires the theory of PDEs, while the H^1 case only depends on the "ODEs" knowledge.

One of the objectives of this paper is to give a mathematical analysis for the L^2 normalized gradient flow of the GP eigenvalue problem. Following the recent work [7], we obtain the well-posedness of the L^2 normalized gradient flow with L^∞ potential. In addition to the well-posedness, similar to the H^1 case [39,45], under some assumptions on the regularity of the solution, we also get several exponential convergences of the solution to the L^2 normalized gradient flow as the time approaches infinity. Another objective of this paper is to consider the numerics of the L^2 normalized gradient flow, including the numerical scheme and its convergence analysis. We propose a normalized implicit-explicit fully discrete scheme for the gradient flow model. A similar temporal semi-discrete scheme has been introduced in [46], combining the spatial Fourier-pseudospectral discretization. Numerical experiments in [46] show that this scheme is very efficient since it only needs to solve a linear elliptic equation with constant coefficients in each iteration. For the convergence analysis, different from [32,38], which considered the convergence and convergence rate of the iterative solutions to the ground state with respect to the iteration numbers, our analysis concentrates on the approximation of the gradient flow model with respect to the mesh size (*cf.* Thm. 4.12), and our numerical analysis can be naturally extended to similar methods such as numerical schemes in [46]. One of the difficulties in the convergence analysis is to estimate the error of the normalized step, which is overcome in a geometric view (*cf.* Lem. 4.9). We obtain also an optimal convergence in $L^\infty(0,T;L^2(\Omega))$ and a suboptimal convergence in $L^\infty(0,T;H^1(\Omega))$.

The organization of this paper is as follows. In Section 2, we introduce the basic knowledge of the GP eigenvalue problem and its gradient flow. In Section 3, we give some mathematical analysis for the L^2 gradient flow of the GP eigenvalue problem, including the well-posedness, the exponential convergence of the energy and the exponential convergence of the solution to the ground state in L^2 norm, as the time approaches infinity. In Section 4, we propose a numerical scheme for the L^2 gradient flow of the GP eigenvalue problem and carry out the convergence analysis with respect to the mesh size. In Section 5, we provide two numerical experiments to validate our theoretic results obtained in Section 4, and give a conclusion in Section 6.

Throughout this paper, the letter C denotes a generic constant that could be different in different occurrences.

2. The gradient flow model

2.1. The Gross–Pitaevskii problem

We consider the following GP eigenvalue problem:

$$-\Delta\varphi + V\varphi + \beta|\varphi|^2\varphi = \lambda\varphi, \qquad \int_{\mathbb{R}^3} |\varphi|^2 \,\mathrm{d}x = 1, \tag{2.1}$$

where V is a real-valued time independent potential function, β is a real number whose symbol represents the repulsive (positive)/attractive (negative) interaction. In this paper, we consider the repulsive interaction case, *i.e.*, $\beta \geq 0$, and without loss of generality, we assume $V \geq 0$. The classical Ljusternik–Schnirelman theory [53] shows that the problem (2.1) has infinitely many eigenvalues $0 < \lambda_1 < \lambda_2 \leq \lambda_3 \leq \cdots < \infty$ and the ground state ϕ_{GS} is the normalized eigenfunction corresponding to the smallest eigenvalue $\lambda_{\mathrm{GS}} := \lambda_1$ [18]. Moreover, the ground state ϕ_{GS} is positive and unique up to a sign [12,18]. In addition, if V satisfies $\lim_{|x|\to\infty} V(x) = +\infty$, then ϕ_{GS} decays exponentially fast as $|x| \to \infty$ [12].

Note that (2.1) is the Euler–Lagrange equation of the GP energy functional:

$$E(v) := \int_{\mathbb{R}^3} \left(\frac{1}{2}|\nabla v|^2 + \frac{1}{2}V|v|^2 + \frac{\beta}{4}|v|^4\right) \mathrm{d}x \qquad v \in H^1(\mathbb{R}^3). \tag{2.2}$$

Then the ground state of a BEC can be rephrased in terms of the solution of the following minimization problem: Find $\varphi \in S$,

$$E(\varphi) = \min_{v \in S} E(v). \tag{2.3}$$

The mathematical analysis of the problem (2.3), such as the existence, uniqueness and other properties, can be found in [12, 18].

2.2. The L^2 gradient flow model

The exponential decay property of the ground state solution mentioned in Section 2.1 suggests that we can consider the GP problem (2.1) on a bounded domain $\Omega \subset \mathbb{R}^3$, together with a homogeneous Dirichlet boundary condition. We adopt the gradient flow approach to calculate the ground state of GP eigenvalue problem, where the ground state solution of GP eigenvalue problem as well as the global minimizer of the problem (2.3) can be viewed as the stationary state of the gradient flow problem. The gradient flow model of the GP problem was first considered in [10] as a mathematical justification for the classical imaginary time method, which has been used in physics literature to calculate the ground state solution of BEC [1, 20, 24]. We recall that the Fréchet derivative of the GP energy functional is given by

$$\langle E'(v), w\rangle = \int_\Omega \Big(\nabla v \cdot \nabla w + Vvw + \beta |v|^2 vw\Big)\,\mathrm{d}x \quad \forall\, v, w \in H_0^1(\Omega), \tag{2.4}$$

where the notation $\langle \cdot, \cdot \rangle$ denotes the dual pair between $H^{-1}(\Omega)$ and $H_0^1(\Omega)$.

The imaginary time approach to solve (2.3) can be read as: for a time sequence $0 = t_0 < t_1 < t_2 < \cdots < t_n < \cdots$,

$$\phi_t = -\frac{\delta E(\phi)}{\delta \phi} = \Delta\phi - V\phi - \beta|\phi|^2\phi, \qquad \text{in } \Omega, \quad t_n < t < t_{n+1}, \quad n \geq 0, \tag{2.5}$$

$$\phi(t_{n+1}) = \frac{\phi(t_{n+1}^-)}{\|\phi(t_{n+1}^-)\|_{L^2(\Omega)}}. \tag{2.6}$$

In fact, (2.5) can be viewed as applying the steepest descent method to the energy functional $E(\phi)$ without constraint and then retracting the solution onto the unit sphere. It is mentioned in [10] that (2.5) and (2.6) can be viewed as a first-order splitting method for the following continuous normalized gradient flow (CNGF):

$$\phi_t = \Delta\phi - V\phi - \beta|\phi|^2\phi + \mu[\phi]\phi, \qquad \text{in } \Omega \times (0,\infty), \tag{2.7}$$

$$\phi = 0, \qquad \text{on } \partial\Omega \times (0,\infty), \tag{2.8}$$

$$\phi = \phi_0, \qquad t = 0 \quad \text{with} \quad \|\phi_0\|_{L^2(\Omega)} = 1, \tag{2.9}$$

where

$$\mu[\phi] := \frac{1}{\|\phi\|^2_{L^2(\Omega)}} \int_\Omega \big(|\nabla\phi|^2 + V|\phi|^2 + \beta|\phi|^4\big)\,\mathrm{d}x. \tag{2.10}$$

Equations (2.7)–(2.10) is called the L^2 gradient flow model of the GP problem, and its mathematical analysis will be presented in the next section.

Remark 2.1 (Projected gradient flow approach)**.** The gradient flow model (2.7)–(2.10) can also be derived from the projected gradient flow approach. In the context of projected Sobolev gradient flow, the critical points of the energy $E(\cdot)$ can be identified by constructing appropriate gradient flows of the form

$$z'(t) = -P_{z,X}(\nabla_X E(z(t))), \tag{2.11}$$

where $\nabla_X E$ is the Sobolev gradient of the energy functional and $P_{z,X}$ is the projection operator. With the choice of $X = L^2(\Omega)$, (2.11) coupled with some initial value $\phi(0) \in H_0^1(\Omega) \cap H^2(\Omega)$ is exactly (2.7)–(2.10) Section 2.2.1 in, cf. [39].

3. Mathematical analysis

In this section, we consider the following nonlinear, parabolic PDEs:

$$\begin{cases} \phi_t = \Delta\phi - V\phi - \beta|\phi|^2\phi + \mu[\phi]\phi, & \text{in } \Omega\times(0,\infty),\\ \phi = 0, & \text{on } \partial\Omega\times(0,\infty),\\ \phi = \phi_0, & t=0, \qquad \|\phi_0\|_{L^2(\Omega)} = 1, \end{cases} \tag{3.1}$$

where $V \geq 0$ and $\beta \geq 0$ and $\mu[\phi]$ is defined in (2.10). For simplicity, we assume $\Omega \subset \mathbb{R}^3$ to be a bounded convex domain with Lipschitz boundary. First, we recall the properties of (3.1) (see Thm. 2.5 of [10] and Prop. 2.2 in [7]).

Proposition 3.1. *Any global solution ϕ of (3.1) with the regularity:*

$$\phi \in C\big([0,\infty); H_0^1(\Omega)\big) \cap C^1\big((0,\infty); L^2(\Omega)\big) \cap C\big((0,\infty); H^2(\Omega)\big)$$

satisfies normalization conservation and energy diminishment, i.e.,

$$\begin{aligned} &\|\phi(\cdot,t)\|_{L^2(\Omega)} = \|\phi_0\|_{L^2(\Omega)} = 1, && t \geq 0,\\ &\frac{\mathrm{d}}{\mathrm{d}t}E(\phi) = -\|\phi_t(\cdot,t)\|^2_{L^2(\Omega)} \leq 0, && t \geq 0. \end{aligned}$$

Let $\{e^{t\Delta}\}_{t>0}$ denote the semigroup generated by the Laplacian operator on $L^2(\Omega)$. The function $u = e^{t\Delta}u_0$ is the solution of the following equation

$$\begin{cases} u_t = \Delta u, & \text{in } \Omega\times(0,\infty),\\ u = 0, & \text{on } \partial\Omega\times(0,\infty),\\ u = u_0 \in H_0^1(\Omega), & t = 0. \end{cases}$$

We recall the properties of $\{e^{t\Delta}\}_{t>0}$ [7,8,44] that will be used in a later theorem.

Proposition 3.2. *For any time independent $f \in L^2(\Omega)$, we have*

$$\sup_{t>0} \|e^{t\Delta}f\|_{L^2(\Omega)} \leq \|f\|_{L^2(\Omega)}.$$

And for any $u_0 \in H_0^1(\Omega)$, we have

$$\|e^{t\Delta}u_0\|^2_{L^2(\Omega)} = \|u_0\|^2_{L^2(\Omega)} - 2\int_0^t \|\nabla e^{s\Delta}u_0\|^2_{L^2(\Omega)}\, \mathrm{d}s.$$

Proposition 3.3. *For any $f \in L^1((0,\infty); L^2(\Omega))$, we have*

$$\left\| \int_0^t e^{(t-s)\Delta} f(s)\, \mathrm{d}s \right\|_{L^\infty((0,\infty);L^2(\Omega))} \leq C\|f\|_{L^1((0,\infty);L^2(\Omega))}.$$

And for any $f \in L^2((0,\infty); L^2(\Omega))$, we have

$$\left\| \nabla \int_0^t e^{(t-s)\Delta} f(s)\, \mathrm{d}s \right\|_{L^\infty((0,\infty);L^2(\Omega))} \leq C\|f\|_{L^2((0,\infty);L^2(\Omega))}.$$

We then carry out the mathematical analysis of (3.1), including the well-posedness and the asymptotic behaviors.

3.1. Well-posedness and global convergence

Following [7], we have

Theorem 3.4. *Let $V \in L^\infty(\Omega)$ with $V \geq 0$ and $\beta \in \mathbb{R}$ be nonnegative. If the initial value $\phi_0 \in H_0^1(\Omega) \cap H^2(\Omega)$ with $\|\phi_0\|_{L^2(\Omega)} = 1$, then there exists a unique global strong solution ϕ satisfying (3.1) with regularity*

$$\phi \in C([0,\infty); H^2(\Omega) \cap H_0^1(\Omega)), \qquad \phi_t \in C([0,\infty); L^2(\Omega)).$$

Moreover, if $\phi_0 \geq 0$, then $\phi(t)$ converges to ϕ_{GS} strongly in $H_0^1(\Omega)$ as $t \to \infty$.

Proof. The proof will be divided into two parts.

Part I (Global well-posedness). We first prove that there exist $T^* > 0$ and a unique local solution $\phi \in C([0,T^*], H_0^1(\Omega))$. Let $M > 0$, $N > 0$, $T > 0$ be some constants that are to be determined. Let

$$\Lambda = \left\{ u \in C\big([0,T]; H_0^1(\Omega)\big) : u(0) = \phi_0,\ \|u\|_{L^\infty\left([0,T]; H^1(\Omega)\right)} \leq M,\ \inf_{t\in[0,T]} \|u\|_{L^2(\Omega)} \geq \frac{N}{2} \right\}$$

be the set equipped with the distance

$$\mathrm{d}(u,v) = \|u - v\|_{L^\infty\left([0,T]; H^1(\Omega)\right)} \qquad \forall\, u, v \in \Lambda.$$

Since $V \in L^\infty(\Omega)$, by continuous embedding $H^1(\Omega) \hookrightarrow L^4(\Omega)$ and Hölder's inequality, we conclude that there exists a constant $C_1(M,N) > 0$ such that

$$\|\mu[u]\|_{L^\infty[0,T]} \leq \frac{C}{N^2}\Big(\|u\|^2_{L^\infty([0,T];H^1(\Omega))} + \|u\|^4_{L^\infty([0,T];H^1(\Omega))} \Big) \leq C_1, \quad u \in \Lambda. \tag{3.2}$$

Note that for all $u, v \in \Lambda$

$$\begin{aligned} |\mu[u] - \mu[v]| &\leq \frac{C}{N^2} \int_\Omega \Big(|\nabla u + \nabla v||\nabla u - \nabla v| + V(x)|u+v||u-v| + \beta|u^4 - v^4| \Big)\,\mathrm{d}x \\ &\quad + \Big| \|u\|^{-2}_{L^2(\Omega)} - \|v\|^{-2}_{L^2(\Omega)} \Big| |\mu[u]| \\ &\leq C_2 \|u - v\|_{H^1(\Omega)}, \end{aligned}$$

here $C_2 = C_2(M,N)$, which leads to

$$\|\mu[u] - \mu[v]\|_{L^\infty[0,T]} \leq C_2 \mathrm{d}(u,v), \quad u, v \in \Lambda. \tag{3.3}$$

For $u \in \Lambda$, define $\mathcal{F}(u)(t)$ as

$$\mathcal{F}(u)(t) = e^{t\Delta}\phi_0 + \int_0^t e^{(t-s)\Delta}(\mu[u]u - \beta|u|^2 u - Vu)\,\mathrm{d}s, \tag{3.4}$$

obviously, $\mathcal{F}(u)(0) = \phi_0$. Combining Properties 3.2 and 3.3, embedding $H^1(\Omega) \hookrightarrow L^6(\Omega)$ and Hölder's inequality, we obtain

$$\begin{aligned} &\|\mathcal{F}(u)\|_{L^\infty([0,T];L^2(\Omega))} \\ &\quad \leq C\big(\|\phi_0\|_{L^2(\Omega)} + \|\mu[u]u - \beta|u|^2u - Vu\|_{L^1([0,T];L^2(\Omega))} \big) \\ &\quad \leq C\big(\|\phi_0\|_{L^2(\Omega)} + T\|\mu[u]u - \beta|u|^2u - Vu\|_{L^\infty([0,T];L^2(\Omega))} \big) \end{aligned} \tag{3.5}$$

$$\begin{aligned}&\leq C\Big(\|\phi_0\|_{L^2(\Omega)}+T(\|\mu[u]\|_{L^\infty[0,T]}+\|V\|_{L^\infty(\Omega)})\|u\|_{L^\infty\big([0,T];L^2(\Omega)\big)}+CT\|u\|^3_{L^\infty([0,T];H^1(\Omega))}\Big)\\&\leq C\|\phi_0\|_{L^2(\Omega)}+C_3(M,N)T,\end{aligned}$$

and

$$\begin{aligned}\|\nabla\mathcal{F}(u)\|_{L^\infty([0,T];L^2(\Omega))}&\leq C\big(\|\phi_0\|_{H^1(\Omega)}+\|\mu[u]u-\beta|u|^2u-Vu\|_{L^2([0,T];L^2(\Omega))}\big)\\&\leq C\Big(\|\phi_0\|_{H^1(\Omega)}+T^{\frac12}\|\mu[u]u-\beta|u|^2u-Vu\|_{L^\infty([0,T];L^2(\Omega))}\Big)\\&\leq C\|\phi_0\|_{H^1(\Omega)}+C_4(M,N)T^{\frac12}.\end{aligned}\tag{3.6}$$

By using (3.2), (3.5) and (3.6), there exist constants $C^*>0$ and $C_5=C_5(M,N)>0$ such that

$$\|\mathcal{F}(u)\|_{L^\infty([0,T],H^1(\Omega))}\leq C^*\|\phi_0\|_{H^1(\Omega)}+C_5\Big(T+T^{\frac12}\Big).\tag{3.7}$$

Meanwhile, we get

$$\begin{aligned}\|\mathcal{F}(u)\|_{L^2(\Omega)}&\geq\|e^{t\Delta}\phi_0\|_{L^2(\Omega)}-\left\|\int_0^t e^{(t-s)\Delta}(\mu[u]u-\beta|u|^2u-Vu)\,\mathrm{d}s\right\|_{L^\infty([0,T];L^2(\Omega))}\\&\geq\left(\|\phi_0\|^2_{L^2(\Omega)}-2\int_0^t\|\nabla e^{s\Delta}\phi_0\|^2_{L^2(\Omega)}\,\mathrm{d}s\right)^{\frac12}-CT\\&\geq\Big(\|\phi_0\|^2_{L^2(\Omega)}-CT\|\nabla\phi_0\|^2_{L^2(\Omega)}\Big)^{\frac12}-CT,\end{aligned}\tag{3.8}$$

which implies

$$\inf_{t\in[0,T]}\|\mathcal{F}(u)\|_{L^2(\Omega)}\geq\|\phi_0\|_{L^2(\Omega)}-C_6(M,N)(T+T^{\frac12}).\tag{3.9}$$

For $u,v\in\Lambda$

$$\begin{aligned}&\|\mathcal{F}(u)-\mathcal{F}(v)\|_{L^\infty([0,T];L^2(\Omega))}\\&\quad\leq C\|\mu[u]u-\mu[v]v-\beta(|u|^2u-|v|^2v)-V(u-v)\|_{L^1([0,T];L^2(\Omega))}\\&\quad\leq C_7(M,N)T\mathrm{d}(u,v),\end{aligned}\tag{3.10}$$

and

$$\begin{aligned}&\|\nabla\mathcal{F}(u)-\nabla\mathcal{F}(v)\|_{L^\infty([0,T];L^2(\Omega))}\\&\quad\leq C\|\mu[u]u-\mu[v]v-\beta(|u|^2u-|v|^2v)-V(u-v)\|_{L^2([0,T];L^2(\Omega))}\\&\quad\leq C_8(M,N)T^{\frac12}\mathrm{d}(u,v).\end{aligned}\tag{3.11}$$

Combining (3.10) and (3.11), we obtain

$$\|\mathcal{F}(u)-\mathcal{F}(v)\|_{L^\infty([0,T];H^1(\Omega))}\leq C_9(M,N)(T+T^{\frac12})\mathrm{d}(u,v).\tag{3.12}$$

First, we choose $M=2C^*\|\phi_0\|_{H^1(\Omega)}$ and $N=\|\phi_0\|_{L^2(\Omega)}$ in (3.7), (3.9) and (3.12), which leads to

$$\|\mathcal{F}(u)\|_{L^\infty([0,T],H^1(\Omega))}\leq\frac{M}{2}+C_1'\Big(T+T^{\frac12}\Big)\qquad\forall\,u\in\Lambda,\tag{3.13}$$

$$\inf_{t\in[0,T]}\|\mathcal{F}(u)\|_{L^2(\Omega)}\geq N-C_2'(T+T^{\frac12})\qquad\forall\,u\in\Lambda,\tag{3.14}$$

$$\|\mathcal{F}(u)-\mathcal{F}(v)\|_{L^\infty([0,T];H^1(\Omega))} \leq C_3'(T+T^{\frac{1}{2}})\mathrm{d}(u,v) \qquad \forall\, u,v\in\Lambda. \tag{3.15}$$

Then, we choose T^* sufficiently small such that, for $0\leq T\leq T^*$

$$C_1'\Big(T+T^{\frac{1}{2}}\Big)\leq \frac{M}{2},\quad C_2'(T+T^{\frac{1}{2}})\leq\frac{N}{2},\quad \text{and}\quad C_3'(T+T^{\frac{1}{2}})\leq\frac{1}{2}$$

which leads to for all $u\in\Lambda$

$$\|\mathcal{F}(u)\|_{L^\infty([0,T],H^1(\Omega))}\leq M,\qquad \inf_{t\in[0,T]}\|\mathcal{F}(u)\|_{L^2(\Omega)}\geq\frac{N}{2}, \tag{3.16}$$

and for all $u,v\in\Lambda$

$$\|\mathcal{F}(u)-\mathcal{F}(v)\|_{L^\infty([0,T];H^1(\Omega))}\leq\frac{1}{2}\mathrm{d}(u,v). \tag{3.17}$$

Inequalities (3.16) and (3.17) show that $\mathcal{F}(\cdot)$ is a contraction map on Λ (the continuity of $\mathcal{F}(\cdot)$ with respect to t can be easily seen from the definition of $\mathcal{F}(\cdot)$.) with $T=T^*$. By Banach Fixed-Point Theorem, there exists a unique $\phi\in\Lambda$ such that $\mathcal{F}(\phi)=\phi$. Proposition 2.2 in [7] tells that ϕ satisfies the additional regularity:

$$\phi\in C\big([0,T^*];H_0^1(\Omega)\big)\cap C^1\big([0,T^*];L^2(\Omega)\big)\cap C\big([0,T^*];H^2(\Omega)\big),$$

which proves the local well-posedness of (3.1).

Let ϕ be the local solution given above. Since β and V are non-negative, we obtain from the energy diminishing property that

$$\|\nabla\phi(t)\|^2_{L^2(\Omega)}\leq 2E(\phi(t))\leq 2E(\phi_0),\quad \forall\, t\in[0,T], \tag{3.18}$$

which shows that the H^1-norm of $\phi(t)$ is bounded with respect to t. Thus we can extend the local solution to a global solution without losing uniqueness. The regularity of $\phi(t)$ directly follows from $\phi_0\in H_0^1(\Omega)\cap H^2(\Omega)$ and Propositions 2.2 and 3.4 in [7].

Part II (Convergence to the ground state). Following Proposition 4.1, Corollary 4.2, and Theorem 4.3 in [7], we are able to prove the convergence to the ground state as $t\to\infty$, under the condition of $\phi_0\geq 0$. The proof will be divided into three steps.

Step 1 (Sequential weak convergence): The energy decay property and Proposition 3.2 show that

$$\phi_t\in L^2([0,\infty);L^2(\Omega)),\quad \sup_{t>0}|\mu[\phi]|\leq C,\quad\text{and}\quad \|\phi\|_{L^\infty([0,\infty);H^1(\Omega))}\leq C.$$

As a result, there exists a sequence $\{t_n\}_{n\in N}$ satisfying $t_n\to\infty$ as $n\to\infty$, $\phi_\infty\in H_0^1(\Omega)$, and $\mu_\infty\in\mathbb{R}$ such that

$$\begin{cases}\phi(t_n)\rightharpoonup\phi_\infty & \text{in } H_0^1(\Omega),\\ \phi_t(t_n)\to 0 & \text{in } L^2(\Omega),\\ \mu[\phi(t_n)]\to\mu_\infty & \text{in } \mathbb{R}.\end{cases}$$

Then under the weak topology of H^{-1},

$$\begin{aligned}&\phi_t(t_n)-\Delta\phi(t_n)+V\phi(t_n)+\beta|\phi(t_n)|^2\phi(t_n)-\mu[\phi(t_n)]\phi(t_n)\\ &\quad\rightharpoonup -\Delta\phi_\infty+V\phi_\infty+\beta|\phi_\infty|^2\phi_\infty-\mu_\infty\phi_\infty\end{aligned}$$

as $n\to\infty$. This implies in H^{-1} sense,

$$-\Delta\phi_\infty+V\phi_\infty+\beta|\phi_\infty|^2\phi_\infty-\mu_\infty\phi_\infty=0. \tag{3.19}$$

Note that $\|\phi(t_n)\|_{L^2(\Omega)} = 1$ for all $n \geq 0$, the weak convergence $\phi(t_n) \rightharpoonup \phi_\infty$ in H_0^1 and the compact embedding $H_0^1(\Omega) \hookrightarrow L^2(\Omega)$ on bounded domain Ω imply $\|\phi_\infty\|_{L^2(\Omega)} = 1$. (3.19) shows that ϕ_∞ is a solution of the GP eigenvalue problem.

Step 2 (Sequential strong convergence): Form (3.19), we conclude that $\mu[\phi_\infty] = \mu_\infty$ and this leads to $\mu[\phi(t_n)] \to \mu[\phi_\infty]$ as $n \to \infty$, which is

$$\int_\Omega \left(|\nabla\phi(t_n)|^2 + V|\phi(t_n)|^2 + \beta|\phi(t_n)|^4\right) \mathrm{d}x \to \int_\Omega \left(|\nabla\phi_\infty|^2 + V|\phi_\infty|^2 + \beta|\phi_\infty|^4\right) \mathrm{d}x$$

when $n \to \infty$. Note that weak convergence in $H_0^1(\Omega)$ implies strong convergence in $L^2(\Omega)$ and $L^4(\Omega)$ (up to subsequences, and we still use the same notation), we have

$$\int_\Omega V|\phi(t_n)|^2 \,\mathrm{d}x \to \int_\Omega V|\phi_\infty|^2 \,\mathrm{d}x \qquad \text{and} \qquad \int_\Omega |\phi(t_n)|^4 \,\mathrm{d}x \to \int_\Omega |\phi_\infty|^4 \,\mathrm{d}x,$$

these convergences further imply

$$\int_\Omega |\nabla\phi(t_n)|^2 \,\mathrm{d}x \to \int_\Omega |\nabla\phi_\infty|^2 \,\mathrm{d}x,$$

which together with the weak convergence, we get $\phi(t_n) \to \phi_\infty$ strongly in $H_0^1(\Omega)$ as $n \to \infty$.

Step 3 (Convergence to the ground state): If the initial value satisfies $\phi_0 \geq 0$, since $V(x) \geq 0$ and $\beta \geq 0$, by the Maximum Principle, see Chapter 2, Section 4 in [33], we have $\phi(t_n) \geq 0$. This implies $\phi_\infty \geq 0$. By Lemma 5.3 in [39], we obtain $\phi_\infty = \phi_{\mathrm{GS}}$. The strong convergence of $\{\phi(t_n)\}_{n\in\mathbb{N}}$ and the energy decay property show that

$$E[\phi(t)] \searrow E[\phi_{\mathrm{GS}}], \qquad \text{as} \;\; t \to \infty.$$

To prove $\phi(t) \to \phi_{\mathrm{GS}}$ in $H_0^1(\Omega)$ as $t \to \infty$, we only need to prove that for every sequence $\{\tilde{t}_k\}_{k\in\mathbb{N}}$ with $\tilde{t}_k \to \infty$ as $k \to \infty$, there exists a subsequence $\{\tilde{t}_{n_k}\}_{k\in\mathbb{N}}$ such that

$$\phi(\tilde{t}_{n_k}) \to \phi_{\mathrm{GS}} \qquad \text{when} \quad k \to \infty. \tag{3.20}$$

Boundedness of $\{\phi(\tilde{t}_k)\}_{k\in\mathbb{N}}$ implies there exist a subsequence $\{\phi(\tilde{t}_{n_k})\}_{k\in\mathbb{N}}$ and $\tilde{\phi}_\infty \in H_0^1(\Omega)$ such that $\phi(\tilde{t}_{n_k}) \rightharpoonup \tilde{\phi}_\infty$ weakly in $H_0^1(\Omega)$ as $k \to \infty$, and hence $\|\tilde{\phi}_\infty\|_{L^2(\Omega)} = 1$. By the lower semi-continuity of $E[\cdot]$, we have

$$E[\tilde{\phi}_\infty] \leq \liminf_{k\to\infty} E[\phi(\tilde{t}_{n_k})] = E[\phi_{\mathrm{GS}}].$$

From the above, we immediately get $\tilde{\phi}_\infty = \phi_{\mathrm{GS}}$ or $\tilde{\phi}_\infty = -\phi_{\mathrm{GS}}$. Again by the Maximum Principle, see Chapter 2, Section 4 in [33], we have $\phi(\tilde{t}_{n_k}) \geq 0$, and hence $\tilde{\phi}_\infty \geq 0$, which is $\tilde{\phi}_\infty = \phi_{\mathrm{GS}}$. Similar to *Step 2*, we obtain $\phi(\tilde{t}_{n_k}) \to \phi_{\mathrm{GS}}$ strongly in $H_0^1(\Omega)$ as $k \to \infty$, which completes the proof. □

Remark 3.5. Under the same assumption in Theorem 3.4, following the regularity theory of elliptic and parabolic PDEs [31,34], we have that if $V \in H^1(\Omega) \cap L^\infty(\Omega)$ and the initial value further satisfies $\Delta\phi_0 \in H_0^1(\Omega)$, then

$$\phi \in C([0,\infty); H^2(\Omega) \cap H_0^1(\Omega)), \qquad \phi_t \in C([0,\infty); H_0^1(\Omega)).$$

Moreover, if $V(x) \in H^2(\Omega)$ and $\Delta\phi_0 \in H^2(\Omega) \cap H_0^1(\Omega)$, then

$$\phi \in C^1([0,\infty); H^2(\Omega) \cap H_0^1(\Omega)), \qquad \phi_{tt} \in C([0,\infty); L^2(\Omega)).$$

3.2. Convergence rate

In this subsection, we will discuss the convergence rate of the solution of (3.1) to the ground state as $t \to \infty$. For simplicity, we make the following assumption.

Assumption 3.6. *The solution of* (3.1) *satisfies* $\phi \in C^1([0,\infty); H_0^1(\Omega)) \cap C([0,\infty); H^2(\Omega))$, *and* $\phi(t)$ *converges to* ϕ_{GS} *strongly in* $H_0^1(\Omega)$ *as* $t \to \infty$.

Remark 3.7. By Remark 3.5, Assumption 3.6 is reasonable for some potential function V and initial value ϕ_0 satisfying some regularity requirements.

Our discussion starts from the following lemma, and we employ a similar proof strategy to that used for establishing the decay rate of the Sobolev gradient flow; see, *e.g.*, Proof of Theorem 3.2 in [39].

Lemma 3.8. *Denote* $g(t) = \frac{1}{2}\|\phi_t(\cdot,t)\|^2_{L^2(\Omega)}$, *then for any* $\epsilon \in (0, \lambda_2 - \lambda_{\mathrm{GS}})$, *there exists* $T_\epsilon > 0$ *such that*

$$g'(t) \le -2(\lambda_2 - \lambda_{\mathrm{GS}} - \epsilon) g(t) \qquad t \ge T_\epsilon, \tag{3.21}$$

where λ_2 *is the second eigenvalue of the following linear eigenvalue problem:*

$$-\Delta u + Vu + \beta|\phi_{\mathrm{GS}}|^2 u = \lambda u.$$

Proof. Note that

$$\phi_{tt} = \Delta\phi_t - V\phi_t - 3\beta\phi^2\phi_t + \left(\frac{\mathrm{d}}{\mathrm{d}t}\mu[\phi]\right)\phi + \mu[\phi]\phi_t,$$

where ϕ_{tt} is understood in H^{-1} sense. We have that

$$\begin{aligned} g'(t) &= \langle \phi_t, \phi_{tt}\rangle_{H^{-1}(\Omega)\times H_0^1(\Omega)} \\ &= -(\nabla\phi_t, \nabla\phi_t)_{L^2(\Omega)} - (V\phi_t, \phi_t)_{L^2(\Omega)} \\ &\quad - \beta(\phi^2\phi_t, \phi_t)_{L^2(\Omega)} \underbrace{-2\beta(\phi^2\phi_t, \phi_t)_{L^2(\Omega)}}_{\le 0} \\ &\quad + \left(\frac{\mathrm{d}}{\mathrm{d}t}\mu[\phi]\right) \underbrace{(\phi, \phi_t)_{L^2(\Omega)}}_{=0} + \mu[\phi](\phi_t, \phi_t)_{L^2(\Omega)} \\ &\le -\int_\Omega \left(|\nabla\phi_t|^2 + V|\phi_t|^2 + \beta|\phi|^2|\phi_t|^2\right) \mathrm{d}x + \mu[\phi]\|\phi_t\|^2_{L^2(\Omega)}. \end{aligned} \tag{3.22}$$

Denote

$$a_\phi(u,v) := \int_\Omega \left(\nabla u\cdot\nabla v + Vuv + \beta|\phi|^2 uv\right) \mathrm{d}x, \qquad C_{\inf} := \liminf_{t\to\infty} \frac{a_\phi(\phi_t,\phi_t)}{\|\phi_t\|^2_{L^2(\Omega)}}.$$

Assume that $(t_n)_{n\in\mathbb{N}}$ with $t_n \to \infty$ satisfies

$$\lim_{n\to\infty} \frac{a_{\phi(t_n)}(\phi_t(t_n), \phi_t(t_n))}{\|\phi_t(t_n)\|^2_{L^2(\Omega)}} = C_{\inf}.$$

Let

$$z_n := \frac{\phi_t(t_n)}{\|\phi_t(t_n)\|_{L^2(\Omega)}},$$

we see that $\{z_n\}_{n\in\mathbb{N}}$ is a bounded sequence in $H_0^1(\Omega)$ and

$$\left|\int_\Omega |\phi(t_n)|^2 z_n^2 \,\mathrm{d}x - \int_\Omega |\phi_{\mathrm{GS}}|^2 z_n^2 \,\mathrm{d}x\right| \le \|\phi(t_n) + \phi_{\mathrm{GS}}\|_{L^4(\Omega)} \|\phi(t_n) - \phi_{\mathrm{GS}}\|_{L^4(\Omega)} \|z_n^2\|_{L^2(\Omega)} \to 0.$$

Hence,

$$\lim_{n\to\infty} \underbrace{\int_\Omega \left(|\nabla z_n|^2 + V|z_n|^2 + \beta|\phi_{\mathrm{GS}}|^2|z_n|^2\right) \mathrm{d}x}_{=:a_{\phi_{\mathrm{GS}}}(z_n,z_n)} = C_{\mathrm{inf}}.$$

Since $\{z_n\}_{n\in\mathbb{N}}$ is bounded in $H^1(\Omega)$, there exists a weak limit

$$z_n \rightharpoonup \hat{z} \qquad \text{weakly in } H^1(\Omega).$$

This indicates $\|\hat{z}\|_{L^2(\Omega)} = 1$ and

$$\begin{aligned}&\left|(\hat{z},\phi_{\mathrm{GS}})_{L^2(\Omega)} - (z_n,\phi(t_n))_{L^2(\Omega)}\right| \\ &\qquad \le \|\hat{z}-z_n\|_{L^2(\Omega)}\|\phi_{\mathrm{GS}}\|_{L^2(\Omega)} + \|z_n\|_{L^2(\Omega)}\|\phi_{\mathrm{GS}}-\phi(t_n)\|_{L^2(\Omega)} \to 0,\end{aligned}$$

which leads to

$$(\hat{z},\phi_{\mathrm{GS}})_{L^2(\Omega)} = 0.$$

Lower semicontinuity of weakly converging sequence implies

$$C_{\mathrm{inf}} = \lim_{n\to\infty} a_{\phi_{\mathrm{GS}}}(z_n,z_n) \ge a_{\phi_{\mathrm{GS}}}(\hat{z},\hat{z}) \ge \inf_{v\in \mathrm{span}\{\phi_{\mathrm{GS}}\}^\perp} \frac{a_{\phi_{\mathrm{GS}}}(v,v)}{\|v\|^2_{L^2(\Omega)}}.$$

With the Courant–Fischer theorem we get

$$C_{\mathrm{inf}} \ge \lambda_2,$$

where λ_2 is the second eigenvalue of linear eigenvalue problem: Find $(u,\lambda)\in H^1_0(\Omega)\times\mathbb{R}$ such that

$$-\Delta u + Vu + \beta|\phi_{\mathrm{GS}}|^2 u = \lambda u.$$

With the fact $\mu[\phi(t)] \to \lambda_{\mathrm{GS}}$ as $t\to\infty$, there exists $T_\epsilon > 0$ such that for $t \ge T_\epsilon$

$$\mu[\phi(t)] \le \lambda_{\mathrm{GS}} + \frac{\epsilon}{2} \tag{3.23}$$

and

$$\frac{a_\phi(\phi_t,\phi_t)}{\|\phi_t\|^2_{L^2(\Omega)}} \ge \lambda_2 - \frac{\epsilon}{2}. \tag{3.24}$$

Combining (3.23) and (3.24), we have that for $t \ge T_\epsilon$,

$$\begin{aligned} g'(t) &\le -\int_\Omega \left(|\nabla\phi_t|^2 + V|\phi_t|^2 + \beta|\phi|^2|\phi_t|^2\right)\mathrm{d}x + \mu[\phi]\|\phi_t\|^2_{L^2(\Omega)} \\ &= \|\phi_t\|^2_{L^2(\Omega)}\left(\mu[\phi] - \frac{a_\phi(\phi_t,\phi_t)}{\|\phi_t\|^2_{L^2(\Omega)}}\right) \\ &\le -(\lambda_2 - \lambda_{\mathrm{GS}} - \epsilon)\|\phi_t\|^2_{L^2(\Omega)} = -2(\lambda_2-\lambda_{\mathrm{GS}}-\epsilon)g(t). \end{aligned}$$

This completes the proof. □

By Grönwall's inequality, we arrive at

Corollary 3.9. *Let $\epsilon\in(0,\lambda_2-\lambda_{GS})$. If $t\ge T_\epsilon$, then*

$$g(t) \le C_\epsilon \exp\big(-2(\lambda_2-\lambda_{GS}-\epsilon)t\big). \tag{3.25}$$

With the inequality (3.25), we obtain the following exponential convergence.

Theorem 3.10. *Let* $\epsilon \in (0, \lambda_2 - \lambda_{GS})$*. If* $t \geq T_\epsilon$*, then*

- *exponential convergence of energy*

$$E(\phi(t)) - E(\phi_{GS}) \leq C_\epsilon \exp\big(-2(\lambda_2 - \lambda_{GS} - \epsilon)t\big), \tag{3.26}$$

- *exponential convergence to ground state*

$$\|\phi(t) - \phi_{GS}\|_{L^2(\Omega)} \leq C_\epsilon \exp\big(-(\lambda_2 - \lambda_{GS} - \epsilon)t\big), \tag{3.27}$$

- *exponential convergence of eigenvalue*

$$|\mu[\phi(t)] - \lambda_{GS}| \leq C_\epsilon \exp\big(-(\lambda_2 - \lambda_{GS} - \epsilon)t\big). \tag{3.28}$$

Proof. Note that

$$E(\phi(t)) - E(\phi_{\mathrm{GS}}) = \int_t^\infty 2g(t)\ \mathrm{d}t,$$

then (3.26) follows from (3.25). Equation (3.27) can be similarly derived by (3.25) and

$$\|\phi(t) - \phi_{\mathrm{GS}}\|_{L^2(\Omega)} \leq \int_t^\infty \|\phi_t\|_{L^2(\Omega)}\ \mathrm{d}t \leq \int_t^\infty \sqrt{2g(t)}\ \mathrm{d}t.$$

With (3.26) and (3.27), we have

$$\begin{aligned}
|\mu[\phi(t)] - \lambda_{\mathrm{GS}}| &\leq 2(E(\phi(t)) - E(\phi_{\mathrm{GS}})) + \left|\frac{\beta}{2}\int_\Omega \Big(|\phi(t)|^4 - |\phi_{\mathrm{GS}}|^4\Big)\ \mathrm{d}x\right| \\
&\leq C_\epsilon \exp\big(-2(\lambda_2 - \lambda_{\mathrm{GS}} - \epsilon)t\big) \\
&\quad + C\|\phi - \phi_{\mathrm{GS}}\|_{L^2(\Omega)}\|\phi + \phi_{\mathrm{GS}}\|_{L^6(\Omega)}\|\phi^2 + \phi_{\mathrm{GS}}^2\|_{L^3(\Omega)} \\
&\leq C_\epsilon \exp\big(-(\lambda_2 - \lambda_{\mathrm{GS}} - \epsilon)t\big).
\end{aligned}$$

This completes the proof of (3.28). □

In addition, we further obtain the strong convergence in $H^2(\Omega)$.

Theorem 3.11. $\phi(t)$ *strongly converges to* ϕ_{GS} *in* $H^2(\Omega)$ *as* $t \to \infty$*, and hence* $\|\phi(t)\|_{H^2(\Omega)}$ *is uniformly bounded.*

Proof. We only need to prove the first claim. The Sobolev embedding $H_0^1(\Omega) \hookrightarrow L^6(\Omega)$ implies that

$$\begin{aligned}
\|\phi^3 - \phi_{\mathrm{GS}}^3\|_{L^2(\Omega)} &= \|(\phi - \phi_{\mathrm{GS}})(\phi^2 + \phi\phi_{\mathrm{GS}} + \phi_{\mathrm{GS}}^2)\|_{L^2(\Omega)} \\
&\leq \|\phi - \phi_{\mathrm{GS}}\|_{L^6(\Omega)}\|\phi^2 + \phi\phi_{\mathrm{GS}} + \phi_{\mathrm{GS}}^2\|_{L^3(\Omega)} \\
&\leq C\Big(\|\phi\|_{H_0^1(\Omega)}^2 + \|\phi_{\mathrm{GS}}\|_{H_0^1(\Omega)}^2\Big)\|\phi - \phi_{\mathrm{GS}}\|_{H_0^1(\Omega)} \qquad \to 0.
\end{aligned}$$

Corollary 3.9 implies $\phi_t \to 0$ in $L^2(\Omega)$, combining (3.28), we have

$$\Delta\phi(t) = \phi_t + V\phi + \beta\phi^3 - \mu[\phi]\phi \to V\phi_{\mathrm{GS}} + \beta\phi_{\mathrm{GS}}^3 - \lambda_{\mathrm{GS}}\phi_{\mathrm{GS}} = \Delta\phi_{\mathrm{GS}} \qquad \text{in } L^2(\Omega).$$

Applying the Miranda–Talenti estimate [35,47], we obtain

$$\|D^2(\phi - \phi_{\mathrm{GS}})\|_{L^2(\Omega)} \leq \|\Delta(\phi - \phi_{\mathrm{GS}})\|_{L^2(\Omega)}.$$

Namely, $\phi(t) \to \phi_{\mathrm{GS}}$ in $H^2(\Omega) \cap H_0^1(\Omega)$. □

4. Numerical analysis

In this section, we introduce the numerical discretization scheme of the L^2 normalized gradient flow corresponding to the GP eigenvalue problem and its convergence analysis. Combining a backward-forward Euler discretization in time and a linear finite element discretization in space, we propose a fully discrete scheme for the model problem, and give local in time convergence results with respect to the temporal mesh τ and spatial mesh h.

4.1. Numerical scheme

We consider the numerical approximation of (3.1) in finite time T and a bounded convex polygon Ω. Taking an inner product with $v \in H_0^1(\Omega)$ in (3.1), we obtain the variational form of (3.1) as follows:

$$(\phi_t, v)_{L^2(\Omega)} + (\nabla\phi, \nabla v)_{L^2(\Omega)} = -(V\phi, v)_{L^2(\Omega)} - \beta(\phi^3, v)_{L^2(\Omega)} + \mu[\phi](\phi, v)_{L^2(\Omega)} \qquad \forall\, t > 0. \tag{4.1}$$

We first consider the temporal semi-discretization. Let $0 = t_0 < t_1 < \cdots < t_N = T$ denote a uniform partition of the time interval $[0, T]$ with stepsize $\tau = T/N$. Let ϕ^n be the approximation of $\phi(t_n)$. By applying the backward-forward Euler discretization to (4.1) at $t = t_{n+1}$, we obtain

$$\begin{aligned}\left(\frac{\tilde{\phi}^{n+1} - \phi^n}{\tau}, v\right)_{L^2(\Omega)} &+ (\nabla\tilde{\phi}^{n+1}, \nabla v)_{L^2(\Omega)} \\ &= -(V\phi^n, v)_{L^2(\Omega)} - \beta((\phi^n)^3, v)_{L^2(\Omega)} + \mu[\phi^n](\phi^n, v)_{L^2(\Omega)} \quad \forall v \in H_0^1(\Omega).\end{aligned} \tag{4.2}$$

Here $\tilde{\phi}^{n+1}$ is a temporary approximation of $\phi(t_{n+1})$. In general, $\|\tilde{\phi}^{n+1}\|_{L^2(\Omega)} \neq 1$. To get a mass conservation approximation, we normalize $\tilde{\phi}^{n+1}$ and set

$$\phi^{n+1} = \frac{\tilde{\phi}^{n+1}}{\left\|\tilde{\phi}^{n+1}\right\|_{L^2(\Omega)}}.$$

We then use the finite element method to perform the spatial discretization of (4.2). Let $\mathcal{T}_h$ be a shape regular and quasi-uniform triangulation of Ω with mesh size h, and denote $S_h \subset H_0^1(\Omega)$ the piecewise linear finite element space corresponding to $\mathcal{T}_h$. The Ritz projection operator $R_h : H_0^1(\Omega) \to S_h$ and the discrete Laplacian operator $\Delta_h : S_h \to S_h$ are defined as follows:

$$\begin{aligned}(\nabla R_h u, \nabla v_h)_{L^2(\Omega)} &= (\nabla u, \nabla v_h)_{L^2(\Omega)} \qquad \forall\, u \in H_0^1(\Omega), \forall\, v_h \in S_h,\\ (\Delta_h u_h, v_h)_{L^2(\Omega)} &= -(\nabla u_h, \nabla v_h)_{L^2(\Omega)} \qquad \forall\, u_h,\, v_h \in S_h.\end{aligned}$$

Combining the finite element discretization in space, we apply the following full-discrete scheme to (3.1).

For $0 \le n \le N-1$ and given $\phi_h^n \in S_h$, we first obtain $\tilde{\phi}_h^{n+1}$ by solving the following equation: Find $\tilde{\phi}_h^{n+1} \in S_h$, such that,

$$\begin{aligned}\left(\frac{\tilde{\phi}_h^{n+1} - \phi_h^n}{\tau}, v_h\right)_{L^2(\Omega)} &+ (\nabla\tilde{\phi}_h^{n+1}, \nabla v_h)_{L^2(\Omega)} \\ &= (-V\phi_h^n, v_h)_{L^2(\Omega)} - \beta\big(|\phi_h^n|^2\phi_h^n, v_h\big)_{L^2(\Omega)} + \mu[\phi_h^n](\phi_h^n, v_h)_{L^2(\Omega)} \qquad \forall\, v_h \in S_h.\end{aligned} \tag{4.3}$$

Then, we get ϕ_h^{n+1} by normalizing $\tilde{\phi}_h^{n+1}$, *i.e.*,

$$\phi_h^{n+1} = \frac{\tilde{\phi}_h^{n+1}}{\left\|\tilde{\phi}_h^{n+1}\right\|_{L^2(\Omega)}}. \tag{4.4}$$

The initial value ϕ_h^0 is given by

$$\phi_h^0 = \frac{R_h\phi_0}{\|R_h\phi_0\|_{L^2(\Omega)}}. \tag{4.5}$$

Remark 4.1 (Well-posedness of the initial value)**.** Equation (A.2) implies that

$$\|\phi_0 - R_h\phi_0\|_{L^2(\Omega)} \le Ch^2\|\phi_0\|_{H^2(\Omega)}.$$

Then for a sufficiently small $h > 0$, we have $\|R_h\phi_0\|_{L^2(\Omega)} > 0$ provided by $\|\phi_0\|_{L^2(\Omega)} = 1$, which indicates the well-posedness of the initial value ϕ_h^0.

The subsequent theorem shows the well-posedness of the numerical scheme (4.3)–(4.5).

Theorem 4.2. *The numerical scheme* (4.3)–(4.5) *is well-posed for any* $\tau > 0$ *and sufficiently small* $h > 0$.

Proof. The numerical scheme (4.3)–(4.5) contains two steps, the first step is to get $\tilde\phi_h^{n+1}$ by solving the following equation

$$\tau(\nabla\tilde\phi_h^{n+1}, \nabla v_h)_{L^2(\Omega)} + (\tilde\phi_h^{n+1}, v_h)_{L^2(\Omega)} = (f^n, v_h)_{L^2(\Omega)} \qquad \forall\, v_h \in S_h,$$

here $f^n \in L^2(\Omega)$ only depends on ϕ_h^n. By noticing that

$$\tau(\nabla u_h, \nabla u_h)_{L^2(\Omega)} + (u_h, u_h)_{L^2(\Omega)} \ge \min\{\tau, 1\}\|u_h\|_{H^1(\Omega)}^2 \qquad \forall u_h \in S_h,$$

then the well-posedness of $\tilde\phi_h^{n+1}$ can be obtained by the Lax–Milgram lemma [15]. The second step is to get ϕ_h^{n+1} by normalizing $\tilde\phi_h^{n+1}$, to show the well-posedness of the second step, we only need to prove that for any $0 \le n \le N-1$

$$\left\|\tilde\phi_h^{n+1}\right\|_{L^2(\Omega)} \ne 0.$$

If not, suppose

$$\left\|\tilde\phi_h^{n+1}\right\|_{L^2(\Omega)} = 0$$

for some $0 \le n \le N-1$, then equation

$$\left(-\frac{\phi_h^n}{\tau}, v_h\right)_{L^2(\Omega)} = \left(-V\phi_h^n - \beta|\phi_h^n|^2\phi_h^n + \mu[\phi_h^n]\phi_h^n, v_h\right)_{L^2(\Omega)} \tag{4.6}$$

holds for any $v_h \in S_h$. Choose $v_h = \phi_h^n$ in (4.6), we can get

$$\underbrace{-\frac{1}{\tau}}_{<0} = \underbrace{\int_\Omega |\nabla\phi_h^n|^2 \,\mathrm{d}x}_{\ge 0},$$

which is a contradiction. $\square$

4.2. Convergence

In this subsection, we will show the convergence of the numerical scheme (4.3)–(4.5). It is well known that error estimates with respect to the mesh size depend on the regularity of the solution. In our analysis, we require the following assumption.

Assumption 4.3. *The potential function* $V \in L^2(\Omega)$*, and the solution of* (3.1) *satisfies*

$$\phi \in C^1([0,\infty); H^2(\Omega) \cap H_0^1(\Omega)), \qquad \phi_{tt} \in C([0,\infty); L^2(\Omega)). \tag{4.7}$$

Remark 4.4. Although the mathematical analysis of the L^2 normalized gradient flow is considered under $V \in L^\infty(\Omega)$, our numerical analysis will show that the convergence also works under a weaker potential function $V \in L^2(\Omega)$ which includes the Coulomb potential.

4.2.1. Technical lemmas

In this part, we will list several technical lemmas which will be used in the convergence analysis, whose proofs are provided in Appendix B. In order to simplify the notation, for $0 \neq v \in L^2(\Omega)$, denote

$$\widehat{v} = \frac{v}{\|v\|_{L^2(\Omega)}}\cdot$$

Lemma 4.5. *For $\|u\|_{H^1(\Omega)} \leq M$, $\|v\|_{H^1(\Omega)} \leq M$, $\|u\|_{L^2(\Omega)} = \|v\|_{L^2(\Omega)} = 1$, there holds*

$$|\mu[u] - \mu[v]| \leq C_M \|u - v\|_{H^1(\Omega)},$$

where C_M depends cubically on M.

Lemma 4.6. *If $u \in H_0^1(\Omega) \cap H^2(\Omega)$ with $\|u\|_{L^2(\Omega)} = 1$, then*

$$\left|\mu[u] - \mu[\widehat{R_h u}]\right| \leq Ch^2,$$

where the constant C only depends on $\|u\|_{H^2(\Omega)}$.

Lemma 4.7 (discrete Gronwall's inequality [42])**.** *Let τ, B and a_k, b_k, c_k, γ_k be nonnegative numbers such that*

$$a_n + \tau \sum_{k=0}^{n} \gamma_k b_k \leq \tau \sum_{k=0}^{n} \gamma_k a_k + \tau \sum_{k=0}^{n} c_k + B.$$

Suppose that $\tau\gamma_k < 1$ for all k, and set $\sigma_k = (1 - \tau\gamma_k)^{-1}$. Then

$$a_n + \tau \sum_{k=0}^{n} \gamma_k b_k \leq \exp\left(\tau \sum_{k=0}^{n} \gamma_k \sigma_k\right)\left(\tau \sum_{k=0}^{n} c_k + B\right).$$

4.2.2. Consistency

Note that the exact solution satisfies: for any $v_h \in S_h$

$$\begin{aligned}&(\phi_t(t_{n+1}), v_h)_{L^2(\Omega)} + (\nabla \phi(t_{n+1}), \nabla v_h)_{L^2(\Omega)} \\ &\quad = -(V\phi(t_{n+1}), v_h)_{L^2(\Omega)} - (\beta \phi(t_{n+1})^3, v_h)_{L^2(\Omega)} + \mu[\phi(t_{n+1})](\phi(t_{n+1}), v_h)_{L^2(\Omega)},\end{aligned}$$

which implies

$$\begin{aligned}&\left(\frac{\widehat{R_h\phi(t_{n+1})} - \widehat{R_h\phi(t_n)}}{\tau}, v_h\right)_{L^2(\Omega)} + (\nabla \widehat{R_h\phi(t_{n+1})}, \nabla v_h)_{L^2(\Omega)} \\ &= -(V\widehat{R_h\phi(t_n)}, v_h)_{L^2(\Omega)} - (\beta(\widehat{R_h\phi(t_n)})^3, v_h)_{L^2(\Omega)} + \mu[\widehat{R_h\phi(t_n)}](\widehat{R_h\phi(t_n)}, v_h)_{L^2(\Omega)} + \mathcal{E}(v_h).\end{aligned}$$

Here, $\mathcal{E}(v_h)$ denotes the truncation error, given by

$$\begin{aligned}\mathcal{E}(v_h) = &\left(\frac{\widehat{R_h\phi(t_{n+1})} - \widehat{R_h\phi(t_n)}}{\tau}, v_h\right)_{L^2(\Omega)} - (\phi_t(t_{n+1}), v_h)_{L^2(\Omega)} \\ &+ \underbrace{\frac{1}{\|R_h\phi(t_{n+1})\|_{L^2(\Omega)}}(\nabla R_h\phi(t_{n+1}) - \nabla\phi(t_{n+1}), \nabla v_h)_{L^2(\Omega)}}_{=0}\end{aligned}$$

$$
\begin{aligned}
&+\left(\frac{1}{\|R_h\phi(t_{n+1})\|_{L^2(\Omega)}}-1\right)(\nabla\phi(t_{n+1}),\nabla v_h)_{L^2(\Omega)}\\
&+(V\widehat{R_h\phi(t_n)},v_h)_{L^2(\Omega)}-(V\phi(t_{n+1}),v_h)_{L^2(\Omega)}\\
&+(\beta(\widehat{R_h\phi(t_n)})^3,v_h)_{L^2(\Omega)}-(\beta\phi(t_{n+1})^3,v_h)_{L^2(\Omega)}\\
&+\mu[\phi(t_{n+1})](\phi(t_{n+1}),v_h)_{L^2(\Omega)}-\mu[\widehat{R_h\phi(t_n)}](\widehat{R_h\phi(t_n)},v_h)_{L^2(\Omega)}\\
=:\;&\mathcal{E}_1(v_h)+\mathcal{E}_2(v_h)+\mathcal{E}_3(v_h)+\mathcal{E}_4(v_h)+\mathcal{E}_5(v_h).
\end{aligned}
\tag{4.8}
$$

The rest of this part is to prove the following estimate of the truncation error $\mathcal{E}(\cdot)$.

Lemma 4.8. *The truncation error of the numerical scheme* (4.3)–(4.5) *is given by*

$$
|\mathcal{E}(v_h)|\le C(\tau+h^2)\|\nabla v_h\|_{L^2(\Omega)}\qquad\forall v_h\in S_h.
\tag{4.9}
$$

Proof. We will estimate for $\mathcal{E}_j(v_h)$, $j=1,2,3,4,5$, respectively, where

$$
\begin{aligned}
\mathcal{E}_1(v_h)&=\left(\frac{\widehat{R_h\phi(t_{n+1})}-\widehat{R_h\phi(t_n)}}{\tau},v_h\right)_{L^2(\Omega)}-(\phi_t(t_{n+1}),v_h)_{L^2(\Omega)},\\
\mathcal{E}_2(v_h)&=\left(\frac{1}{\|R_h\phi(t_{n+1})\|_{L^2(\Omega)}}-1\right)(\nabla\phi(t_{n+1}),\nabla v_h)_{L^2(\Omega)},\\
\mathcal{E}_3(v_h)&=(V\widehat{R_h\phi(t_n)},v_h)_{L^2(\Omega)}-(V\phi(t_{n+1}),v_h)_{L^2(\Omega)},\\
\mathcal{E}_4(v_h)&=(\beta(\widehat{R_h\phi(t_n)})^3,v_h)_{L^2(\Omega)}-(\beta\phi(t_{n+1})^3,v_h)_{L^2(\Omega)},\\
\mathcal{E}_5(v_h)&=\mu[\phi(t_{n+1})](\phi(t_{n+1}),v_h)_{L^2(\Omega)}-\mu[\widehat{R_h\phi(t_n)}](\widehat{R_h\phi(t_n)},v_h)_{L^2(\Omega)}.
\end{aligned}
$$

First, we have

$$
\begin{aligned}
|\mathcal{E}_1(v_h)|\le{}&\left\|\frac{\widehat{R_h\phi(t_{n+1})}-\widehat{R_h\phi(t_n)}}{\tau}-\frac{R_h\phi(t_{n+1})-R_h\phi(t_n)}{\tau}\right\|_{L^2(\Omega)}\|v_h\|_{L^2(\Omega)}\\
&+\left\|\frac{R_h\phi(t_{n+1})-R_h\phi(t_n)}{\tau}-\frac{\phi(t_{n+1})-\phi(t_n)}{\tau}\right\|_{L^2(\Omega)}\|v_h\|_{L^2(\Omega)}\\
&+\left\|\frac{\phi(t_{n+1})-\phi(t_n)}{\tau}-\phi_t(t_{n+1})\right\|_{L^2(\Omega)}\|v_h\|_{L^2(\Omega)}\\
\le{}&I_1\|v_h\|_{L^2(\Omega)}+Ch^2\|v_h\|_{L^2(\Omega)}+Ch^2\left\|\frac{\phi(t_{n+1})-\phi(t_n)}{\tau}\right\|_{H^2(\Omega)}\|v_h\|_{L^2(\Omega)}+C\tau\|v_h\|_{L^2(\Omega)}\\
\le{}&I_1\|v_h\|_{L^2(\Omega)}+Ch^2\|v_h\|_{L^2(\Omega)}+C\tau\|v_h\|_{L^2(\Omega)},
\end{aligned}
\tag{4.10}
$$

where

$$
I_1=\left\|\frac{(\phi(t_{n+1})/\|R_h\phi(t_{n+1})\|_{L^2(\Omega)}-\phi(t_{n+1}))-(\phi(t_n)/\|R_h\phi(t_n)\|_{L^2(\Omega)}-\phi(t_n))}{\tau}\right\|_{L^2(\Omega)}.
$$

It is seen that

$$
I_1\le\max_{t_n\le t\le t_{n+1}}\left\|\partial_t\big(\phi(t)/\|R_h\phi(t)\|_{L^2(\Omega)}-\phi(t)\big)\right\|_{L^2(\Omega)}.
$$

Since

$$\begin{aligned}
&\partial_t(\phi(t)/\|R_h\phi(t)\|_{L^2(\Omega)} - \phi(t))\\
&= \partial_t\phi(t)(1/\|R_h\phi(t)\|_{L^2(\Omega)} - 1) + \phi\left(\frac{1}{\|R_h\phi(t)\|_{L^2(\Omega)}} - \frac{1}{\|\phi(t)\|_{L^2(\Omega)}}\right)'\\
&= \phi_t(t)(1/\|R_h\phi(t)\|_{L^2(\Omega)} - 1) + \phi\left(\frac{(R_h\phi(t), R_h\phi_t(t))_{L^2(\Omega)}}{\|R_h\phi(t)\|^3_{L^2(\Omega)}} - \frac{(\phi(t),\phi_t(t))_{L^2(\Omega)}}{\|\phi(t)\|^3_{L^2(\Omega)}}\right),
\end{aligned}$$

we are able to estimate as follows

$$\|\phi_t(t)(1/\|R_h\phi(t)\|_{L^2(\Omega)} - 1)\|_{L^2(\Omega)} \le C\|\phi(t) - R_h\phi(t)\|_{L^2(\Omega)} \le Ch^2,$$

and

$$\begin{aligned}
&\left|\frac{(R_h\phi(t), R_h\phi_t(t))_{L^2(\Omega)}}{\|R_h\phi(t)\|^3_{L^2(\Omega)}} - \frac{(\phi(t),\phi_t(t))_{L^2(\Omega)}}{\|\phi(t)\|^3_{L^2(\Omega)}}\right|\\
&\le \left|\frac{(R_h\phi(t), R_h\phi_t(t))_{L^2(\Omega)}}{\|R_h\phi(t)\|^3_{L^2(\Omega)}} - \frac{(\phi(t),\phi_t(t))_{L^2(\Omega)}}{\|R_h\phi(t)\|^3_{L^2(\Omega)}}\right|\\
&\quad + \left|\frac{(\phi(t),\phi_t(t))_{L^2(\Omega)}}{\|R_h\phi(t)\|^3_{L^2(\Omega)}} - \frac{(\phi(t),\phi_t(t))_{L^2(\Omega)}}{\|\phi(t)\|^3_{L^2(\Omega)}}\right|\\
&\le C\big|(R_h\phi(t), R_h\phi_t(t))_{L^2(\Omega)} - (\phi(t),\phi_t(t))_{L^2(\Omega)}\big| + Ch^2\\
&\le C\big|(R_h\phi(t), R_h\phi_t(t) - \phi_t(t))_{L^2(\Omega)}\big| + C\big|(R_h\phi(t) - \phi(t), \phi_t)_{L^2(\Omega)}\big| + Ch^2\\
&\le Ch^2\|\phi_t\|_{H^2(\Omega)} + Ch^2\|\phi\|_{H^2(\Omega)} + Ch^2,
\end{aligned}$$

we get $I_1 \le Ch^2$, which implies

$$|\mathcal{E}_1(v_h)| \le C(\tau + h^2)\|v_h\|_{L^2(\Omega)}. \tag{4.11}$$

Second, it is easy to show that

$$\begin{aligned}
|\mathcal{E}_2(v_h)| &= \left|\left(\frac{1}{\|R_h\phi(t_{n+1})\|_{L^2(\Omega)}} - 1\right)(\nabla\phi(t_{n+1}), \nabla v_h)_{L^2(\Omega)}\right|\\
&\le \left|\frac{1}{\|R_h\phi(t_{n+1})\|_{L^2(\Omega)}} - 1\right|\|\nabla\phi(t_{n+1})\|_{L^2(\Omega)}\|\nabla v_h\|_{L^2(\Omega)} \le Ch^2\|v_h\|_{H^1(\Omega)}.
\end{aligned} \tag{4.12}$$

Third, by Sololev embedding inequality, there holds

$$\begin{aligned}
|\mathcal{E}_3(v_h)| &= \left|(V\widehat{R_h\phi(t_n)}, v_h)_{L^2(\Omega)} - (V\phi(t_{n+1}), v_h)_{L^2(\Omega)}\right|\\
&\le \left|(V\widehat{R_h\phi(t_n)} - V\widehat{R_h\phi(t_{n+1})}, v_h)_{L^2(\Omega)}\right| + \left|(V\widehat{R_h\phi(t_{n+1})} - V\phi(t_{n+1}), v_h)_{L^2(\Omega)}\right|\\
&\le \|V\|_{L^2(\Omega)}\left\|\widehat{R_h\phi(t_{n+1})} - \widehat{R_h\phi(t_n)}\right\|_{L^3(\Omega)}\|v_h\|_{L^6(\Omega)}\\
&\quad + \|V\|_{L^2(\Omega)}\|\widehat{R_h\phi(t_{n+1})} - \phi(t_{n+1})\|_{L^3(\Omega)}\|v_h\|_{L^6(\Omega)}\\
&\le C\tau\|v_h\|_{H^1(\Omega)} + Ch^2\|v_h\|_{H^1(\Omega)}.
\end{aligned} \tag{4.13}$$

Fourth,

$$|\mathcal{E}_4(v_h)| = \left|(\beta(\widehat{R_h\phi(t_n)})^3, v_h)_{L^2(\Omega)} - (\beta\phi(t_{n+1})^3, v_h)_{L^2(\Omega)}\right|$$

$$\begin{aligned}&\leq |(\beta(\widehat{R_h\phi(t_n)})^3-\beta(\widehat{R_h\phi(t_{n+1})})^3,v_h)_{L^2(\Omega)}|\\&\quad+|(\beta(\widehat{R_h\phi(t_{n+1})})^3-\beta\phi(t_{n+1})^3,v_h)_{L^2(\Omega)}|\\&\leq C\tau\|v_h\|_{L^2(\Omega)}+Ch^2\|v_h\|_{H^1(\Omega)}.\end{aligned}\tag{4.14}$$

Finally, by Lemmas 4.5 and 4.6, we can estimate as follows

$$\begin{aligned}|\mathcal{E}_5(v_h)|&=\left|\mu[\phi(t_{n+1})](\phi(t_{n+1}),v_h)_{L^2(\Omega)}-\mu[\widehat{R_h\phi(t_n)}](\widehat{R_h\phi(t_n)},v_h)_{L^2(\Omega)}\right|\\&\leq|\mu[\phi(t_{n+1})]-\mu[\phi(t_n)]||(\phi(t_{n+1}),v_h)_{L^2(\Omega)}|\\&\quad+|\mu[\phi(t_n)]||(\phi(t_{n+1})-\phi(t_n),v_h)_{L^2(\Omega)}|\\&\quad+|\mu[\phi(t_n)]-\mu[\widehat{R_h\phi(t_n)}]||(\phi(t_n),v_h)_{L^2(\Omega)}|\\&\quad+|\mu[\widehat{R_h\phi(t_n)}]||(\phi(t_n)-\widehat{R_h\phi(t_n)},v_h)_{L^2(\Omega)}|\\&\leq C\|\phi(t_{n+1})-\phi(t_n)\|_{H^1(\Omega)}\|v_h\|_{L^2(\Omega)}+C\tau\|v_h\|_{L^2(\Omega)}\\&\quad+Ch^2\|v_h\|_{L^2(\Omega)}+Ch^2\|v_h\|_{L^2(\Omega)}\\&\leq C\tau\|v_h\|_{L^2(\Omega)}+Ch^2\|v_h\|_{L^2(\Omega)}.\end{aligned}\tag{4.15}$$

Combining estimates of $\mathcal{E}_1$–$\mathcal{E}_5$, we arrive at the given conclusion. □

4.2.3. Error equation

We define the following two types of error functions:

$$e_h^n=\widehat{R_h\phi(t_n)}-\phi_h^n$$

for $0\leq n\leq N$, and

$$\tilde{e}_h^n=\widehat{R_h\phi(t_n)}-\tilde{\phi}_h^n$$

for $1\leq n\leq N$, with $\tilde{e}_h^0=0$. Then the error equation can be written as: For $0\leq n\leq N-1$

$$\begin{aligned}&\left(\frac{\tilde{e}_h^{n+1}-e_h^n}{\tau},v_h\right)_{L^2(\Omega)}+(\nabla\tilde{e}_h^{n+1},\nabla v_h)_{L^2(\Omega)}\\&\quad=-(Ve_h^n,v_h)_{L^2(\Omega)}-(\beta(\widehat{R_h\phi(t_n)})^3-\beta(\phi_h^n)^3,v_h)_{L^2(\Omega)}\\&\qquad+\mu[\widehat{R_h\phi(t_n)}](\widehat{R_h\phi(t_n)},v_h)_{L^2(\Omega)}-\mu[\phi_h^n](\phi_h^n,v_h)_{L^2(\Omega)}+\mathcal{E}(v_h)\end{aligned}\tag{4.16}$$

holds for any $v_h\in S_h$.

To carry out the error estimate, we do several preparations.

Lemma 4.9. *For $0\leq n\leq N$, there hold*

$$\|e_h^n\|_{L^2(\Omega)}\leq C\|\tilde{e}_h^n\|_{L^2(\Omega)},\tag{4.17}$$

$$\|e_h^n\|_{L^2(\Omega)}\leq\|\tilde{e}_h^n\|_{L^2(\Omega)}+C\|\tilde{e}_h^n\|_{L^2(\Omega)}^3.\tag{4.18}$$

Proof. Left in Appendix B. □

Lemma 4.10. *There exist τ_0 and h_0 sufficiently small such that for $\tau\leq\tau_0$ and $h\leq h_0$, with an additional "inverse" CFL condition $\tau\geq\kappa h^4$ where κ is a constant sufficiently large, such that*

$$\|\tilde{e}_h^n\|_{L^2(\Omega)}\leq\sqrt{\tau},\tag{4.19}$$

$$\|\tilde{e}_h^n\|_{H^1(\Omega)}\leq 1,\tag{4.20}$$

$$\|\tilde{e}_h^n\|_{L^\infty(\Omega)}\leq 1,\tag{4.21}$$

for $0\leq n\leq N$.

We will prove Lemma 4.10 by mathematical induction, for $n = 0$, since $\tilde{e}_h^0 = 0$, (4.19)–(4.21) naturally hold. Assume (4.19)–(4.21) hold for $0 \le k \le n$, in the next subsection, we will show that (4.19)–(4.21) also hold for $k = n+1$. Before that, we have the following results under assumptions of the mathematical induction.

Lemma 4.11. *For $0 \le k \le n$, the following estimates hold for e_h^k:*

$$\|e_h^k\|_{H^1(\Omega)} \le C\|\tilde{e}_h^k\|_{H^1(\Omega)} + Ch^2 \tag{4.22}$$

and

$$\|e_h^k\|_{L^\infty(\Omega)} \le C. \tag{4.23}$$

Proof. By directly calculating and assumption (4.20)

$$\begin{aligned}
\|e_h^k\|_{H^1(\Omega)} &\le \|\tilde{e}_h^k\|_{H^1(\Omega)} + \|\phi_h^k - \tilde{\phi}_h^k\|_{H^1(\Omega)} = \|\tilde{e}_h^k\|_{H^1(\Omega)} + \left| \frac{1}{\|\tilde{\phi}_h^k\|_{L^2(\Omega)}} - 1 \right| \|\tilde{\phi}_h^k\|_{H^1(\Omega)} \\
&\le \|\tilde{e}_h^k\|_{H^1(\Omega)} + C\|\phi(t_k) - \tilde{\phi}_h^k\|_{L^2(\Omega)} \\
&\le \|\tilde{e}_h^k\|_{H^1(\Omega)} + C\|\phi(t_k) - \widehat{R_h\phi(t_k)}\|_{L^2(\Omega)} + C\|\widehat{R_h\phi(t_k)} - \tilde{\phi}_h^k\|_{L^2(\Omega)} \\
&\le C\|\tilde{e}_h^k\|_{H^1} + Ch^2.
\end{aligned}$$

This completes the proof of (4.22). The proof of (4.23) follows from a similar argument with assumption (4.21). ☐

4.2.4. Proof of Lemma 4.10

Taking $v_h = \tilde{e}_h^{n+1}$ in the error equation (4.16) yields,

$$\begin{aligned}
&\frac{\|\tilde{e}_h^{n+1}\|_{L^2(\Omega)}^2 - \|e_h^n\|_{L^2(\Omega)}^2}{2\tau} + \frac{\|\tilde{e}_h^{n+1} - e_h^n\|_{L^2(\Omega)}^2}{2\tau} + (\nabla \tilde{e}_h^{n+1}, \nabla v_h)_{L^2(\Omega)} \\
&\quad = -(V e_h^n, \tilde{e}_h^{n+1})_{L^2(\Omega)} - (\beta(\widehat{R_h\phi(t_n)})^3 - \beta(\phi_h^n)^3, \tilde{e}_h^{n+1})_{L^2(\Omega)} \\
&\qquad + \mu[\widehat{R_h\phi(t_n)}](\widehat{R_h\phi(t_n)}, \tilde{e}_h^{n+1})_{L^2(\Omega)} - \mu[\phi_h^n](\phi_h^n, \tilde{e}_h^{n+1})_{L^2(\Omega)} + \mathcal{E}(\tilde{e}_h^{n+1}).
\end{aligned}$$

Discarding the nonnegative term $\|\tilde{e}_h^{n+1} - e_h^n\|_{L^2(\Omega)}^2/(2\tau)$ and applying the Hölder's inequality yield

$$\begin{aligned}
&\frac{\|\tilde{e}_h^{n+1}\|_{L^2(\Omega)}^2 - \|e_h^n\|_{L^2(\Omega)}^2}{2\tau} + \|\nabla \tilde{e}_h^{n+1}\|_{L^2(\Omega)}^2 \\
&\le \|V\|_{L^2(\Omega)} \|e_h^n\|_{L^3(\Omega)} \|\tilde{e}_h^{n+1}\|_{L^6(\Omega)} \\
&\quad + C\|(\widehat{R_h\phi(t_n)})^2 + \widehat{R_h\phi(t_n)}\phi_h^n + (\phi_h^n)^2\|_{L^3(\Omega)} \|e_h^n\|_{L^2(\Omega)} \|\tilde{e}_h^{n+1}\|_{L^6(\Omega)} \\
&\quad + |\mu[\widehat{R_h\phi(t_n)}]| |(e_h^n, \tilde{e}_h^{n+1})_{L^2(\Omega)}| + |\mu[\phi_h^n] - \mu[\widehat{R_h\phi(t_n)}]| |(\phi_h^n, \tilde{e}_h^{n+1})_{L^2(\Omega)}| + |\mathcal{E}(\tilde{e}_h^{n+1})| \\
&=: \mathcal{E}_1 + \mathcal{E}_2 + \mathcal{E}_3 + \mathcal{E}_4 + |\mathcal{E}(\tilde{e}_h^{n+1})|.
\end{aligned}$$

Applying Young's inequality, we may estimate as follows,

$$\begin{aligned}
\mathcal{E}_1 &\le C\|e_h^n\|_{L^2(\Omega)}^{1/2} \|e_h^n\|_{L^6(\Omega)}^{1/2} \|\tilde{e}_h^{n+1}\|_{H^1(\Omega)} \le C\|\tilde{e}_h^n\|_{L^2(\Omega)}^{1/2} \|e_h^n\|_{H^1(\Omega)}^{1/2} \|\tilde{e}_h^{n+1}\|_{H^1(\Omega)} \\
&\le C\|\tilde{e}_h^n\|_{L^2(\Omega)}^{1/2} (\|\tilde{e}_h^n\|_{H^1(\Omega)}^{1/2} + h) \|\tilde{e}_h^{n+1}\|_{H^1(\Omega)} \\
&\le C_\epsilon \|\tilde{e}_h^n\|_{L^2(\Omega)}^2 + \epsilon\|\tilde{e}_h^n\|_{H^1(\Omega)}^2 + \epsilon\|\tilde{e}_h^{n+1}\|_{H^1(\Omega)}^2 + C_\epsilon h^4,
\end{aligned}$$

here ϵ is a small constant that to be determined later. It is easy to see that

$$\mathcal{E}_2 \le C_\epsilon \|\tilde{e}_h^n\|_{L^2(\Omega)}^2 + \epsilon \|\tilde{e}_h^{n+1}\|_{H^1(\Omega)}^2,$$

and

$$\mathcal{E}_3 \le C\|\tilde{e}_h^n\|_{L^2(\Omega)}^2 + C\|\tilde{e}_h^{n+1}\|_{L^2(\Omega)}^2.$$

As for $\mathcal{E}_4$, we have

$$\begin{aligned}\mathcal{E}_4 &\le C\|e_h^n\|_{H^1(\Omega)}\|\tilde{e}_h^{n+1}\|_{L^2(\Omega)} \le C(\|\tilde{e}_h^n\|_{H^1(\Omega)} + h^2)\|\tilde{e}_h^{n+1}\|_{L^2(\Omega)}\\ &\le \epsilon\|\tilde{e}_h^n\|_{H^1(\Omega)}^2 + C_\epsilon h^4 + C_\epsilon\|\tilde{e}_h^{n+1}\|_{L^2(\Omega)}^2.\end{aligned}$$

Combining estimates of $\mathcal{E}_1$–$\mathcal{E}_4$, using Lemma 4.8, equations (4.18) and (4.19), we obtain

$$\begin{aligned}&\frac{\|\tilde{e}_h^{n+1}\|_{L^2(\Omega)}^2 - \|\tilde{e}_h^n\|_{L^2(\Omega)}^2}{2\tau} + \|\nabla\tilde{e}_h^{n+1}\|_{L^2(\Omega)}^2\\ &\le C_\epsilon(\tau^2 + h^4) + C_\epsilon(\|\tilde{e}_h^n\|_{L^2(\Omega)}^2 + \|\tilde{e}_h^{n+1}\|_{L^2(\Omega)}^2) + \epsilon(\|\tilde{e}_h^n\|_{H^1(\Omega)}^2 + \|\tilde{e}_h^{n+1}\|_{H^1(\Omega)}^2).\end{aligned} \tag{4.24}$$

Summing equation (4.24) from 0 to $n+1$, we obtain

$$\|\tilde{e}_h^{n+1}\|_{L^2(\Omega)}^2 + \tau\sum_{k=1}^{n+1}\|\nabla\tilde{e}_h^k\|_{L^2(\Omega)}^2 \le C_\epsilon(\tau^2 + h^4) + C_\epsilon\tau\sum_{k=1}^{n+1}\|\tilde{e}_h^k\|_{L^2(\Omega)}^2 + C\epsilon\tau\sum_{k=1}^{n+1}\|\nabla\tilde{e}_h^k\|_{L^2(\Omega)}^2. \tag{4.25}$$

Choosing ϵ sufficiently small such that $C\epsilon \le \frac{1}{2}$ and applying the discrete Gronwall inequality to (4.25), we arrive at

$$\max_{0\le k\le n+1}\|\tilde{e}_h^k\|_{L^2(\Omega)}^2 + \tau\sum_{k=0}^{n+1}\|\nabla\tilde{e}_h^k\|_{L^2(\Omega)}^2 \le C(\tau + h^2)^2.$$

Then under an "inverse" CFL condition $\tau \ge \kappa h^4$ for sufficiently large κ with τ and h sufficiently small:

$$\begin{aligned}\|\tilde{e}_h^{n+1}\|_{L^2(\Omega)} &\le C(\tau + h^2) \le C\tau + C(h^2/\sqrt{\tau})\sqrt{\tau} \le (C\sqrt{\tau} + C/\kappa)\sqrt{\tau} \le \sqrt{\tau},\\ \|\nabla\tilde{e}_h^{n+1}\|_{L^2(\Omega)} &\le C\left(\sqrt{\tau} + \frac{h^2}{\sqrt{\tau}}\right) \le C(\sqrt{\tau} + \kappa^{-1}) \le 1.\end{aligned}$$

This completes the proof of (4.19) and (4.20) for $k = n+1$. If we are able to prove

$$\|\Delta_h\tilde{e}_h^{n+1}\|_{L^2(\Omega)} \le C, \tag{$*$}$$

we then obtain from (A.5) that

$$\|\tilde{e}_h^{n+1}\|_{L^\infty(\Omega)} \le \|\tilde{e}_h^{n+1}\|_{L^2(\Omega)}^{1/4}\|\Delta_h\tilde{e}_h^{n+1}\|_{L^2(\Omega)}^{3/4} \le C(\tau + h^2)^{1/4},$$

which proves (4.21) for $k = n+1$, and the proof of mathematical induction is complete.

To prove ($*$), we divide into two cases:

$$\tau \le h^2 \quad \text{and} \quad \tau \ge h^2.$$

If $\tau \le h^2$, by the inverse inequality, we can get

$$\|\Delta\tilde{e}_h^{n+1}\|_{L^2(\Omega)} \le Ch^{-2}\|\tilde{e}_h^{n+1}\|_{L^2(\Omega)} \le Ch^{-2}(\tau + h^2) \le C.$$

If $\tau \geq h^2$, we rewrite the error equation (4.16) as

$$\begin{aligned}(\Delta_h \tilde{e}_h^{n+1}, v_h)_{L^2(\Omega)} = {}& \left(\frac{\tilde{e}_h^{n+1} - e_h^n}{\tau}, v_h\right)_{L^2(\Omega)} + (V e_h^n, v_h)_{L^2(\Omega)} + (\beta(\widehat{R_h\phi(t_n)})^3 - \beta(\phi_h^n)^3, v_h)_{L^2(\Omega)} \\ & - \mu[\widehat{R_h\phi(t_n)}](\widehat{R_h\phi(t_n)}, v_h)_{L^2(\Omega)} + \mu[\phi_h^n](\phi_h^n, v_h)_{L^2(\Omega)} - \mathcal{E}(v_h) \\ =:{}& \mathcal{G}_1 + \mathcal{G}_2 + \mathcal{G}_3 + \mathcal{G}_4 + \mathcal{G}_5 + \mathcal{G}_6.\end{aligned}$$

We estimate $\mathcal{G}_1$ as follows

$$\begin{aligned}|\mathcal{G}_1| &\leq \left\| \frac{\tilde{e}_h^{n+1} - e_h^n}{\tau} \right\|_{L^2(\Omega)} \|v_h\|_{L^2(\Omega)} \leq \tau^{-1}(\|\tilde{e}_h^{n+1}\|_{L^2(\Omega)} + \|e_h^n\|_{L^2(\Omega)})\|v_h\|_{L^2(\Omega)} \\ &\leq C\tau^{-1}(\tau + h^2)\|v_h\|_{L^2(\Omega)} \leq C\|v_h\|_{L^2(\Omega)}.\end{aligned}$$

Obviously,

$$|\mathcal{G}_2| \leq C\|V\|_{L^2(\Omega)}\|e_h^n\|_{L^\infty(\Omega)}\|v_h\|_{L^2(\Omega)} \leq C\|v_h\|_{L^2(\Omega)}$$

and

$$|\mathcal{G}_j| \leq C\|v_h\|_{L^2(\Omega)}, \qquad j = 3, \ldots, 5.$$

With slightly modified estimates of the truncation error (*i.e.*, in the proof of Lem. 4.8, we apply the inverse inequality $\|v_h\|_{H^1(\Omega)} \leq Ch^{-1}\|v_h\|_{L^2(\Omega)}$ to estimates of $|\mathcal{E}_2(v_h)|$, $|\mathcal{E}_3(v_h)|$ and $|\mathcal{E}_4(v_h)|$, and further use Lemma A.2 for the estimate of $|\mathcal{E}_3(v_h)|$ which yields $|\mathcal{E}_3(v_h)| \leq C\|v_h\|_{L^2(\Omega)}$), we have

$$|\mathcal{G}_6| \leq C\|v_h\|_{L^2(\Omega)}.$$

Estimates of $\mathcal{G}_1$–$\mathcal{G}_6$ imply

$$\|\Delta_h \tilde{e}_h^{n+1}\|_{L^2(\Omega)} \leq C.$$

The proof is completed by combining estimates of two cases.

4.2.5. Error estimate

From the proof of Lemma 4.10, we have the following convergence results.

Theorem 4.12. *Under the same assumptions in Lemma 4.10, there holds*

$$\max_{0 \leq n \leq N} \|\phi(t_n) - \phi_h^n\|_{L^2(\Omega)} \leq C(\tau + h^2).$$

Proof. We obtain from Lemma 4.9 that

$$\|e_h^n\|_{L^2(\Omega)} \leq C\|\tilde{e}_h^n\|_{L^2(\Omega)} \leq C(\tau + h^2),$$

which leads to

$$\begin{aligned}\|\phi(t_n) - \phi_h^n\|_{L^2(\Omega)} &\leq \|\phi(t_n) - \widehat{R_h\phi(t_n)}\|_{L^2(\Omega)} + \|e_h^n\|_{L^2(\Omega)} \\ &\leq Ch^2 + C(\tau + h^2) \leq C(\tau + h^2),\end{aligned}$$

and completes the proof. □

Theorem 4.13 (discrete H^2 stability)**.** *Under the same assumptions in Lemma 4.10, there holds*

$$\max_{0 \leq n \leq N} \|\Delta_h \phi_h^n\|_{L^2(\Omega)} \leq C.$$

Proof. Note that

$$\phi_h^n = \frac{\tilde{\phi}_h^n}{\|\tilde{\phi}_h^n\|_{L^2(\Omega)}},$$

we obtain from $(*)$ that

$$\|\Delta_h \phi_h^n\|_{L^2(\Omega)} \leq C\|\Delta_h \tilde{\phi}_h^n\|_{L^2(\Omega)} \leq C\|\Delta_h \widehat{R_h\phi(t_n)}\|_{L^2(\Omega)} + C\|\Delta_h \tilde{e}_h^n\|_{L^2(\Omega)} \leq C,$$

which completes the proof. □

Corollary 4.14. *Under the same assumptions in Lemma 4.10, there holds*

$$\max_{0\leq n\leq N} \|\phi(t_n) - \phi_h^n\|_{H^1(\Omega)} \leq C(\sqrt{\tau} + h).$$

Proof. With inequality (A.4), we obtain

$$\|\nabla e_h^n\|_{L^2(\Omega)} \leq \|e_h^n\|_{L^2(\Omega)}^{\frac{1}{2}} \|\Delta_h e_h^n\|_{L^2(\Omega)}^{\frac{1}{2}} \leq C(\sqrt{\tau} + h),$$

which leads to

$$\|\phi(t_n) - \phi_h^n\|_{H^1(\Omega)} \leq \|\phi(t_n) - \widehat{R_h\phi(t_n)}\|_{H^1(\Omega)} + C\|\nabla e_h^n\|_{L^2(\Omega)} \leq C(\sqrt{\tau} + h).$$

This completes the proof. □

5. NUMERICAL EXPERIMENTS

In this section, we will provide two numerical experiments to verify our convergence results of numerical scheme (4.3)–(4.5) corresponding to the gradient flow model, *i.e.*, Theorem 4.12 and Corollary 4.14. All computations are performed on $\Omega = (0,1)^3$ up to time $T = 1$. The numerical error is quantified in the following norms:

$$e_{L^2} = \|\phi_h^N - \phi_{\text{ref}}(t_N)\|_{L^2(\Omega)} \qquad e_{H^1} = \|\phi_h^N - \phi_{\text{ref}}(t_N)\|_{H^1(\Omega)},$$

where $t_N = T$ is the final time and ϕ_{ref} denotes a reference solution computed by using the same numerical scheme as for ϕ_h^N with a finer time step or spatial mesh size. The corresponding code is designed based on the toolbox PHG (Parallel Hierarchical Grid) [48] and the computations are carried out on LSSC–IV cluster in the State Key Laboratory of Mathematical Sciences of the Chinese Academy of Sciences.

5.1. Example I. Harmonic potential

We consider the system (3.1) with $\beta = 10$, the initial function ϕ_0 and potential function V are as follows:

$$\phi_0 = cx(1-x)y(1-y)z(1-z), \qquad V = \frac{1}{2}(x^2 + y^2 + z^2), \tag{5.1}$$

where $c > 0$ is a constant such that $\|\phi_0\|_{L^2(\Omega)} = 1$.

Tables 1 and 2 show the temporal discretization errors e_{L^2} and e_{H^1} and the temporal convergence orders, respectively. In each case, the reference solution ϕ_{ref} is computed using the scheme (4.3)–(4.5) with the same spatial mesh as that used in computing ϕ_h^N and a smaller time step $\tau = \frac{1}{2000}$.

Tables 3 and 4 show the spatial discretization errors and convergence orders of e_{L^2} and e_{H^1}, respectively. In each case, the reference solution ϕ_{ref} is computed using the scheme (4.3)–(4.5) with the same temporal mesh as that used in computing ϕ_h^N and a smaller spatial mesh $h = 0.027063$.

From Tables 1–4, we can see that the scheme exhibits first-order temporal convergence under the L^2 and H^1 norms, first-order spatial convergence under the H^1 norm, and second-order spatial convergence under the L^2 norm.

TABLE 1. L^2 temporal discretization errors of scheme (4.3)–(4.5) with reference time step $\tau = \frac{1}{2000}$.

h	τ	e_{L^2}	Order
0.216506	1/90	2.0951E-02	–
	1/180	1.0940E-02	0.9374
	1/360	5.1690E-03	1.0817
0.108253	1/90	2.0952E-02	–
	1/180	1.0972E-02	0.9333
	1/360	5.1920E-03	1.0795

TABLE 2. H^1 temporal discretization errors of scheme (4.3)–(4.5) with reference time step $\tau = \frac{1}{2000}$.

h	τ	e_{H^1}	Order
0.216506	1/90	2.4147E-01	–
	1/180	1.2583E-01	0.9404
	1/360	5.9384E-02	1.0833
0.108253	1/90	2.3044E-01	–
	1/180	1.2037E-01	0.9369
	1/360	5.6883E-02	1.0814

TABLE 3. L^2 spatial discretization errors of scheme (4.3)–(4.5) with reference spatial mesh size $h = 0.027063$.

τ	h	e_{L^2}	Order
$\frac{1}{1000}$	0.433013	1.4300E-01	–
	0.216506	3.7730E-02	1.9222
	0.108253	9.1250E-03	2.0478
$\frac{1}{2000}$	0.433013	1.4298E-01	–
	0.216506	3.7687E-02	1.9237
	0.108253	9.1241E-03	2.0463

TABLE 4. H^1 spatial discretization errors of scheme (4.3)–(4.5) with reference spatial mesh size $h = 0.027063$ and corresponding orders.

τ	h	e_{H^1}	Order
$\frac{1}{1000}$	0.433013	2.9615	–
	0.216506	1.4438	1.0365
	0.108253	0.6971	1.0504
$\frac{1}{2000}$	0.433013	2.9599	–
	0.216506	1.4419	1.0376
	0.108253	0.6962	1.0504

TABLE 5. L^2 temporal discretization errors of scheme (4.3)–(4.5) with reference time step $\tau = \frac{1}{2000}$.

h	τ	e_{L^2}	Order
0.216506	1/70	5.9623E-02	–
	1/140	3.0171E-02	0.9827
	1/280	1.4200E-02	1.0873
0.108253	1/70	6.2760E-02	–
	1/140	3.2162E-02	0.9645
	1/280	1.5221E-03	1.0793

TABLE 6. H^1 temporal discretization errors of scheme (4.3)–(4.5) with reference time step $\tau = \frac{1}{2000}$.

h	τ	e_{H^1}	Order
0.216506	1/70	6.9833E-01	–
	1/140	3.5162E-01	0.9899
	1/280	1.6507E-01	1.0909
0.108253	1/70	6.9649E-01	–
	1/140	3.5514E-01	0.9717
	1/280	1.6765E-01	1.0829

5.2. Example II. Lattice potential

We consider the system (3.1) with $\beta = 10$, the initial function ϕ_0 and potential function V are as follows:

$$\begin{aligned} \phi_0 &= cx(1-x)y(1-y)z(1-z), \\ V &= \frac{(x^2+y^2+z^2)}{2} + 20 + 20\sin(2\pi x)\sin(2\pi y)\sin(2\pi z), \end{aligned}$$

where $c > 0$ is a constant such that $\|\phi_0\|_{L^2(\Omega)} = 1$.

We present the temporal discretization errors and spatial discretization errors of the scheme (4.3)–(4.5) in Tables 5–8.

The temporal convergence orders of e_{L^2} and e_{H^1} are shown in Tables 5 and 6. The reference solution ϕ_{ref} is computed by the scheme (4.3)–(4.5) with the same spatial mesh as in the computation of ϕ_h^N and a smaller time step $\tau = \frac{1}{2000}$. Tables 7 and 8 show spatial convergence orders of e_{L^2} and e_{H^1} while the reference solution ϕ_{ref} is derived with the same temporal mesh in computing ϕ_h^N and a smaller spatial mesh $h = 0.017469$.

Similar to Example I, Tables 5–8 show that the convergence order of e_{L^2} is $O(\tau + h^2)$, which validates the conclusion in Theorem 4.12. The convergence order of e_{H^1} is $O(\tau + h)$, showing that the result in Corollary 4.14 is sub-optimal.

6. CONCLUSION

In this paper, we have carried out the mathematical analysis of the L^2 normalized gradient flow model for the GP eigenvalue problem and given a normalized implicit-explicit full-discrete scheme. We prove the well-posedness of the scheme and establish the optimal-order $L^\infty(0,T;L^2(\Omega))$ convergence of the approximations. Under a mild inverse CFL condition, we have proven the convergence rate is of order $O(\tau + h^2)$ in $L^\infty(0,T;L^2(\Omega))$-norm. With this convergence result, combining the H^2-stability, we have proved that the numerical scheme has a

TABLE 7. L^2 spatial discretization errors of scheme (4.3)–(4.5) with reference spatial mesh size $h = 0.017469$.

τ	h	e_{L^2}	Order
$\frac{1}{500}$	0.279508	6.0835E-02	–
	0.139754	1.4965E-02	2.0233
	0.069877	3.6470E-03	2.0368
$\frac{1}{1000}$	0.279508	5.9719E-02	–
	0.139754	1.4734E-02	2.0190
	0.069877	3.6120E-03	2.0283

TABLE 8. H^1 spatial discretization errors of scheme (4.3)–(4.5) with reference spatial mesh size $h = 0.017469$.

τ	h	e_{H^1}	Order
$\frac{1}{500}$	0.279508	1.6535	–
	0.139754	7.9726E-01	1.0524
	0.069877	3.8740E-01	1.0412
$\frac{1}{1000}$	0.279508	1.6381	–
	0.139754	7.9058E-01	1.0510
	0.069877	3.8341E-01	1.0440

sub-optimal convergence of the form $O(\sqrt{\tau}+h)$ in $L^\infty(0,T;H^1(\Omega))$-norm. Numerical experiments validate our theories and show that the theoretical convergence order in $L^\infty(0,T;H^1(\Omega))$-norm is not sharp. The analysis of the optimal-order convergence in $L^\infty(0,T;H^1(\Omega))$-norm will be left as future work.

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Appendix A. Properties of discrete operators

Lemma A.1 ([15])**.** *Let Ω be a bounded convex polygon. For the Ritz projection operator R_h and $u \in H^2(\Omega) \cap H_0^1(\Omega)$, there hold:*

$$\|\nabla(u - R_h u)\|_{L^2(\Omega)} \leq Ch\|D^2 u\|_{L^2(\Omega)}, \tag{A.1}$$

$$\|u - R_h u\|_{L^2(\Omega)} \leq Ch^2\|D^2 u\|_{L^2(\Omega)}. \tag{A.2}$$

Lemma A.2. *Let Ω be a bounded convex polygon. If $u \in H^2(\Omega) \cap H_0^1(\Omega)$, then*

$$\|R_h u\|_{L^\infty(\Omega)} \leq C\|u\|_{H^2(\Omega)}. \tag{A.3}$$

Proof. Denote $I_h u \in S_h$ the interpolation of u, we have

$$\begin{aligned}\|R_h u\|_{L^\infty(\Omega)} &\leq \|I_h u\|_{L^\infty(\Omega)} + \|I_h u - R_h u\|_{L^\infty(\Omega)}\\ &\leq \|u\|_{L^\infty(\Omega)} + Ch^{-\frac{3}{2}}\|I_h u - R_h u\|_{L^2(\Omega)} \quad \text{(inverse inequality)}\\ &\leq C\|u\|_{H^2(\Omega)} + Ch^{-\frac{3}{2}}\|I_h u - u\|_{L^2(\Omega)} + Ch^{-\frac{3}{2}}\|u - R_h u\|_{L^2(\Omega)}\\ &\leq C\|u\|_{H^2(\Omega)},\end{aligned}$$

where we have used the Sobolev embedding inequality and the approximation property of the interpolation operator [15] in the last line. □

Lemma A.3. *The discrete Laplacian operator satisfies*

$$\|\nabla u_h\|_{L^2(\Omega)} \leq \|u_h\|_{L^2(\Omega)}^{\frac{1}{2}}\|\Delta_h u_h\|_{L^2(\Omega)}^{\frac{1}{2}} \qquad \forall\, u_h \in S_h, \tag{A.4}$$

and

$$\|u_h\|_{L^\infty(\Omega)} \leq C\|u_h\|_{L^2(\Omega)}^{\frac{1}{4}}\|\Delta_h u_h\|_{L^2(\Omega)}^{\frac{3}{4}} \qquad \forall\, u_h \in S_h. \tag{A.5}$$

Proof. By the definition of Δ_h and Hölder's inequality, we obtain

$$\|\nabla u_h\|_{L^2(\Omega)}^2 = -(\Delta_h u_h, u_h)_{L^2(\Omega)} \leq \|u_h\|_{L^2(\Omega)}\|\Delta_h u_h\|_{L^2(\Omega)},$$

which completes the proof of (A.4).

To prove (A.5), let $u \in H^2(\Omega) \cap H_0^1(\Omega)$ such that

$$\Delta u = \Delta_h u_h.$$

Then we have $\|u\|_{H^2(\Omega)} \leq C\|\Delta_h u_h\|_{L^2(\Omega)}$. Next we show that $\|u\|_{L^2(\Omega)} \leq C\|u_h\|_{L^2(\Omega)}$.

Note that

$$\begin{aligned}\|u\|_{L^2(\Omega)} &\leq \|u_h\|_{L^2(\Omega)} + \|u - u_h\|_{L^2(\Omega)}\\ &\leq \|u_h\|_{L^2(\Omega)} + h^2\|u\|_{H^2(\Omega)} \qquad \text{(here (A.2) is used)}\\ &\leq \|u_h\|_{L^2(\Omega)} + Ch^2\|\Delta_h u_h\|_{L^2(\Omega)}\\ &\leq C\|u_h\|_{L^2(\Omega)},\end{aligned} \tag{A.6}$$

where the inverse inequality is applied to obtain the last line. Similarly, we can prove that

$$\|I_h u\|_{L^2(\Omega)} \leq C\|u_h\|_{L^2(\Omega)}. \tag{A.7}$$

Then by the triangle inequality, we get

$$\begin{aligned}\|u_h\|_{L^\infty(\Omega)} &\leq \|u\|_{L^\infty(\Omega)} + \|u - u_h\|_{L^\infty(\Omega)}\\ &\leq \|u\|_{L^\infty(\Omega)} + \|u - I_h u\|_{L^\infty(\Omega)} + \|I_h u - u_h\|_{L^\infty(\Omega)}\end{aligned}$$

$$\begin{aligned}&\le C\|u\|_{L^\infty(\Omega)} + \|I_h u - u_h\|_{L^\infty(\Omega)}\\&\le C\|u\|^{\frac{1}{4}}_{L^2(\Omega)}\|u\|^{\frac{3}{4}}_{H^2(\Omega)} + h^{-\frac{3}{2}}\|I_h u - u_h\|_{L^2(\Omega)},\end{aligned}$$

which together with Sobolev interpolation inequality, inverse inequality, equations (A.6) and (A.7) yields

$$\begin{aligned}\|u_h\|_{L^\infty(\Omega)} &\le C\|u_h\|^{\frac{1}{4}}_{L^2(\Omega)}\|\Delta_h u\|^{\frac{3}{4}}_{L^2(\Omega)} + h^{-\frac{3}{2}}\|I_h u - u_h\|^{\frac{1}{4}}_{L^2(\Omega)}\|I_h u - u_h\|^{\frac{3}{4}}_{L^2(\Omega)}\\&\le C\|u_h\|^{\frac{1}{4}}_{L^2(\Omega)}\|\Delta_h u\|^{\frac{3}{4}}_{L^2(\Omega)}\\&\quad + h^{-\frac{3}{2}}\|I_h u - u_h\|^{\frac{1}{4}}_{L^2(\Omega)}\big(\|I_h u - u\|_{L^2(\Omega)} + \|u - u_h\|_{L^2(\Omega)}\big)^{\frac{3}{4}}\\&\le C\|u_h\|^{\frac{1}{4}}_{L^2(\Omega)}\|\Delta_h u\|^{\frac{3}{4}}_{L^2(\Omega)} + h^{-\frac{3}{2}}\|u_h\|^{\frac{1}{4}}_{L^2(\Omega)}\big(h^2\|\Delta_h u_h\|_{L^2(\Omega)}\big)^{\frac{3}{4}}\\&\le C\|u_h\|^{\frac{1}{4}}_{L^2(\Omega)}\|\Delta_h u\|^{\frac{3}{4}}_{L^2(\Omega)}.\end{aligned}$$

This completes the proof of (A.5). □

APPENDIX B. DETAILED PROOFS

B.1. Proof of Lemma 4.5

Proof. A direct calculation shows that

$$\begin{aligned}\mu[u] - \mu[v] &= \int_\Omega \Big((|\nabla u|^2 - |\nabla v|^2) + V(u^2 - v^2) + \beta(u^4 - v^4)\Big)\mathrm{d}x\\&= \int_\Omega \Big((\nabla u + \nabla v)\cdot(\nabla u - \nabla v) + V(u+v)(u-v)\\&\quad + \beta(u^2+v^2)(u+v)(u-v)\Big)\mathrm{d}x.\end{aligned}$$

We then obtain from Hölder's inequality that

$$\begin{aligned}|\mu[u] - \mu[v]| &\le M\|u - v\|_{H^1(\Omega)} + \|V\|_{L^2(\Omega)}\|u+v\|_{L^4(\Omega)}\|u-v\|_{L^4(\Omega)}\\&\quad + \beta\|u^2+v^2\|_{L^3(\Omega)}\|u+v\|_{L^6(\Omega)}\|u-v\|_{L^2(\Omega)}\\&\le C_M\|u-v\|_{H^1(\Omega)},\end{aligned}$$

where the Sobolev embedding $H^1(\Omega) \hookrightarrow L^6(\Omega)$ has been used. □

B.2. Proof of Lemma 4.6

Proof. Denote

$$A := \int_\Omega \Big(|\nabla R_h u|^2 + V|R_h u|^2 + \beta|R_h u|^4\Big)\,\mathrm{d}x.$$

Then we obtain

$$\begin{aligned}|\mu[u] - A| &\le \left|\int_\Omega (|\nabla u|^2 - |\nabla R_h u|^2)\,\mathrm{d}x\right| + \|V\|_{L^2(\Omega)}\|u + R_h u\|_{L^\infty(\Omega)}\|u - R_h u\|_{L^2(\Omega)}\\&\quad + \beta\|u^2 + (R_h u)^2\|_{L^3(\Omega)}\|u + R_h u\|_{L^6(\Omega)}\|u - R_h u\|_{L^2(\Omega)}\\&=: I_1 + I_2 + I_3.\end{aligned}$$

Properties of the Ritz projection show that

$$I_2 \le C_1 h^2, \qquad I_3 \le C_2 h^2,$$

here constants C_1 and C_2 depend on $\|u\|_{H^2(\Omega)}$. For I_1, we get

$$\begin{aligned} I_1 &= \left|\int_\Omega (\nabla u + \nabla R_h u)\cdot(\nabla u - \nabla R_h u)\ \mathrm{d}x\right| = \left|\int_\Omega \nabla u\cdot(\nabla u - \nabla R_h u)\ \mathrm{d}x\right| \\ &= \left|\int_\Omega \Delta u(u - R_h u)\ \mathrm{d}x\right| \le C_3 h^2, \end{aligned}$$

with C_3 depends on $\|u\|_{H^2(\Omega)}$.

The last is the estimate of $\left|A - \mu[\widehat{R_h u}]\right|$,

$$\begin{aligned} \left|A - \mu[\widehat{R_h u}]\right| &\le \left|1 - \frac{1}{\|R_h u\|^2_{L^2(\Omega)}}\right|\left|\int_\Omega \left(|\nabla R_h u|^2 + V|R_h u|^2\right)\ \mathrm{d}x\right| \\ &\quad + \left|1 - \frac{1}{\|R_h u\|^4_{L^2(\Omega)}}\right|\left|\int_\Omega \beta|R_h u|^4\ \mathrm{d}x\right| \\ &\le C_4 h^2, \end{aligned}$$

here C_4 depends on $\|u\|_{H^2(\Omega)}$. Combining the above estimates, we complete the proof. □

B.3. Proof of Lemma 4.9

Proof. Denote

$$\alpha = \arccos\left((\widehat{R_h\phi(t_n)}, \phi_h^n)_{L^2(\Omega)}\right) \in [0,\pi]$$

be the angle between vectors $\widehat{R_h\phi(t_n)}$ and ϕ_h^n, then for $\alpha \in (\pi/6, \pi]$, we have $\|\tilde{e}_h^n\|_{L^2(\Omega)} \ge 1/2$, with the fact $\|e_h^n\|_{L^2(\Omega)} \le 2$, we can complete the proof of (4.17) and (4.18) for the case $\alpha \in (\pi/6, \pi]$.

For the case $\alpha \in [0, \pi/6]$, we have $\|\tilde{e}_h^n\|_{L^2(\Omega)} \ge \sin\alpha$, and

$$\|e_h^n\|_{L^2(\Omega)} = 2\sin(\alpha/2) \le \alpha \le C\sin\alpha \le C\|\tilde{e}_h^n\|_{L^2(\Omega)}.$$

Meanwhile,

$$\begin{aligned} \|e_h^n\|_{L^2(\Omega)} - \|\tilde{e}_h^n\|_{L^2(\Omega)} &\le \|e_h^n\|_{L^2(\Omega)} - \|e_h^n\|_{L^2(\Omega)}\cos(\alpha/2) \\ &= \|e_h^n\|_{L^2(\Omega)} 2\sin^2(\alpha/4) \le C\|\tilde{e}_h^n\|^3_{L^2(\Omega)}, \end{aligned}$$

which completes the proof. □