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Error estimate for structure-preserving finite difference schemes of the one-dimensional Cahn–Hilliard system coupled with viscoelasticity

By

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Abstract

In this article we give an observation for the solution to the Cahn-Hilliard system coupled with viscoelastic equation in one-space dimension, through the numerical analysis of the system. We shall introduce an example of structure-preserving finite difference scheme for the system and give a proof of the error estimate between the strict solution and solution for the finite difference scheme.

§ 1. Introduction

In [7], to study phase separation phenomenon arising in viscoelastic materials, the Cahn-Hilliard system coupled with viscoelasticity is considered. In the case of one spatial dimension, the system is written as follows:

$$(1.1)\qquad \partial_t^2 u = \partial_x \left\{ \frac{\partial W}{\partial \varepsilon}(\varepsilon, \chi) + \nu \partial_t \varepsilon \right\},$$

$$(1.2)\qquad \partial_t \chi = \partial_x^2 p,$$

$$(1.3)\qquad p = -\gamma \partial_x^2 \chi + \psi'(\chi) + \frac{\partial W}{\partial \chi}(\varepsilon, \chi), \qquad (t,x) \in (0,T] \times (0,L),$$

$$(1.4)\qquad u(t,x) = \partial_x \chi(t,x) = \partial_x p(t,x) = 0, \qquad (t,x) \in [0,T] \times \{0,L\},$$

$$(1.5)\qquad u(0,\cdot) = u_0, \quad \partial_t u(0,\cdot) = u_1, \quad \chi(0,\cdot) = \chi_0, \qquad x \in (0,L),$$

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where ν and γ are positive constants. The system describes a phase separation process in a binary deformable alloy quenched below a critical temperature. For the physical background we refer to [3], [4] and [5]. The unknowns u, ε, χ and p are the displacement, the linearized strain given as $\varepsilon = \partial_x u$, the order parameter (or phase ratio) and the chemical potential difference between the components, respectively. We regard that $\chi = -1$ and $\chi = 1$ correspond to the phase a and b of binary a-b alloy, respectively. The elastic energy $W(\varepsilon, \chi)$ is given as the following form;

$$W(\varepsilon, \chi) := \frac{1}{2}|\varepsilon - \overline{\varepsilon}(\chi)|^2, \tag{1.6}$$

where the function $\overline{\varepsilon}$ denotes the stress-free strain corresponding to the order parameter χ, defined by

$$\overline{\varepsilon}(\chi) = (1 - z(\chi))\overline{\varepsilon}_a + z(\chi)\overline{\varepsilon}_b \tag{1.7}$$

with constants $\overline{\varepsilon}_a$, $\overline{\varepsilon}_b$ which represent eigenstrains of phases a and b, and sufficient smooth given function z satisfying

$$z(\chi) = \begin{cases} 0 & \text{for } \chi \leq -1, \\ 1 & \text{for } \chi \geq 1. \end{cases}$$

In the same as the assumption in [7], we here suppose that the chemical energy takes the standard double-well form:

$$\psi(\chi) = \frac{1}{4}(1 - \chi^2)^2.$$

In order to give a simplified numerical scheme, let us transform the system (1.1)–(1.5) to the first order system by introducing the velocity $v = \partial_t u$ as a new unknown. Observe that

$$\frac{\partial W}{\partial \varepsilon}(\varepsilon, \chi) = \varepsilon - \overline{\varepsilon}(\chi), \qquad \frac{\partial W}{\partial \chi}(\varepsilon, \chi) = -\overline{\varepsilon}'(\chi) \cdot (\varepsilon - \overline{\varepsilon}(\chi)).$$

We thus rewrite the system (1.1)–(1.5) as follows:

$$
\begin{aligned}
&(1.8) && \partial_t \varepsilon = \partial_x v, && \\
&(1.9) && \partial_t v = \partial_x \varepsilon + \nu \partial_x^2 v - \partial_x \overline{\varepsilon}(\chi), && \\
&(1.10) && \partial_t \chi = \partial_x^2 p, && \\
&(1.11) && p = -\gamma \partial_x^2 \chi + \psi'(\chi) - \overline{\varepsilon}'(\chi) \cdot (\varepsilon - \overline{\varepsilon}(\chi)), && (t, x) \in (0, T] \times (0, L), \\
&(1.12) && v(t, x) = \partial_x \chi(t, x) = \partial_x p(t, x) = 0, && (t, x) \in [0, T] \times \{0, L\}, \\
&(1.13) && \varepsilon(0, \cdot) = \varepsilon_0, \quad v(0, \cdot) = v_0, \quad \chi(0, \cdot) = \chi_0, && x \in (0, L).
\end{aligned}
$$

We remark that it will be more complicated in vain in the case without this transformation although a similar analysis to this article work out (see e.g. [10]). Let us denote the momentum M and the total energy E by

$$M := \int_0^L \chi dx, \qquad E := \int_0^L \left(\frac{1}{2}|v|^2 + W(\varepsilon, \chi) + \frac{\gamma}{2}|\partial_x \chi|^2 + \psi(\chi) \right) dx. \tag{1.14}$$

It is easily seen that the smooth solution (ε, v, χ) of this system satisfies the total density conservation law and the energy decreasing law:

$$\frac{d}{dt}M = 0, \quad \frac{d}{dt}E + \nu \int_0^L |\partial_x v|^2 dx + \int_0^L |\partial_x p|^2 dx = 0. \tag{1.15}$$

In this article we give a simple example of structure-preserving finite difference scheme whose solution also satisfies the momentum conservation and the energy decreasing laws (1.15) in the discrete sense. We call numerical schemes which inherit the energy structure for the differential equations *structure-preserving numerical schemes*. There are a lot of aspects of the structure-preserving numerical scheme and derivation of it such as [1], [2] and [8]. Actually, we shall later use the discrete variational derivative method (DVDM) introduced in [1] to derive the numerical scheme. When we consider the numerical study for the nonlinear partial differential equations (PDEs), the structure-preserving property is often helpful. For example, the inherited structure plays the role as the a priori estimate as the same as PDEs. In addition, with the help of the structure, we can apply the energy method to the numerical scheme in a similar way to the method for PDEs. For more precise information about the energy method for the structure-preserving finite difference schemes, we refer to the second author's results [11] and [12]. According to these, as an application of the energy method, we can show not only the existence of solution for the scheme but also the error estimate between the strict solution for (1.8)-(1.13) and the approximate solution for the scheme. Our method can be applied to more complicated schemes including the case of the Cahn-Hilliard-elasticity system (without viscosity term), and can give the proof of the global existence result of the solution for these schemes. However, for the sake of brevity, we restrict ourselves to introduce the simple structure-preserving finite difference scheme for (1.8)–(1.13) and its error estimate here. We shall give the completed result including the result given here in forthcoming paper [9].

The rest of this article is organized as follows: in the next section we prepare the settings for the discrete notation and so on, and some lemmas. In the section 3 we introduce the structure-preserving finite difference scheme for (1.8)–(1.13) and prove the error estimate. In the last section we exhibit the numerical results.

§ 2. Setting and Preliminaries

Let us consider the problem in space-time domain $[0, L] \times [0, T] (\ni (x, t))$. We define $C^m(\Omega)$ as the function space of m-times continuous differentiable functions on $\Omega \subset \mathbb{R}$. We remark that the domain Ω will be used in various situations, for instance, in some place as a subset of $[0, L]$ or in other place as a bounded ball $\{\xi \mid |\xi| \leq R\}$, and so on. We denote partial differential operators with respect to space variable x and time variable t by ∂_x and ∂_t, and similarly we define the differential operators with respect to ξ, η, γ by ∂_ξ, ∂_η, ∂_γ respectively. In particular, in the case of single variable function we may also denote the derivatives such as F', F'' and F'''. Let K and N be any natural numbers. We split space interval $[0, L]$ into K-th parts and time interval $[0, T]$ into N-th parts with space and time mesh sizes Δx and Δt, and hence the following relations hold $L = K\Delta x$ and $T = N\Delta t$. In the finite difference method we pursue values at $(k\Delta x, n\Delta t)$ with $k = 0, 1, \ldots, K$ and $n = 0, 1, \ldots, N$. We use a notation such as $f_k^{(n)}$ as the value at $(k\Delta x, n\Delta t)$. We also use expression in bold print to denote vectors with respect to the space variable such as $\boldsymbol{f}^{(n)} := (f_k^{(n)})_{k=0}^K$ and especially in a single variable case $\boldsymbol{f} := (f_k)_{k=0}^K$. For the approximation to derivatives and integral, we follow the notation in [1], namely, the difference operators δ_n^+, δ_k^+, δ_k^-, $\delta_k^{\langle 1 \rangle}$ and $\delta_k^{\langle 2 \rangle}$ are defined by

$$\begin{aligned}
&\delta_n^+ f_k^{(n)} := \frac{f_k^{(n+1)} - f_k^{(n)}}{\Delta t}, \quad \delta_k^+ f_k^{(n)} := \frac{f_{k+1}^{(n)} - f_k^{(n)}}{\Delta x}, \quad \delta_k^- f_k^{(n)} := \frac{f_k^{(n)} - f_{k-1}^{(n)}}{\Delta x}, \\
&\delta_k^{\langle 1 \rangle} f_k^{(n)} := \frac{f_{k+1}^{(n)} - f_{k-1}^{(n)}}{2\Delta x}, \quad \delta_k^{\langle 2 \rangle} f_k^{(n)} := \frac{f_{k+1}^{(n)} - 2f_k^{(n)} + f_{k-1}^{(n)}}{\Delta x^2},
\end{aligned} \tag{2.1}$$

and we adopt the trapezoidal rule:

$$\sum_{k=0}^{K}{}'' f_k \Delta x := \sum_{k=0}^{K-1} \frac{f_k + f_{k+1}}{2} \Delta x, \tag{2.2}$$

as an approximation to integration with respect to space variable. We use a notation of product of vectors $\boldsymbol{fg}$ as the sense $\boldsymbol{fg} := (f_k g_k)_{k=0}^K$.

When we derive the structures such as an energy conservation law, the integration by parts formula plays an essential role. Correspondingly, we prepare its discrete version called the *summation by parts formula*.

Lemma 2.1 ([1, Propositions 3.2 and 3.3]). *It holds that*

$$\sum_{k=0}^{K}{}'' f_k^{(n)} \cdot \delta_k^{\langle 1\rangle} g_k^{(n)} \Delta x + \sum_{k=0}^{K}{}'' \delta_k^{\langle 1\rangle} f_k^{(n)} \cdot g_k^{(n)} \Delta x = \left[\frac{f_k^{(n)} \cdot s_k^{\langle 1\rangle} g_k^{(n)} + s_k^{\langle 1\rangle} f_k^{(n)} \cdot g_k^{(n)}}{2} \right]_{k=0}^{K}, \tag{2.3}$$

$$\sum_{k=0}^{K}{}'' f_k^{(n)} \cdot \delta_k^{\langle 2\rangle} g_k^{(n)} \Delta x + \sum_{k=0}^{K}{}'' \left(\frac{\delta_k^+ f_k^{(n)} \cdot \delta_k^+ g_k^{(n)} + \delta_k^- f_k^{(n)} \cdot \delta_k^- g_k^{(n)}}{2} \right) \Delta x = \left[\frac{\mu_k^+ f_k^{(n)} \cdot \delta_k^+ g_k^{(n)} + \mu_k^- f_k^{(n)} \cdot \delta_k^- g_k^{(n)}}{2} \right]_{k=0}^{K}, \tag{2.4}$$

where $s_k^{\langle 1\rangle} f_k^{(n)} := (f_{k+1}^{(n)} + f_{k-1}^{(n)})/2$ *and* $\mu_k^{\pm} f_k^{(n)} := (f_k^{(n)} + f_{k\pm 1}^{(n)})/2$.

Obviously, (2.3) and (2.4) correspond to

$$\int_0^L f(t,x) \cdot \partial_x g(t,x) dx + \int_0^L \partial_x f(t,x) \cdot g(t,x) dx = [f(t,x) \cdot g(t,x)]_{x=0}^{L},$$

$$\int_0^L f(t,x) \cdot \partial_x^2 g(t,x) dx + \int_0^L \partial_x f(t,x) \cdot \partial_x g(t,x) dx = [f(t,x) \cdot \partial_x g(t,x)]_{x=0}^{L},$$

respectively. The formula corresponding to the fundamental formula of calculus

$$\sum_{k=0}^{K}{}'' \delta_k^{\langle 2\rangle} g_k \Delta x = \left[\delta_k^{\langle 1\rangle} g_k \right]_{k=0}^{K} \tag{2.5}$$

also holds, which is easily seen by putting $f_k = 1$ $(k = -1, 0, 1, \ldots, K, K+1)$ in (2.4).

Let Ω be a domain in $\mathbb{R}$. For $F \in C^1(\Omega)$ and ξ, $\eta \in \Omega$ we define *difference quotient* of F at (ξ, η) by

$$\frac{\partial F}{\partial(\xi,\eta)} := \begin{cases} \frac{F(\xi)-F(\eta)}{\xi-\eta}, & \xi \neq \eta, \\ F'(\eta), & \xi = \eta. \end{cases}$$

It often appears naturally in structure-preserving numerical schemes (see e.g. [1]). For example, in the case that $F(\xi) = \frac{1}{p+1}\xi^{p+1}$ for $p \in \mathbb{N}$, its difference quotient is given as $\frac{\partial F}{\partial(\xi,\eta)} = \frac{1}{p+1}\sum_{j=0}^{p} \xi^j \eta^{p-j}$. Obviously, from the mean value theorem we have for any $\xi, \eta \in \Omega$

$$\inf_{\xi \in \Omega} F'(\xi) \leq \frac{\partial F}{\partial(\xi,\eta)} \leq \sup_{\xi \in \Omega} F'(\xi). \tag{2.6}$$

Subtraction between two difference quotients often appears in both proofs of existence of solution and error estimate. In order to treat these calculations simply and systematically, we define $\overline{F}''(\xi,\widetilde{\xi};\eta,\widetilde{\eta})$ for $F \in C^2$ by

$$\overline{F}''(\xi,\widetilde{\xi};\eta,\widetilde{\eta}) := \frac{\partial}{\partial(\xi,\widetilde{\xi})}\left(\frac{\partial F}{\partial(\cdot,\eta)} + \frac{\partial F}{\partial(\cdot,\widetilde{\eta})}\right)$$
$$= \begin{cases} \frac{1}{\xi-\widetilde{\xi}}\left\{\left(\frac{\partial F}{\partial(\xi,\eta)} + \frac{\partial F}{\partial(\xi,\widetilde{\eta})}\right) - \left(\frac{\partial F}{\partial(\widetilde{\xi},\eta)} + \frac{\partial F}{\partial(\widetilde{\xi},\widetilde{\eta})}\right)\right\}, & \xi \neq \widetilde{\xi}, \\ \partial_\xi\left(\frac{\partial F}{\partial(\xi,\eta)} + \frac{\partial F}{\partial(\xi,\widetilde{\eta})}\right)\Big|_{\xi=\widetilde{\xi}}, & \xi = \widetilde{\xi}, \end{cases}$$

which is a kind of 2nd order difference quotient. For example, $\overline{F}''$ in the case $F(\xi) = \frac{1}{p+1}\xi^{p+1}$ is

$$\overline{F}''(\xi,\widetilde{\xi};\eta,\widetilde{\eta}) = \frac{1}{p+1}\sum_{j=1}^{p}\left\{\left(\eta^{p-j} + \widetilde{\eta}^{p-j}\right)\sum_{k=0}^{j-1}\xi^k\widetilde{\xi}^{j-1-k}\right\}.$$

It satisfies the following properties.

Lemma 2.2 ([11]). *Let $F \in C^2(\Omega)$. For any ξ, $\widetilde{\xi}$, η, $\widetilde{\eta} \in \Omega$ it holds that*

$$\frac{\partial F}{\partial(\xi,\eta)} - \frac{\partial F}{\partial(\widetilde{\xi},\widetilde{\eta})} = \frac{1}{2}\overline{F}''(\xi,\widetilde{\xi};\eta,\widetilde{\eta})\cdot(\xi-\widetilde{\xi}) + \frac{1}{2}\overline{F}''(\eta,\widetilde{\eta};\xi,\widetilde{\xi})\cdot(\eta-\widetilde{\eta}).$$

Lemma 2.3 ([12]). *If $F \in C^2(\Omega)$, then $\overline{F}'' \in C(\Omega)$. Moreover, for any ξ, $\widetilde{\xi}$, η, $\widetilde{\eta} \in \Omega$ it holds that*

$$\inf_{\xi\in\Omega} F''(\xi) \le \overline{F}''(\xi,\widetilde{\xi};\eta,\widetilde{\eta}) \le \sup_{\xi\in\Omega} F''(\xi).$$

In the same fashion, *partial difference quotients* are defined by

$$\frac{\partial F(\cdot,\eta)}{\partial(\xi,\widetilde{\xi})} := \begin{cases} \frac{F(\xi,\eta)-F(\widetilde{\xi},\eta)}{\xi-\widetilde{\xi}}, & \xi \neq \widetilde{\xi}, \\ \partial_\xi F(\xi,\eta), & \xi = \widetilde{\xi}, \end{cases} \qquad \frac{\partial F(\xi,\cdot)}{\partial(\eta,\widetilde{\eta})} := \begin{cases} \frac{F(\xi,\eta)-F(\xi,\widetilde{\eta})}{\eta-\widetilde{\eta}}, & \eta \neq \widetilde{\eta}, \\ \partial_\eta F(\xi,\eta), & \eta = \widetilde{\eta}, \end{cases}$$

and analogous lemmas hold as above for the partial difference quotients from the same observation.

Let us define the discrete Lebesgue norm $\|\cdot\|_{L^p_d}$ and the discrete Dirichlet semi-norm $\|D\cdot\|$ by

$$\|\boldsymbol{f}\|_{L^p_d} := \begin{cases} \left(\sum_{k=0}^{K}{}''|f_k|^p\Delta x\right)^{\frac{1}{p}}, & p \in [1,\infty), \\ \max_{k=0,1,\dots,K}|f_k|, & p = \infty, \end{cases} \qquad \|D\boldsymbol{f}\| := \sqrt{\sum_{k=0}^{K-1}|\delta_k^+ f_k|^2\Delta x}.$$

It is easily checked that the discrete Hölder inequality $\|\boldsymbol{f}\boldsymbol{g}\|_{L^r_d} \le \|\boldsymbol{f}\|_{L^p_d}\|\boldsymbol{g}\|_{L^q_d}$ with $1/r = 1/p + 1/q$ holds. We remark that for any $\boldsymbol{f}$ satisfying boundary condition $\delta_k^{\langle 1\rangle} f_k|_{k=0,K} = 0$

$$\|D\boldsymbol{f}\|^2 = \sum_{k=0}^{K}{}''\frac{|\delta_k^+ f_k|^2 + |\delta_k^- f_k|^2}{2}\Delta x$$

holds.

§ 3. A Structure-Preserving Scheme and Error Estimate

From the standard observation with the help of DVDM in [1], we deduce the following numerical scheme:

$$\delta_n^+ \mathcal{E}_k^{(n)} = \delta_k^{\langle 1\rangle} \left(\frac{V_k^{(n+1)} + V_k^{(n)}}{2} \right), \tag{3.1}$$

$$\delta_n^+ V_k^{(n)} = \delta_k^{\langle 1\rangle} \left(\frac{\mathcal{E}_k^{(n+1)} + \mathcal{E}_k^{(n)}}{2} \right) + \nu \delta_k^{\langle 2\rangle} \left(\frac{V_k^{(n+1)} + V_k^{(n)}}{2} \right) - \delta_k^{\langle 1\rangle} \overline{\varepsilon}(\mathcal{X}_k^{(n)}), \tag{3.2}$$

$$\delta_n^+ \mathcal{X}_k^{(n)} = \delta_k^{\langle 2\rangle} P_k^{(n)}, \tag{3.3}$$

$$P_k^{(n)} = -\gamma \delta_k^{\langle 2\rangle} \left(\frac{\mathcal{X}_k^{(n+1)} + \mathcal{X}_k^{(n)}}{2} \right) + \frac{\partial \psi}{\partial(\mathcal{X}_k^{(n+1)}, \mathcal{X}_k^{(n)})} + \frac{\partial W(\mathcal{E}_k^{(n+1)}, \cdot)}{\partial(\mathcal{X}_k^{(n+1)}, \mathcal{X}_k^{(n)})} \tag{3.4}$$

$$(k = 0, 1, \ldots, K, \ n = 0, 1, \ldots, N-1),$$

$$V_k^{(n)}|_{k=0,K} = s_k^{\langle 1\rangle} V_k^{(n)}|_{k=0,K} = \delta_k^{\langle 1\rangle} \mathcal{X}_k^{(n)}|_{k=0,K} = \delta_k^{\langle 1\rangle} P_k^{(n)}|_{k=0,K} = 0 \tag{3.5}$$

$$(n = 0, 1, \ldots, N),$$

$$\mathcal{E}_k^{(0)} = \varepsilon_0(k\Delta x), \quad V_k^{(0)} = v_0(k\Delta x), \quad \mathcal{X}_k^{(0)} = \chi_0(k\Delta x) \quad (k = 0, 1, \ldots, K), \tag{3.6}$$

where $s_k^{\langle 1\rangle}$ is defined in Lemma 2.1. The boundary condition for $V_k^{(n)}$ in (3.5) may seem to be strange or over-determined. However, we use both assumptions to remove the boundary integral term of (2.3) as we will see in the proof of Theorem 3.1 later. From this the boundary condition for $\mathcal{E}_k^{(n)}$:

$$\delta_k^{\langle 1\rangle} \left(\frac{\mathcal{E}_k^{(n+1)} + \mathcal{E}_k^{(n)}}{2} \right) \Bigg|_{k=0,K} = 0$$

is also derived, due to (3.2) at $k = 0, K$ with the boundary condition (3.4).

The scheme inherits the structure of the system (1.8)–(1.13) in the following sense.

Theorem 3.1. *The solution for the scheme* (3.1)–(3.5) *satisfies*

$$\delta_n^+ M_d^{(n)} = 0, \tag{3.7}$$

$$\delta_n^+ E_d^{(n)} + \nu \sum_{k=0}^{K}{}'' \frac{\left|\delta_k^+ \left(\frac{V_k^{(n+1)}+V_k^{(n)}}{2}\right)\right|^2 + \left|\delta_k^- \left(\frac{V_k^{(n+1)}+V_k^{(n)}}{2}\right)\right|^2}{2} \Delta x + \sum_{k=0}^{K}{}'' \frac{|\delta_k^+ P_k^{(n)}|^2 + |\delta_k^- P_k^{(n)}|^2}{2} \Delta x = 0, \tag{3.8}$$

where the discrete momentum $M_d^{(n)}$ *and energy* $E_d^{(n)}$ *are defined by*

$$M_d^{(n)} := \sum_{k=0}^{K}{}'' \mathcal{X}_k^{(n)} \Delta x,$$
$$E_d^{(n)} := \sum_{k=0}^{K}{}'' \left(\frac{1}{2}|V_k^{(n)}|^2 + W(\mathcal{E}_k^{(n)}, \mathcal{X}_k^{(n)}) + \frac{\gamma}{2} \frac{|\delta_k^+ \mathcal{X}_k^{(n)}|^2 + |\delta_k^- \mathcal{X}_k^{(n)}|^2}{2} + \psi(\mathcal{X}_k^{(n)}) \right) \Delta x.$$

Proof. It follows from (2.5) and the boundary condition (3.5) that

$$\delta_n^+ M_d^{(n)} = \sum_{k=0}^{K}{}'' \delta_k^{\langle 2\rangle} P_k^{(n)} \Delta x = [\delta_k^{\langle 1\rangle} P_k^{(n)}]_{k=0}^{K} = 0,$$

which implies (3.7). Next, we show (3.8). It follows from (2.4) that

$$\begin{aligned}
&\delta_n^+ \left(\sum_{k=0}^{K}{}'' \frac{|\delta_k^+ \mathcal{X}_k^{(n)}|^2 + |\delta_k^- \mathcal{X}_k^{(n)}|^2}{2} \Delta x \right) \\
&= \sum_{k=0}^{K}{}'' \frac{\delta_n^+ \delta_k^+ \mathcal{X}_k^{(n)} \cdot \delta_k^+ (\mathcal{X}_k^{(n+1)} + \mathcal{X}_k^{(n)}) + \delta_n^+ \delta_k^- \mathcal{X}_k^{(n)} \cdot \delta_k^- (\mathcal{X}_k^{(n+1)} + \mathcal{X}_k^{(n)})}{2} \Delta x \\
&= \left[\frac{\mu_k^+ \delta_n^+ \mathcal{X}_k^{(n)} \cdot \delta_k^+ (\mathcal{X}_k^{(n+1)} + \mathcal{X}_k^{(n)}) + \mu_k^- \delta_n^+ \mathcal{X}_k^{(n)} \cdot \delta_k^- (\mathcal{X}_k^{(n+1)} + \mathcal{X}_k^{(n)})}{2} \right]_{k=0}^{K} \\
&\quad - \sum_{k=0}^{K}{}'' \delta_n^+ \mathcal{X}_k^{(n)} \cdot \delta_k^{\langle 2\rangle} (\mathcal{X}_k^{(n+1)} + \mathcal{X}_k^{(n)}) \Delta x.
\end{aligned}$$

Thanks to the boundary condition $\delta_k^{\langle 1\rangle} \mathcal{X}_k^{(n)}|_{k=0,K} = 0$, we see that $\delta_k^+ \mathcal{X}_k^{(n)}|_{k=0,K} = -\delta_k^- \mathcal{X}_k^{(n)}|_{k=0,K}$ and $\mu_k^+ \mathcal{X}_k^{(n)}|_{k=0,K} = \mu_k^- \mathcal{X}_k^{(n)}|_{k=0,K}$. Then from (2.4) we arrive at

$$\delta_n^+ \left(\sum_{k=0}^{K}{}'' \frac{|\delta_k^+ \mathcal{X}_k^{(n)}|^2 + |\delta_k^- \mathcal{X}_k^{(n)}|^2}{2} \Delta x \right) = -2 \sum_{k=0}^{K}{}'' \delta_n^+ \mathcal{X}_k^{(n)} \cdot \delta_k^{\langle 2\rangle} \left(\frac{\mathcal{X}_k^{(n+1)} + \mathcal{X}_k^{(n)}}{2} \right) \Delta x.$$

Observe that

$$\psi(\mathcal{X}_k^{(n+1)}) - \psi(\mathcal{X}_k^{(n)}) = \frac{\partial \psi}{\partial(\mathcal{X}_k^{(n+1)}, \mathcal{X}_k^{(n)})} \cdot (\mathcal{X}_k^{(n+1)} - \mathcal{X}_k^{(n)}),$$

$$\begin{aligned}
&W(\mathcal{E}_k^{(n+1)}, \mathcal{X}_k^{(n+1)}) - W(\mathcal{E}_k^{(n)}, \mathcal{X}_k^{(n)}) \\
&\quad = \frac{\partial W(\mathcal{E}_k^{(n+1)}, \cdot)}{\partial(\mathcal{X}_k^{(n+1)}, \mathcal{X}_k^{(n)})} \cdot (\mathcal{X}_k^{(n+1)} - \mathcal{X}_k^{(n)}) + \frac{\partial W(\cdot, \mathcal{X}_k^{(n)})}{\partial(\mathcal{E}_k^{(n+1)}, \mathcal{E}_k^{(n)})} \cdot (\mathcal{E}_k^{(n+1)} - \mathcal{E}_k^{(n)}),
\end{aligned}$$

due to the definition of the difference quotient. Since

$$\frac{\partial W(\cdot, \mathcal{X}_k^{(n)})}{\partial(\mathcal{E}_k^{(n+1)}, \mathcal{E}_k^{(n)})} = \frac{\mathcal{E}_k^{(n+1)} + \mathcal{E}_k^{(n)}}{2} - \overline{\varepsilon}(\mathcal{X}_k^{(n)}),$$

we have

$$\begin{aligned}\delta_n^+ E_d^{(n)} &= \sum_{k=0}^{K}{}'' \delta_n^+ V_k^{(n)} \cdot \frac{V_k^{(n+1)} + V_k^{(n)}}{2}\Delta x + \sum_{k=0}^{K}{}'' \delta_n^+ \mathcal{X}_k^{(n)} \cdot \frac{\partial W(\mathcal{E}_k^{(n+1)}, \cdot)}{\partial(\mathcal{X}_k^{(n+1)}, \mathcal{X}_k^{(n)})}\Delta x \\ &+ \sum_{k=0}^{K}{}'' \delta_n^+ \mathcal{E}_k^{(n)} \cdot \frac{\mathcal{E}_k^{(n+1)} + \mathcal{E}_k^{(n)}}{2}\Delta x - \sum_{k=0}^{K}{}'' \delta_n^+ \mathcal{E}_k^{(n)} \cdot \overline{\varepsilon}(\mathcal{X}_k^{(n)})\Delta x \\ &- \gamma \sum_{k=0}^{K}{}'' \delta_n^+ \mathcal{X}_k^{(n)} \cdot \delta_k^{\langle 2\rangle} \left(\frac{\mathcal{X}_k^{(n+1)} + \mathcal{X}_k^{(n)}}{2}\right)\Delta x + \sum_{k=0}^{K}{}'' \delta_n^+ \mathcal{X}_k^{(n)} \cdot \frac{\partial \psi}{\partial(\mathcal{X}_k^{(n+1)}, \mathcal{X}_k^{(n)})}\Delta x.\end{aligned}$$

Substituting (3.1)–(3.4) into this and using the summation by parts (2.3) and (2.4) yield

$$\begin{aligned}\delta_n^+ E_d^{(n)} &= \sum_{k=0}^{K}{}'' \delta_k^{\langle 1\rangle} \left(\frac{\mathcal{E}_k^{(n+1)} + \mathcal{E}_k^{(n)}}{2}\right) \cdot \frac{V_k^{(n+1)} + V_k^{(n)}}{2}\Delta x \\ &\quad + \nu \sum_{k=0}^{K}{}'' \delta_k^{\langle 2\rangle} \left(\frac{V_k^{(n+1)} + V_k^{(n)}}{2}\right) \cdot \frac{V_k^{(n+1)} + V_k^{(n)}}{2}\Delta x \\ &\quad - \sum_{k=0}^{K}{}'' \delta_k^{\langle 1\rangle} \overline{\varepsilon}(\mathcal{X}_k^{(n)}) \cdot \frac{V_k^{(n+1)} + V_k^{(n)}}{2}\Delta x \\ &\quad + \sum_{k=0}^{K}{}'' \delta_k^{\langle 2\rangle} P_k^{(n)} \cdot P_k^{(n)}\Delta x + \sum_{k=0}^{K}{}'' \delta_k^{\langle 1\rangle} \left(\frac{V_k^{(n+1)} + V_k^{(n)}}{2}\right) \cdot \frac{\mathcal{E}_k^{(n+1)} + \mathcal{E}_k^{(n)}}{2}\Delta x \\ &\quad - \sum_{k=0}^{K}{}'' \delta_k^{\langle 1\rangle} \left(\frac{V_k^{(n+1)} + V_k^{(n)}}{2}\right) \cdot \overline{\varepsilon}(\mathcal{X}_k^{(n)})\Delta x \\ &= \nu \sum_{k=0}^{K}{}'' \delta_k^{\langle 2\rangle} \left(\frac{V_k^{(n+1)} + V_k^{(n)}}{2}\right) \cdot \frac{V_k^{(n+1)} + V_k^{(n)}}{2}\Delta x + \sum_{k=0}^{K}{}'' \delta_k^{\langle 2\rangle} P_k^{(n)} \cdot P_k^{(n)}\Delta x \\ &= -\nu \sum_{k=0}^{K}{}'' \frac{\left|\delta_k^+ \left(\frac{V_k^{(n+1)} + V_k^{(n)}}{2}\right)\right|^2 + \left|\delta_k^- \left(\frac{V_k^{(n+1)} + V_k^{(n)}}{2}\right)\right|^2}{2}\Delta x \\ &\qquad - \sum_{k=0}^{K}{}'' \frac{|\delta_k^+ P_k^{(n)}|^2 + |\delta_k^- P_k^{(n)}|^2}{2}\Delta x,\end{aligned}$$

which completes the proof. □

From now on we show the error estimate. Let us denote the error $(\mathcal{E}_k^{(n)}, V_k^{(n)}, \mathcal{X}_k^{(n)}) - (\varepsilon, v, \chi)(n\Delta t, k\Delta x)$ by $(e_{\varepsilon,k}^{(n)}, e_{v,k}^{(n)}, e_{\chi,k}^{(n)})$, and the error vector

$$(\boldsymbol{e}_\varepsilon^{(n)}, \boldsymbol{e}_v^{(n)}, \boldsymbol{e}_\chi^{(n)}) := ((e_{\varepsilon,k}^{(n)}, e_{v,k}^{(n)}, e_{\chi,k}^{(n)}))_{k=0}^K$$

by $\boldsymbol{e}^{(n)}$ with the norm $\|\boldsymbol{e}^{(n)}\|_{(L_d^2)^3} := \|\boldsymbol{e}_\varepsilon^{(n)}\|_{L_d^2} + \|\boldsymbol{e}_v^{(n)}\|_{L_d^2} + \|\boldsymbol{e}_\chi^{(n)}\|_{L_d^2}$.

Theorem 3.2. *Let $T < \infty$ be fixed. Assume that the initial value $(\varepsilon_0, v_0, \chi_0)$ be sufficiently smooth. Let us denote by C_1 the bound for the solutions $\varepsilon_k^{(n)} := \varepsilon(k\Delta x, n\Delta t)$, $\chi_k^{(n)} := \chi(k\Delta x, n\Delta t)$, $\mathcal{E}_k^{(n)}$ and $\mathcal{X}_k^{(n)}$, that is,*

$$\|\boldsymbol{\varepsilon}^{(n)}\|_{L_d^\infty},\ \|\boldsymbol{\chi}^{(n)}\|_{L_d^\infty},\ \|\boldsymbol{\mathcal{E}}^{(n)}\|_{L_d^\infty}, \|\boldsymbol{\mathcal{X}}^{(n)}\|_{L_d^\infty} \le C_1.$$

Then there exists some constant R determined by C_1 such that if $\Delta t < R$ then

$$\max_{n=0,1,2,\dots,N} \|\boldsymbol{e}^{(n)}\|_{(L_d^2)^3} \le C \cdot (\Delta t + \Delta x^2),$$

where C depends on T and L.

Proof. Subtracting (3.1)–(3.4) from (1.8)–(1.11) at $(k\Delta x, (n+1)\Delta t)$ gives

$$\delta_n^+ e_{\varepsilon,k}^{(n)} = \delta_k^{\langle 1\rangle}\left(\frac{e_{v,k}^{(n+1)} + e_{v,k}^{(n)}}{2}\right) + \zeta_{1,k}^{(n)}, \tag{3.9}$$

$$\delta_n^+ e_{v,k}^{(n)} = \delta_k^{\langle 1\rangle}\left(\frac{e_{\varepsilon,k}^{(n+1)} + e_{\varepsilon,k}^{(n)}}{2}\right) + \nu\delta_k^{\langle 2\rangle}\left(\frac{e_{v,k}^{(n+1)} + e_{v,k}^{(n)}}{2}\right) - \delta_k^{\langle 1\rangle} N_{1,k}^{(n)} + \zeta_{2,k}^{(n)} \tag{3.10}$$

$$\delta_n^+ e_{\chi,k}^{(n)} = \delta_k^{\langle 2\rangle} e_{p,k}^{(n)} + \zeta_{3,k}^{(n)}, \tag{3.11}$$

$$e_{p,k}^{(n)} = -\gamma\delta_k^{\langle 2\rangle}\left(\frac{e_{\chi,k}^{(n+1)} + e_{\chi,k}^{(n)}}{2}\right) + N_{2,k}^{(n)} + N_{3,k}^{(n)} + \zeta_{4,k}^{(n)}, \tag{3.12}$$

where

$$N_{1,k}^{(n)} := \overline{\varepsilon}(\mathcal{X}_k^{(n)}) - \overline{\varepsilon}(\chi_k^{(n)}), \qquad N_{2,k}^{(n)} := \frac{\partial\psi}{\partial(\mathcal{X}_k^{(n+1)}, \mathcal{X}_k^{(n)})} - \frac{\partial\psi}{\partial(\chi_k^{(n+1)}, \chi_k^{(n)})},$$
$$N_{3,k}^{(n)} := \frac{\partial W(\mathcal{E}_k^{(n+1)}, \cdot)}{\partial(\mathcal{X}_k^{(n+1)}, \mathcal{X}_k^{(n)})} - \frac{\partial W(\varepsilon_k^{(n+1)}, \cdot)}{\partial(\chi_k^{(n+1)}, \chi_k^{(n)})}.$$

It is easily checked that the residue terms $\zeta_{i,k}^{(n)}$ $(i = 1, \dots, 4)$ are dependent on the solution (ε, v, χ) and estimated by $O(\Delta t + \Delta x^2)$ under sufficient smoothness condition for the solution. The existence of sufficiently smooth solution (ε, v, χ) under a smooth initial value is assured by the standard parabolic theory (see e.g. [6]).

Multiplying $\frac{e_{\chi,k}^{(n+1)} + e_{\chi,k}^{(n)}}{2}$ by (3.11) with (3.12) and taking summation following trapezoidal rule, we have

$$\begin{aligned}
&\frac{1}{2}\delta_n^+\|\boldsymbol{e}_\chi^{(n)}\|_{L_d^2}^2 + \gamma\left\|\delta_k^{\langle 2\rangle}\left(\frac{\boldsymbol{e}_\chi^{(n+1)}+\boldsymbol{e}_\chi^{(n)}}{2}\right)\right\|_{L_d^2}^2 \\
&\quad = \sum_{k=0}^{K}{}'' \frac{e_{\chi,k}^{(n+1)}+e_{\chi,k}^{(n)}}{2}\cdot\zeta_{3,k}^{(n)}\Delta x + \sum_{k=0}^{K}{}''\frac{e_{\chi,k}^{(n+1)}+e_{\chi,k}^{(n)}}{2}\cdot\delta_k^{\langle 2\rangle}\left(N_{2,k}^{(n)}-N_{3,k}^{(n)}+\zeta_{4,k}^{(n)}\right)\Delta x \\
&\quad \le \left\|\delta_k^{\langle 2\rangle}\left(\frac{\boldsymbol{e}_\chi^{(n+1)}+\boldsymbol{e}_\chi^{(n)}}{2}\right)\right\|_{L_d^2}(\|\boldsymbol{N}_2^{(n)}\|_{L_d^2}+\|\boldsymbol{N}_3^{(n)}\|_{L_d^2}) \\
&\qquad + \left\|\frac{\boldsymbol{e}_\chi^{(n+1)}+\boldsymbol{e}_\chi^{(n)}}{2}\right\|_{L_d^2}(\|\boldsymbol{\zeta}_3^{(n)}\|_{L_d^2}+\|\delta_k^{\langle 2\rangle}\boldsymbol{\zeta}_4^{(n)}\|_{L_d^2}).
\end{aligned}$$

From the Young inequality we have

$$\begin{aligned}
\frac{1}{2}\delta_n^+\|\boldsymbol{e}_\chi^{(n)}\|_{L_d^2}^2 &\le \frac{1}{4\gamma}(\|\boldsymbol{N}_2^{(n)}\|_{L_d^2}+\|\boldsymbol{N}_3^{(n)}\|_{L_d^2})^2 \\
&\qquad + C\left(\|\boldsymbol{e}_\chi^{(n+1)}\|_{L_d^2}+\|\boldsymbol{e}_\chi^{(n)}\|_{L_d^2}\right)\cdot(\Delta t+\Delta x^2).
\end{aligned}\tag{3.13}$$

In a similar way, calculating $\frac{e_{\varepsilon,k}^{(n+1)}+e_{\varepsilon,k}^{(n)}}{2}$ by (3.9) and $\frac{e_{v,k}^{(n+1)}+e_{v,k}^{(n)}}{2}$ by (3.10), and summing the resulting equations, we obtain

$$\begin{aligned}
&\frac{1}{2}\delta_n^+\left(\|\boldsymbol{e}_\varepsilon^{(n)}\|_{L_d^2}^2+\|\boldsymbol{e}_v^{(n)}\|_{L_d^2}^2\right)+\nu\left\|D\left(\frac{\boldsymbol{e}_v^{(n+1)}+\boldsymbol{e}_v^{(n)}}{2}\right)\right\|^2 \\
&\quad = \sum_{k=0}^{K}{}''\frac{e_{\varepsilon,k}^{(n+1)}+e_{\varepsilon,k}^{(n)}}{2}\cdot\zeta_{1,k}^{(n)}\Delta x+\sum_{k=0}^{K}{}''\frac{e_{v,k}^{(n+1)}+e_{v,k}^{(n)}}{2}\cdot\left(-\delta_k^{\langle 1\rangle}N_{1,k}^{(n)}+\zeta_{2,k}^{(n)}\right)\Delta x \\
&\quad \le \left\|\delta_k^{\langle 1\rangle}\left(\frac{\boldsymbol{e}_v^{(n+1)}+\boldsymbol{e}_v^{(n)}}{2}\right)\right\|_{L_d^2}\|\boldsymbol{N}_1^{(n)}\|_{L_d^2}+\left\|\frac{\boldsymbol{e}_\varepsilon^{(n+1)}+\boldsymbol{e}_\varepsilon^{(n)}}{2}\right\|_{L_d^2}\|\boldsymbol{\zeta}_1^{(n)}\|_{L_d^2} \\
&\qquad + \left\|\frac{\boldsymbol{e}_v^{(n+1)}+\boldsymbol{e}_v^{(n)}}{2}\right\|_{L_d^2}\|\boldsymbol{\zeta}_2^{(n)}\|_{L_d^2}.
\end{aligned}$$

Lemma 3.3. *For any* $\boldsymbol{f}=(f_k)_{k=-1}^{K+1}\in\mathbb{R}^{K+3}$ *with* $f_{-1}=f_1$ *and* $f_{K-1}=f_{K+1}$ *it holds that*

$$\|\delta_k^{\langle 1\rangle}\boldsymbol{f}\|_{L_d^2}\le\|D\boldsymbol{f}\|.$$

Proof. It follows from $2\delta_k^{\langle 1\rangle}f_k=\delta_k^+f_k+\delta_k^-f_k$ and $(a+b)^2\le 2(a^2+b^2)$ that

$$\|\delta_k^{\langle 1\rangle}\boldsymbol{f}\|_{L_d^2}^2=\frac{1}{4}\sum_{k=0}^{K}{}''|\delta_k^+f_k+\delta_k^-f_k|^2\Delta x\le\frac{1}{2}\sum_{k=0}^{K}{}''\left(|\delta_k^+f_k|^2+|\delta_k^-f_k|^2\right)\Delta x.$$

Observe that $\delta_k^+ f_K = -\delta_k^+ f_{K-1}$ and $\delta_k^- f_0 = -\delta_k^+ f_0$ from the boundary condition. Since $\delta_k^- f_k = \delta_k^+ f_{k-1}$ for $k = 1, 2, \ldots, K$ holds, we see that

$$\begin{aligned}
&\sum_{k=0}^{K}{}'' \left(|\delta_k^+ f_k|^2 + |\delta_k^- f_k|^2\right) \Delta x \\
&= \frac{1}{2}\left(|\delta_k^+ f_0|^2 + |\delta_k^- f_0|^2\right) \Delta x + \sum_{k=1}^{K-1} \left(|\delta_k^+ f_k|^2 + |\delta_k^- f_k|^2\right) \Delta x + \frac{1}{2}\left(|\delta_k^+ f_K|^2 + |\delta_k^- f_K|^2\right) \Delta x \\
&= |\delta_k^+ f_0|^2 \Delta x + \left(|\delta_k^+ f_0|^2 \Delta x + 2\sum_{k=1}^{K-2} |\delta_k^+ f_k|^2 \Delta x + |\delta_k^+ f_{K-1}|^2 \Delta x\right) + |\delta_k^+ f_{K-1}|^2 \Delta x \\
&= \sum_{k=0}^{K-1} |\delta_k^+ f_k|^2 \Delta x = \|D\boldsymbol{f}\|^2,
\end{aligned}$$

which completes the proof. $\square$

From the Young inequality with this lemma, we obtain

$$\begin{aligned}
\frac{1}{2}\delta_n^+ \left(\|\boldsymbol{e}_\varepsilon^{(n)}\|_{L_d^2}^2 + \|\boldsymbol{e}_v^{(n)}\|_{L_d^2}^2\right) &\le \frac{1}{4\nu}\|\boldsymbol{N}_1^{(n)}\|_{L_d^2}^2 \\
&+ C\left(\|\boldsymbol{e}_\varepsilon^{(n+1)}\|_{L_d^2} + \|\boldsymbol{e}_\varepsilon^{(n)}\|_{L_d^2} + \|\boldsymbol{e}_v^{(n+1)}\|_{L_d^2} + \|\boldsymbol{e}_v^{(n)}\|_{L_d^2}\right) \cdot (\Delta t + \Delta x^2).
\end{aligned} \tag{3.14}$$

From now on, we shall estimate the nonlinear terms $\|\boldsymbol{N}_i^{(n)}\|_{L_d^2}$ $(i = 1, 2, 3)$. From the definition of the difference quotient and its property (2.6), we have

$$\|\boldsymbol{N}_1^{(n)}\|_{L_d^2} \le \left\|\frac{\partial\overline{\varepsilon}}{\partial(\boldsymbol{\mathcal{X}}^{(n)}, \boldsymbol{\chi}^{(n)})}\right\|_{L_d^\infty} \|\boldsymbol{e}_\chi^{(n)}\|_{L_d^2} \le \max_{|r|\le C_1} |\overline{\varepsilon}'(r)| \|\boldsymbol{e}_\chi^{(n)}\|_{L_d^2}.$$

It follows from Lemmas 2.2 and 2.3 that

$$\|\boldsymbol{N}_2^{(n)}\|_{L_d^2} \le \max_{|r|\le C_1} |\psi''(r)| \left(\|\boldsymbol{e}_\chi^{(n+1)}\|_{L_d^2} + \|\boldsymbol{e}_\chi^{(n)}\|_{L_d^2}\right).$$

Similarly, we also obtain

$$\begin{aligned}
\|\boldsymbol{N}_3^{(n)}\|_{L_d^2} &\le \left\|\frac{\partial W(\boldsymbol{\mathcal{E}}^{(n+1)}, \cdot)}{\partial(\boldsymbol{\mathcal{X}}^{(n+1)}, \boldsymbol{\mathcal{X}}^{(n)})} - \frac{\partial W(\boldsymbol{\mathcal{E}}^{(n+1)}, \cdot)}{\partial(\boldsymbol{\chi}^{(n+1)}, \boldsymbol{\chi}^{(n)})}\right\|_{L_d^2} \\
&\qquad + \left\|\frac{\partial W(\boldsymbol{\mathcal{E}}^{(n+1)}, \cdot)}{\partial(\boldsymbol{\chi}^{(n+1)}, \boldsymbol{\chi}^{(n)})} - \frac{\partial W(\boldsymbol{\varepsilon}^{(n+1)}, \cdot)}{\partial(\boldsymbol{\chi}^{(n+1)}, \boldsymbol{\chi}^{(n)})}\right\|_{L_d^2} \\
&\le \max_{|r_1|,|r_2|\le C_1} |\partial_\chi^2 W(r_1, r_2)|(\|\boldsymbol{e}_\chi^{(n+1)}\|_{L_d^2} + \|\boldsymbol{e}_\chi^{(n)}\|_{L_d^2}) \\
&\qquad + \max_{|r_1|,|r_2|\le C_1} |\partial_\chi\partial_\varepsilon W(r_1, r_2)| \|\boldsymbol{e}_\varepsilon^{(n+1)}\|_{L_d^2}.
\end{aligned}$$

Remark that $\max_{|r_1|,|r_2|\leq C_1}|\partial_\chi\partial_\varepsilon W(r_1,r_2)|=\max_{|r|\leq C_1}|\overline{\varepsilon}'(r)|$ holds from the definition of W. Combining (3.13) with (3.14) yields

$$
\begin{aligned}
&\frac{1}{2}\delta_n^+\|\boldsymbol{e}^{(n)}\|^2_{(L^2_d)^3}\\
&\leq \frac{1}{4\nu}\|\boldsymbol{N}_1^{(n)}\|^2_{L^2_d}+\frac{1}{4\gamma}(\|\boldsymbol{N}_2^{(n)}\|_{L^2_d}+\|\boldsymbol{N}_3^{(n)}\|_{L^2_d})^2\\
&\quad +C\left(\|\boldsymbol{e}^{(n+1)}\|_{(L^2_d)^3}+\|\boldsymbol{e}^{(n)}\|_{(L^2_d)^3}\right)\cdot(\Delta t+\Delta x^2)\\
&\leq \frac{\max_{|r|\leq C_1}|\overline{\varepsilon}'(r)|^2}{4\nu}\|\boldsymbol{e}_\chi^{(n)}\|^2_{L^2_d}+\frac{1}{4\gamma}\Bigg(\max_{|r|\leq C_1}|\psi''(r)|\left(\|\boldsymbol{e}_\chi^{(n+1)}\|_{L^2_d}+\|\boldsymbol{e}_\chi^{(n)}\|_{L^2_d}\right)\\
&\quad +\max_{|r_1|,|r_2|\leq C_1}|\partial_\chi^2 W(r_1,r_2)|(\|\boldsymbol{e}_\chi^{(n+1)}\|_{L^2_d}+\|\boldsymbol{e}_\chi^{(n)}\|_{L^2_d})+\max_{|r|\leq C_1}|\overline{\varepsilon}'(r)|\|\boldsymbol{e}_\varepsilon^{(n+1)}\|_{L^2_d}\Bigg)^2\\
&\quad +C\left(\|\boldsymbol{e}^{(n+1)}\|_{(L^2_d)^3}+\|\boldsymbol{e}^{(n)}\|_{(L^2_d)^3}\right)\cdot(\Delta t+\Delta x^2)\\
&\leq \Bigg[\left\{\frac{1}{2\sqrt{\nu}}\max_{|r|\leq C_1}|\overline{\varepsilon}'(r)|+\frac{1}{2\sqrt{\gamma}}\left(\max_{|r|\leq C_1}|\psi''(r)|+\max_{|r_1|,|r_2|\leq C_1}|\partial_\chi^2 W(r_1,r_2)|\right)\right\}\|\boldsymbol{e}^{(n)}\|_{(L^2_d)^3}\\
&\quad +\frac{1}{2\sqrt{\gamma}}\max\left\{\max_{|r|\leq C_1}|\psi''(r)|+\max_{|r_1|,|r_2|\leq C_1}|\partial_\chi^2 W(r_1,r_2)|,\ \max_{|r|\leq C_1}|\overline{\varepsilon}'(r)|\right\}\|\boldsymbol{e}^{(n+1)}\|_{(L^2_d)^3}\Bigg]^2\\
&\quad +C\left(\|\boldsymbol{e}^{(n+1)}\|_{(L^2_d)^3}+\|\boldsymbol{e}^{(n)}\|_{(L^2_d)^3}\right)\cdot(\Delta t+\Delta x^2)\\
&\leq A(\|\boldsymbol{e}^{(n+1)}\|^2_{(L^2_d)^3}+\|\boldsymbol{e}^{(n)}\|^2_{(L^2_d)^3})+C\left(\|\boldsymbol{e}^{(n+1)}\|_{(L^2_d)^3}+\|\boldsymbol{e}^{(n)}\|_{(L^2_d)^3}\right)\cdot(\Delta t+\Delta x^2)\\
&\leq (A+\epsilon)\cdot(\|\boldsymbol{e}^{(n+1)}\|^2_{(L^2_d)^3}+\|\boldsymbol{e}^{(n)}\|^2_{(L^2_d)^3})+C(\epsilon)\cdot(\Delta t^2+\Delta x^4).
\end{aligned}
$$

From the standard procedure in [12] (that is, by using the discrete Gronwall inequality), we arrive at the desired result. Remark that R in the assumption in this theorem is fixed value satisfying $R<1/2A$, and ϵ is chosen satisfying $R<1/2(A+\epsilon)<1/2A$. We have thus completed the proof. □

§ 4. Numerical Simulation

In this section, by using the scheme (3.1)–(3.6), we practically simulate dynamics of solutions for the Cahn-Hilliard system coupled with viscoelasticity (1.8)–(1.13) through a numerical computation. Through the simulation we expect to observe the phase separation in viscoelastic materials. We shall here give two results of numerical experiments. In the first numerical result (Case 1), we can observe that a pattern of the phase separation actually arises in not only order parameter χ but also shear strain ε, although it is well-known that the solution ε for the linear single viscoelastic equation tends to 0. Moreover, in the second numerical result (Case 2), we give the example of generation of a pattern for identically zero initial value of $\varepsilon_0=0$ but small perturbed initial value of χ_0.

Let us introduce settings of the numerical simulations. We set the given function $z = z(\chi)$ in the definition of $\bar{\varepsilon}$ as follows:

$$z(\chi) = \begin{cases} 0, & \chi \le -1, \\ \frac{1}{2}\left(\sin\frac{\pi x}{2} + 1\right), & -1 < \chi < 1, \\ 1, & \chi \ge 1, \end{cases}$$

with $\bar{\varepsilon}_a = 1$ and $\bar{\varepsilon}_b = 2$. We set parameters as follows: $\gamma = 0.001$, $\nu = 0.1$, $L = 1$, $T = 0.3$, $K = 20$ and $N = 10000$. We thus see that $\Delta x = 1/20$, $\Delta t = 3/100000$. In all the numerical computations here we have simulated by using Sci lab. In order to obtain next time-step of solutions using our nonlinear scheme, we use the function "`fsolve`" in Scilab.

As mentioned above, we give two kinds of numerical experiment for two initial values. The first result is the experiments under the following initial value:

$$\text{(Case 1)} \begin{cases} \varepsilon_0 = -0.4\cos\pi x + 0.2\cos 2\pi x - 0.01\cos 5\pi x, \qquad v_0 = 0, \\ \chi_0 = 0.16\cos\pi x + 0.11\cos 2\pi x + 0.05\cos 3\pi x. \end{cases}$$

In the case 1, we observe that a pattern appears in not only χ but also ε, which means the phase separation phenomena in alloy (see Figure 1).

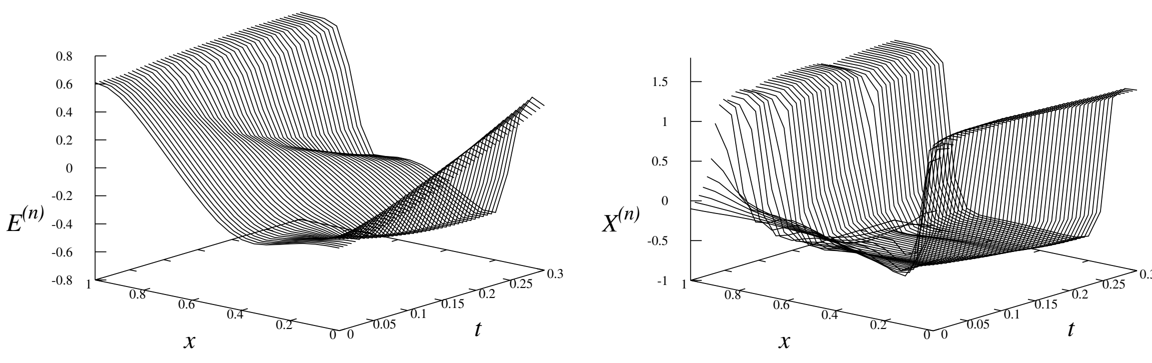

Figure 1. Numerical solution $(\boldsymbol{\mathcal{E}}^{(n)}, \boldsymbol{\mathcal{X}}^{(n)})$ in Case 1

Next, we give another result of the numerical simulation.

$$\text{(Case 2)} \begin{cases} \varepsilon_0 = 0, \qquad v_0 = 0, \\ \chi_0 = 0.1\xi \qquad (\xi \text{ is a uniform random variable in } [0,1]). \end{cases}$$

Figure 2 is the profiles of the numerical solutions in Case 2. This implies that the pattern appears even if the initial values ε_0 and v_0 are identically zero but χ_0 has some small perturbation. To replicate the experiment we give the concrete value of ξ: $\xi = (\xi_k)_{k=0}^{20}$ is given as

$$\begin{aligned}\xi = (&0.021132, 0.075604, 0.000022, 0.033033, 0.066538, 0.062839, 0.084975,\\ &0.068573, 0.087822, 0.006837, 0.056085, 0.066236, 0.072635, 0.019851,\\ &0.054426, 0.023207, 0.023122, 0.021646, 0.088339, 0.065251, 0.030761)\end{aligned}$$

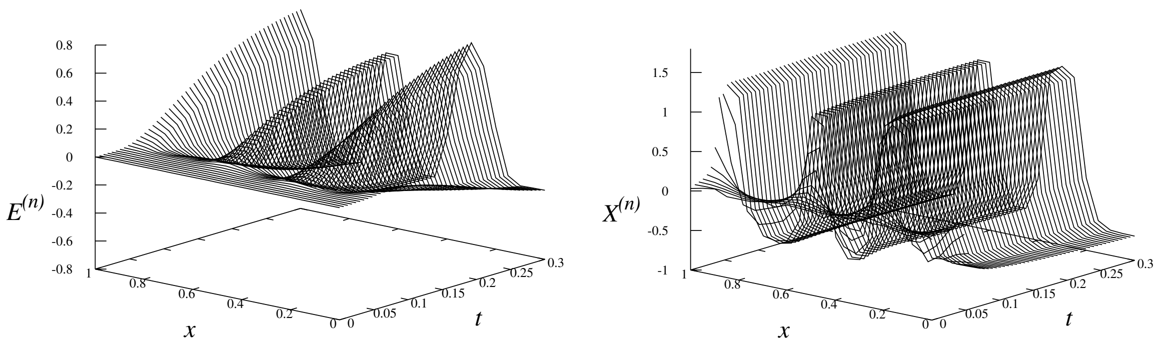

Figure 2. Numerical solution $(\boldsymbol{\mathcal{E}}^{(n)}, \boldsymbol{\mathcal{X}}^{(n)})$ in Case 2

By the conservation law (3.7), we have $M_d^{(n)} = M_d^{(0)}$ for any $n = 0, 1, 2, \ldots$. From the energy decreasing law (3.8) we see that $E_d^{(n)} \le E_d^{(0)}$ for any $n = 0, 1, 2, \ldots$. Moreover, by summing (3.8) with respect to $\ell = 0, 1, 2, \ldots, n-1$ and defining the total energy $T_d^{(n)}$ by

$$\begin{aligned} T_d^{(n)} :=& E_d^{(n)} + \nu \sum_{\ell=0}^{n-1} \sum_{k=0}^{K}{}'' \frac{\left|\delta_k^+ \left(\frac{V_k^{(\ell+1)}+V_k^{(\ell)}}{2}\right)\right|^2 + \left|\delta_k^- \left(\frac{V_k^{(\ell+1)}+V_k^{(\ell)}}{2}\right)\right|^2}{2} \Delta x \Delta t \\ &+ \sum_{\ell=0}^{n-1} \sum_{k=0}^{K}{}'' \frac{|\delta_k^+ P_k^{(\ell)}|^2 + |\delta_k^- P_k^{(\ell)}|^2}{2} \Delta x \Delta t, \end{aligned}$$

we also obtain the total energy conservation law: $T_d^{(n)} = E_d^{(0)}$ for any $n = 0, 1, 2, \ldots$. The fluctuations of $T_d^{(n)}$ and $M_d^{(n)}$ are shown in Figures 3 and 4. From this we can confirm that $T_d^{(n)}$ and $M_d^{(n)}$ are conserved well. For more details and other simulations we will give in forthcoming paper [9].

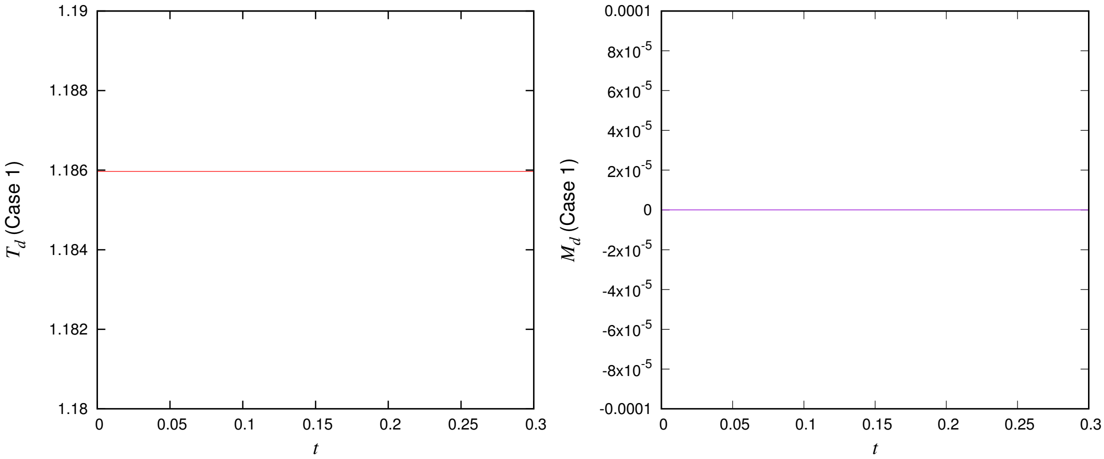

Figure 3. $T_d^{(n)}$ and $M_d^{(n)}$ in Case 1

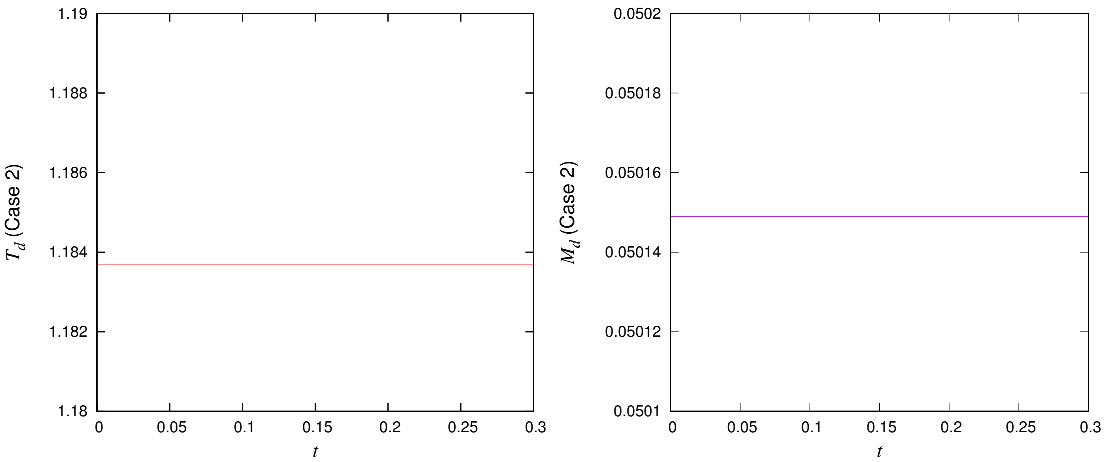

Figure 4. $T_d^{(n)}$ and $M_d^{(n)}$ in Case 2

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