

ENTROPY-STABLE AND ENTROPY-DISSIPATIVE APPROXIMATIONS OF A FOURTH-ORDER QUANTUM DIFFUSION EQUATION

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ABSTRACT. Structure-preserving numerical schemes for a nonlinear parabolic fourth-order equation, modeling the electron transport in quantum semiconductors, with periodic boundary conditions are analyzed. First, a two-step backward differentiation formula (BDF) semi-discretization in time is investigated. The scheme preserves the nonnegativity of the solution, is entropy stable and dissipates a modified entropy functional. The existence of a weak semi-discrete solution and, in a particular case, its temporal second-order convergence to the continuous solution is proved. The proofs employ an algebraic relation which implies the G-stability of the two-step BDF. Second, an implicit Euler and q -step BDF discrete variational derivative method are considered. This scheme, which exploits the variational structure of the equation, dissipates the discrete Fisher information (or energy). Numerical experiments show that the discrete (relative) entropies and Fisher information decay even exponentially fast to zero.

1. INTRODUCTION

This paper is devoted to the study of novel structure-preserving temporal higher-order numerical schemes for the fourth-order quantum diffusion equation

$$(1) \quad n_t + \operatorname{div} \left(n \nabla \left(\frac{\Delta \sqrt{n}}{\sqrt{n}} \right) \right) = 0, \quad x \in \mathbb{T}^d, \quad t > 0, \quad n(0) = n_0,$$

where \mathbb{T}^d is the d -dimensional torus. This equation is the zero-temperature and zero-field limit of the quantum drift-diffusion model, which describes the evolution of the electron density $n(t) = n(t, \cdot)$ in a quantum semiconductor device; see [21]. It was derived in [7] from a relaxation-time Wigner equation using a Chapman-Enskog expansion around the quantum equilibrium. For smooth positive solutions, (1) can be written in a symmetric form for the variable $\log n$:

$$(2) \quad n_t + \frac{1}{2} \partial_{ij}^2 (n \partial_{ij}^2 \log n) = 0, \quad x \in \mathbb{T}^d, \quad t > 0, \quad n(0) = n_0,$$

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where here and in the following, we employ the summation convention over repeated indices and the notation $\partial_i = \partial/\partial x_i$, $\partial_{ij}^2 = \partial^2/\partial x_i \partial x_j$. This is the multidimensional form of the so-called Derrida-Lebowitz-Speer-Spohn (DLSS) equation. Its one-dimensional version was derived in [8] in a suitable scaling limit from the time-discrete Toom model and the variable n is related to a limit random variable.

The main difficulties in the analysis of (1) (or (2)) are the highly nonlinear structure, originating from the quantum potential term $\Delta\sqrt{n}/\sqrt{n}$ in (1), and the fourth-order differential operator, which lacks a maximum principle.

These difficulties have been overcome by exploiting the rich mathematical structure of (2). First, equation (2) preserves the nonnegativity of the solutions [22]: Starting from a nonnegative initial datum, the weak solution stays nonnegative for all time. Second, (2) allows for a class of Lyapunov functionals and so-called entropy dissipation estimates. More precisely, the functionals

$$E_\alpha[n] = \frac{1}{\alpha(\alpha-1)} \int_{\mathbb{T}^d} n^\alpha dx \quad (\alpha \neq 0, 1), \quad E_1[n] = \int_{\mathbb{T}^d} (n(\log n - 1) + 1) dx$$

are Lyapunov functionals along solutions to (2), i.e. $dE_\alpha[n]/dt \leq 0$ if $(\sqrt{d}-1)^2/(d+2) \leq \alpha \leq (\sqrt{d}+1)^2/(d+2)$, and the entropy dissipation inequality

$$(3) \quad \frac{d}{dt} E_\alpha[n] + 2\kappa_\alpha \int_{\mathbb{T}^d} (\Delta n^{\alpha/2})^2 dx \leq 0$$

holds if $(\sqrt{d}-1)^2/(d+2) < \alpha < (\sqrt{d}+1)^2/(d+2)$. The constant $\kappa_\alpha > 0$ can be computed explicitly, see Lemma 6 below. For $\alpha = 1$, inequality (3) can be interpreted as the dissipation of the physical entropy. Third, equation (1) is the gradient flow of the Fisher information

$$(4) \quad F[n] = \int_{\mathbb{T}^d} |\nabla \sqrt{n}|^2 dx$$

with respect to the Wasserstein metric [14]. As the variational derivative of the Fisher information equals $\delta F[n]/\delta n = -\Delta\sqrt{n}/\sqrt{n}$, a straightforward computation shows that the Fisher information is dissipated along solutions to (1),

$$(5) \quad \frac{d}{dt} F[n] + \int_{\mathbb{T}^d} n \left| \nabla \left(\frac{\delta F[n]}{\delta n} \right) \right|^2 dx = 0.$$

Since the Fisher information can be interpreted as the quantum energy, the latter can be seen as an energy dissipation identity.

Whereas the local-in-time existence of positive classical solutions for strictly positive $W^{1,p}(\mathbb{T}^d)$ initial data with $p > d$ could be proved using semigroup theory [2], global-in-time existence results were based on estimates (3) and (5). More precisely, the global existence of a nonnegative weak solution was achieved in [24] in the one-dimensional case. This result was extended later to several space dimensions in [22], employing entropy dissipation inequalities, and in [14], exploring the variational structure of the equation.

From a numerical viewpoint, it is desirable to design numerical approximations which preserve the above structural properties like positivity preservation, entropy stability, and

entropy or energy dissipation on a discrete level. For a constant time step size $\tau > 0$, let $t_k = k\tau$ ($k \geq 0$). If n_k approximates the solution $n(t_k)$ to (2) at time t_k , we call a numerical scheme *entropy dissipating* if $E_\alpha[n_{k+1}] \leq E_\alpha[n_k]$ for all $k \geq 0$ with α in a certain parameter range, and *entropy stable* if there exists a constant $C > 0$ such that $E_\alpha[n_k] \leq C$ for all $k \geq 0$. In this paper, we investigate the entropy stability and entropy dissipation of backward differentiation formulas (BDF).

In the literature, most of the numerical schemes proposed for (2) are based on an implicit Euler discretization in one space dimension. In [25], the convergence of a positivity-preserving semi-discrete Euler scheme was shown. A fully discrete finite-difference scheme which preserves the positivity, mass, and physical entropy was derived in [4]. Düring et al. [9] employed the variational structure of (2) on a fully discrete level and introduced a discrete minimizing movement scheme. This approach implies the decay of the discrete Fisher information and the nonnegativity of the discrete solutions. Finally, a positivity-preserving finite-volume scheme in several space dimensions for a stationary quantum drift-diffusion model was suggested in [5].

Positivity preserving and entropy consistent numerical schemes have been investigated in the literature also for other nonlinear fourth- and second-order equations. For instance, a positivity preserving finite difference approximation of the thin-film equation was proposed by Zhornitskaya and Bertozzi [31]. Finite element techniques for the same equation were employed by Barrett, Blowley, and Garcke [1], imposing the nonnegativity property as a constraint such that at each time level a variational inequality has to be solved. Furthermore, entropy consistent finite volume–finite element schemes were suggested and analyzed by Grün and Rumpf [17, 18]. Furihata and Matsuo [13] developed the discrete variational derivative method to derive conservative or dissipative schemes for a variety of evolution equations possessing a variational structure. Entropy dissipative fully discrete schemes for electro-reaction-diffusion systems were derived by Glitzky and Gärtner [16].

In most of these works, the time discretization is restricted to the implicit Euler method, motivated by the fact that the solutions often lack regularity. However, high-order schemes often still yield smaller time errors than the Euler scheme, and this improved accuracy is vital to match the spatial approximation errors. A difficulty of the analysis is that the time discretization has to be compatible with the entropy structure of the equation. This is the case for the first-order implicit Euler discretization. Indeed, multiplying the semi-discrete scheme

$$(6) \quad \frac{1}{\tau}(n_{k+1} - n_k) + \frac{1}{2}\partial_{ij}^2(n_{k+1}\partial_{ij}^2 \log n_{k+1}) = 0, \quad k \geq 0,$$

where $\tau > 0$ is the time step and n_k approximates $n(t_k)$ with $t_k = \tau k$, by $\log n_{k+1}$ and using the elementary inequality

$$(7) \quad (x - y) \log x \geq x \log x - y \log y \quad \text{for } x, y > 0$$

(which follows from the convexity of $x \mapsto x \log x$), it was shown in [22, Lemma 4.1] that

$$E_\alpha[n_{k+1}] + 2\tau\kappa_\alpha \int_{\mathbb{T}^d} (\Delta n_{k+1}^{\alpha/2})^2 dx \leq E_\alpha[n_k], \quad k \geq 0.$$

As a consequence, $k \mapsto E_\alpha[n_k]$ is nonincreasing and the entropy dissipation structure is preserved. It is less clear whether higher-order approximations yield entropy dissipating numerical schemes. In this paper, we prove this property for the two-step BDF method.

Two-step BDF (or BDF2) methods have been employed in the literature to approximate various evolution equations in different contexts. We just mention numerical schemes for incompressible Navier-Stokes problems [10, 15, 19], semilinear and quasilinear parabolic equations [11, 28], and nonlinear evolution problems governed by monotone operators [12, 20]. To our knowledge, temporal higher-order schemes for the quantum diffusion equation (1) have been not considered so far.

In the following, we detail our main results. First, we analyze the BDF2 time approximation of the DLSS equation, written in the form

$$(8) \quad \frac{2}{\alpha} n^{1-\alpha/2} (n^{\alpha/2})_t + \frac{1}{2} \partial_{ij}^2 (n \partial_{ij}^2 \log n) = 0,$$

which was already used in [27] in a different context. Introducing the variable $v_k := n_k^{\alpha/2}$, which approximates $n(t_k)^{\alpha/2}$, the semi-discrete BDF2 scheme for (8) reads as

$$(9) \quad \frac{2}{\alpha\tau} v_{k+1}^{2/\alpha-1} \left(\frac{3}{2} v_{k+1} - 2v_k + \frac{1}{2} v_{k-1} \right) + \frac{1}{2} \partial_{ij}^2 (n_{k+1} \partial_{ij}^2 \log n_{k+1}) = 0 \quad \text{in } \mathbb{T}^d, \quad k \geq 1.$$

Here, $v_0 = n_0^{\alpha/2}$ is given by the initial datum n_0 , and v_1 is the solution to the implicit Euler scheme

$$(10) \quad \frac{2}{\alpha\tau} v_1^{2/\alpha-1} (v_1 - v_0) + \frac{1}{2} \partial_{ij}^2 (n_1 \partial_{ij}^2 \log n_1) = 0 \quad \text{in } \mathbb{T}^d.$$

The existence of a weak solution to the scheme (9)–(10) is provided by the following theorem.

Theorem 1 (Existence of solutions and entropy stability). *Let $1 \leq d \leq 3$, $1 \leq \alpha < (\sqrt{d} + 1)^2 / (d + 2)$, and let $n_0 \in L^3(\mathbb{T}^d)$ be a nonnegative function. Then there exists a weak solution $v_1 = n_1^{\alpha/2}$ of the implicit Euler scheme (10) and a sequence $(v_k) = (n_k^{\alpha/2})$ of weak nonnegative solutions to (9) satisfying $v_k \geq 0$ in \mathbb{T}^d , $v_k \in H^2(\mathbb{T}^d)$, and for all $\phi \in W^{2,\infty}(\mathbb{T}^d)$,*

$$(11) \quad \frac{1}{\alpha\tau} \int_{\mathbb{T}^d} v_{k+1}^{2/\alpha-1} \left(\frac{3}{2} v_{k+1} - 2v_k + \frac{1}{2} v_{k-1} \right) \phi dx + \int_{\mathbb{T}^d} \left(\frac{1}{2\alpha} v_{k+1}^{2/\alpha-1} \partial_{ij}^2 v_{k+1} - \frac{\alpha}{2} \partial_i (v_{k+1}^{1/\alpha}) \partial_j (v_{k+1}^{1/\alpha}) \right) \partial_{ij}^2 \phi dx = 0.$$

If $\alpha > 1$, the scheme (9) is entropy stable and the a priori estimate

$$(12) \quad E_\alpha[n_m] + \frac{4}{3} \kappa_\alpha \tau \sum_{k=1}^m \int_{\mathbb{T}^d} (\Delta(n_k^{\alpha/2}))^2 dx \leq E_\alpha[n_0], \quad m \geq 1,$$

holds, where $\kappa_\alpha > 0$ is defined in Lemma 6.

When we redefine the entropy, we are able to prove entropy dissipation of the semi-discrete scheme. For this, introduce the modified entropy

$$E_\alpha^G[n_k, n_{k-1}] = \frac{1}{2\alpha(\alpha-1)} \int_{\mathbb{T}^d} (n_k^\alpha + (2n_k^{\alpha/2} - n_{k-1}^{\alpha/2})^2) dx, \quad k \geq 1.$$

This definition is motivated by the inequality

$$2 \left(\frac{3}{2}a - 2b + \frac{1}{2}c \right) a \geq \frac{1}{2}(a^2 + (2a-b)^2) - \frac{1}{2}(b^2 + (2b-c)^2) \quad \text{for all } a, b, c \in \mathbb{R},$$

which implies the G-stability of the BDF2 method; see [6] and Lemma 5. The entropies E_α and E_α^G are formally related by $E_\alpha^G[n_k, n_{k-1}] = E_\alpha[n_k] + O(\tau)$ as $\tau \rightarrow 0$ for $k \geq 2$.

Corollary 2 (Entropy dissipation). *Let the assumptions of Theorem 1 hold for $\alpha > 1$. Then the scheme (9) is entropy dissipative in the sense of*

$$(13) \quad E_\alpha^G[n_{k+1}, n_k] + 2\kappa_\alpha \tau \int_{\mathbb{T}^d} (\Delta(n_{k+1}^{\alpha/2}))^2 dx \leq E_\alpha^G[n_k, n_{k-1}], \quad k \geq 1.$$

In particular, $k \mapsto E_\alpha^G[n_k, n_{k-1}]$ is nonincreasing.

We stress the fact that the implicit Euler scheme (6) dissipates *all* admissible entropies, whereas the BDF2 scheme just dissipates *one* entropy, $E_\alpha^G[n_k]$, where α has been fixed in the scheme.

The proof of Theorem 1 is based on the semi-discrete entropy stability inequality (12) and the Leray-Schauder fixed-point theorem. Instead of (7), we employ the algebraic inequalities (18) and (19) (see Section 2). We have not been able to obtain similar inequalities for BDF k methods with $3 \leq k \leq 6$. The reason might be the fact that the only G-stable BDF methods are the BDF1 (implicit Euler) and BDF2 discretizations [6]. Moreover, we have not been able to prove entropy dissipation for $\alpha = 1$ since in this case, inequalities (18) and (19) cannot be used.

If $\alpha = 1$, we prove that the semi-discrete solution to the BDF2 scheme converges to the continuous solution with second-order rate.

Theorem 3 (Second-order convergence). *Let the assumptions of Theorem 1 hold, let $\alpha = 1$, and let (v_k) be the sequence of solutions to (9)-(10) constructed in Theorem 1. We assume that there exist values $\mu_k > 0$ such that $v_k \geq \mu_k > 0$ in \mathbb{T}^d . Furthermore, let n be a strictly positive solution to (2) satisfying $\sqrt{n} \in H^3(0, T; L^2(\mathbb{T}^d)) \cap W^{2,\infty}(0, T; L^2(\mathbb{T}^d))$. Then there exists a constant $C > 0$, depending only on the $L^2(0, T; L^2(\mathbb{T}^d))$ norm of $(\sqrt{n})_{ttt}$, the $L^\infty(0, T; L^2(\mathbb{T}^d))$ norm of $(\sqrt{n})_{tt}$, and T , but not on τ , such that*

$$\|v_k - \sqrt{n(t_k, \cdot)}\|_{L^2(\mathbb{T}^d)} \leq C\tau^2,$$

where $0 < \tau < 1/8$ is the time step and $t_k = \tau k$, $k \geq 0$.

It is shown in [2, Theorem 6.2] that the solution n to (2) is smooth locally in time if the initial datum is positive and an element of $W^{1,\infty}(\mathbb{T}^d)$. The proof of Theorem 3 is based on local truncation error estimates and the monotonicity of the formal operator $A(v) = v^{1-2/\alpha} \partial_{ij}^2 (v^2 \partial_{ij}^2 \log v)$ for $\alpha = 1$ [26]. If $\alpha \neq 1$, the operator A seems to be not

monotone, and our proof does not apply. Possibly, the second-order convergence for $\alpha \neq 1$ could be achieved by applying suitable nonlinear semigroup estimates.

Next, we investigate a fully discrete numerical scheme which dissipates the Fisher information. To this end, we employ the discrete variational derivative method of Furihata and Matsuo [13]. The method is based on the variational structure of the DLSS equation,

$$(14) \quad n_t + \operatorname{div} \left(n \nabla \frac{\delta F[n]}{\delta n} \right) = 0, \quad t > 0.$$

The dissipation of the Fisher information $F[n]$ (see (4)) follows from (formally) integrating by parts in

$$\frac{d}{dt} F[n] = \int_{\mathbb{T}^d} \frac{\delta F[n]}{\delta n} n_t dx = - \int_{\mathbb{T}^d} n \left| \nabla \left(\frac{\delta F[n]}{\delta n} \right) \right|^2 dx \leq 0$$

(see (5)). The idea of the method is to derive a discrete formula for the variational derivative $\delta F[n]/\delta n$ in such a way that the above integration by parts formula and consequently the dissipation property hold on a discrete level. We provide such formulas for spatial finite difference and temporally higher-order BDF approximations.

The numerical approximation for equation (1), derived in [9], takes advantage of the gradient-flow structure in the sense that the variational structure was discretized instead of equation (1) itself. The method is based on the minimizing movement (steepest descent) scheme and consequently dissipates the discrete Fisher information. In each time step, a constrained quadratic optimization problem for the Fisher information needs to be solved on a finite-dimensional space. Each subproblem has to be solved iteratively, leading to a sequential quadratic programming method. In general, this structure-preserving approach, known as “first discretize, then minimize”, has good stability properties and captures well other structural features of equations, like those presented in [29].

The strategy of the discrete variational derivative method is the standard “first minimize, then discretize” approach, i.e., the discretization of equation (1), as the minimality condition in the variational setting, is performed. To some extent this is simpler than the above approach, since in each time step only a discrete nonlinear system has to be solved, and the main structural property remains preserved. Furthermore, we derive temporally higher-order discretizations, whereas the scheme in [9] is of first order only.

To simplify the notation, we consider the spatially one-dimensional case only. The extension to the multidimensional situation is straightforward if we assume rectangular grids. Let x_0, \dots, x_N be equidistant grid points of \mathbb{T} with mesh size $h > 0$ and $x_0 \cong x_N$. Let U_i^k be an approximation of $n(t_k, x_i)$ and set $U^k = (U_0^k, \dots, U_{N-1}^k)$, $U_N = U_0$. Furthermore, let $\delta_k^{1,q}$ be the q -step BDF operator at time t_k ; for instance,

$$(15) \quad \delta_{k+1}^{1,q} U_i^{k+1} = \frac{1}{\tau} (U_i^{k+1} - U_i^k) \quad \text{if } q = 1,$$

$$(16) \quad \delta_{k+1}^{1,q} U_i^{k+1} = \frac{1}{\tau} \left(\frac{3}{2} U_i^{k+1} - 2U_i^k + \frac{1}{2} U_i^{k-1} \right) \quad \text{if } q = 2.$$

We denote by $\delta_i^{(1)}$ the central finite-difference operator at x_i , i.e. $\delta_i^{(1)}U^k = (U_{i+1}^k - U_{i-1}^k)/h$. Then, following (14), we propose the fully discrete scheme

$$(17) \quad \delta_{k+1}^{1,q}U_i^{k+1} = \delta_i^{(1)} \left(U^{k+1} \delta_i^{(1)} \left(\frac{\delta F_d}{\delta(U^{k+1}, \dots, U^{k-q+1})} \right) \right), \quad k \geq q-1,$$

where $i = 0, \dots, N-1$. The discrete variational derivative $\delta F_d / \delta(U^{k+1}, \dots, U^{k-q+1}) \in \mathbb{R}^N$ is defined in such a way that a discrete chain rule holds (see (39) and (42) in Section 3 for the precise definitions), yielding the dissipation of the discrete Fisher information $F_d[U^k]$ in the sense of the following theorem.

Theorem 4 (Dissipation of the Fisher information). *Let $N \in \mathbb{N}$, $U^0 \in \mathbb{R}^N$ be some nonnegative initial datum with unit mass, $\sum_{i=0}^{N-1} U_i^0 h = 1$, and let $U^1, \dots, U^{q-1} \in \mathbb{R}^N$ be starting values with unit mass and $F_d[U^{q-1}] \leq \dots \leq F_d[U^0] < \infty$. Then scheme (17), with the discrete variational derivative $\delta F_d / \delta(U^{k+1}, \dots, U^{k-q+1})$ defined by (42), is consistent of order $(q, 2)$ with respect to the time-space discretization. Furthermore, U^k is bounded uniformly in k , has unit mass, and the discrete Fisher information is dissipated in the sense of*

$$\delta_k^{1,q} F_d[U^k] \leq 0 \quad \text{for all } k \geq q.$$

Furthermore, for $q = 1$ the discrete variational derivative is defined by (39), scheme (17) is consistent of order $(1, 2)$ and the discrete Fisher information is nonincreasing, $F_d[U^{k+1}] \leq F_d[U^k]$ for all $k \geq 1$.

We say that a scheme is consistent of order (q, m) if the truncation error is of the order $O(\tau^q) + O(h^m)$ for $\tau \rightarrow 0$ and $h \rightarrow 0$.

The paper is organized as follows. The analysis of the BDF2 time approximation is performed in Section 2, and Theorems 1 and 3 are proved. The fully discrete variational derivative method is detailed in Section 3, and Theorem 4 is proved. Numerical experiments in Section 4 illustrate the entropy stability, entropy dissipation, and energy (Fisher information) dissipation, even in situations not covered by the above theorems.

2. BDF2 TIME APPROXIMATION

First, we collect some auxiliary results. The following lemma is needed to show a priori bounds for the semi-discrete solutions to the DLSS equation.

Lemma 5. *It holds for all $a, b, c \in \mathbb{R}$,*

$$(18) \quad 2 \left(\frac{3}{2}a - 2b + \frac{1}{2}c \right) a \geq \frac{3}{2}a^2 - 2b^2 + \frac{1}{2}c^2 + (a-b)^2 - (b-c)^2,$$

$$(19) \quad 2 \left(\frac{3}{2}a - 2b + \frac{1}{2}c \right) a \geq \frac{1}{2}(a^2 + (2a-b)^2) - \frac{1}{2}(b^2 + (2b-c)^2).$$

Proof. We calculate

$$2 \left(\frac{3}{2}a - 2b + \frac{1}{2}c \right) a = \frac{3}{2}a^2 - 2b^2 + \frac{1}{2}c^2 + (a-b)^2 - (b-c)^2 + \frac{1}{2}(a-2b+c)^2,$$

which proves the first assertion. Because of

$$2 \left(\frac{3}{2}a - 2b + \frac{1}{2}c \right) a = \frac{1}{2}(a^2 + (2a - b)^2) - \frac{1}{2}(b^2 + (2b - c)^2) + \frac{1}{2}(a - 2b + c)^2,$$

the second assertion follows as well. \square

We also recall the following inequality (see [22, Lemma 2.2] for a proof).

Lemma 6. *Let $d \geq 2$ and $\sqrt{n} \in H^2(\mathbb{T}^d) \cap W^{1,4}(\mathbb{T}^d) \cap L^\infty(\mathbb{T}^d)$ with $\inf_{\mathbb{T}^d} n > 0$. Then, for any $(\sqrt{d} - 1)^2/(d + 2) < \alpha < (\sqrt{d} + 1)^2/(d + 2)$, $\alpha \neq 1$,*

$$\frac{1}{4(\alpha - 1)} \int_{\mathbb{T}^d} n \partial_{ij}^2(\log n) \partial_{ij}^2(n^{\alpha-1}) dx \geq \kappa_\alpha \int_{\mathbb{T}^d} (\Delta n^{\alpha/2})^2 dx$$

and for $\alpha = 1$,

$$\frac{1}{4} \int_{\mathbb{T}^d} n (\partial_{ij}^2(\log n))^2 dx \geq \kappa_1 \int_{\mathbb{T}^d} (\Delta \sqrt{n})^2 dx,$$

where

$$\kappa_\alpha = \frac{p(\alpha)}{\alpha^2(p(\alpha) - p(0))} > 0 \quad \text{and} \quad p(\alpha) = -\alpha^2 + \frac{2(d+1)}{d+2}\alpha - \left(\frac{d-1}{d+2}\right)^2.$$

Proof of Theorem 1. Given $v_0 = n_0^{\alpha/2}$, the existence of a nonnegative weak solution $v_1 \in H^2(\mathbb{T}^d)$ to (10) is shown in [22]. Assume that $v_2, \dots, v_k \in H^2(\mathbb{T}^d)$ are solutions to (11). We introduce the variable y by $v_{k+1} = e^{\alpha y/2}$ such that $n_{k+1} = e^y$. First, we prove the existence of a weak solution $y \in H^2(\mathbb{T}^d)$ to the regularized equation

$$(20) \quad \frac{2}{\alpha\tau} e^{(1-\alpha/2)y} \left(\frac{3}{2} e^{\alpha y/2} - 2v_k + \frac{1}{2}v_{k-1} \right) + \frac{1}{2} \partial_{ij}^2(e^y \partial_{ij}^2 y) + \varepsilon L(y) = 0,$$

where $\varepsilon > 0$ and

$$L(y) = \Delta^2 y - \operatorname{div}(|\nabla y|^2 \nabla y) + y.$$

Step 1: Definition of the fixed-point operator. Given $z \in W^{1,4}(\mathbb{T}^d)$ and $\sigma \in [0, 1]$, we define on $H^2(\mathbb{T}^d)$ the forms

$$\begin{aligned} a(y, \phi) &= \frac{1}{2} \int_{\mathbb{T}^d} e^z \partial_{ij}^2 y \partial_{ij}^2 \phi dx + \varepsilon \int_{\mathbb{T}^d} (\Delta y \Delta \phi + |\nabla z|^2 \nabla y \cdot \nabla \phi + y \phi) dx, \\ f(\phi) &= -\frac{2\sigma}{\alpha\tau} \int_{\mathbb{T}^d} e^{(1-\alpha/2)z} \left(\frac{3}{2} e^{\alpha z/2} - 2v_k + \frac{1}{2}v_{k-1} \right) \phi dx. \end{aligned}$$

Since $H^2(\mathbb{T}^d) \hookrightarrow W^{1,4}(\mathbb{T}^d) \hookrightarrow L^\infty(\mathbb{T}^d)$ with continuous embeddings (remember that $d \leq 3$), these mappings are well defined and continuous. Furthermore, by the Poincaré inequality

for periodic functions with constant $C_P > 0$, the bilinear form a is coercive,

$$\begin{aligned} \varepsilon \|y\|_{H^2(\mathbb{T}^d)}^2 &= \varepsilon \int_{\mathbb{T}^d} (|\nabla^2 y|^2 + |\nabla y|^2 + y^2) dx \leq \varepsilon \int_{\mathbb{T}^d} ((C_P^2 + 1)|\nabla^2 y|^2 + y^2) dx \\ &= \varepsilon \int_{\mathbb{T}^d} ((C_P^2 + 1)(\Delta y)^2 + y^2) dx \leq \varepsilon (C_P^2 + 1) \int_{\mathbb{T}^d} ((\Delta y)^2 + y^2) dx \\ &\leq (C_P^2 + 1)a(y, y). \end{aligned}$$

By Lax-Milgram's lemma, there exists a unique solution $y \in H^2(\mathbb{T}^d)$ to

$$a(y, \phi) = f(\phi) \quad \text{for all } \phi \in H^2(\mathbb{T}^d).$$

This defines the fixed-point operator $S : W^{1,4}(\mathbb{T}^d) \times [0, 1] \rightarrow W^{1,4}(\mathbb{T}^d)$, $S(z, \sigma) = y$. It holds $S(y, 0) = 0$ for all $y \in W^{1,4}(\mathbb{T}^d)$, and S is continuous and compact, in view of the compact embedding $H^2(\mathbb{T}^d) \hookrightarrow W^{1,4}(\mathbb{T}^d)$. In order to apply the Leray-Schauder theorem, it remains to show that there exists a uniform bound in $W^{1,4}(\mathbb{T}^d)$ for all fixed points of $S(\cdot, \sigma)$.

Step 2: A priori bound. Let $y \in H^2(\mathbb{T}^d)$ be a fixed point of $S(\cdot, \sigma)$ for some $\sigma \in [0, 1]$. We employ the test function $\phi = y$ in (20). This gives

$$(21) \quad \begin{aligned} 0 &= \frac{2\sigma}{\alpha\tau} \int_{\mathbb{T}^d} e^{(1-\alpha/2)y} \left(\frac{3}{2}e^{\alpha y/2} - 2v_k + \frac{1}{2}v_{k-1} \right) y dx \\ &\quad + \frac{1}{2} \int_{\mathbb{T}^d} e^y (\partial_{ij}^2 y)^2 dx + \varepsilon \int_{\mathbb{T}^d} ((\Delta y)^2 + |\nabla y|^4 + y^2) dx. \end{aligned}$$

To estimate the first integral, we distinguish the domains $\{y < 0\}$ and $\{y \geq 0\}$:

$$\begin{aligned} \frac{2\sigma}{\alpha\tau} \int_{\mathbb{T}^d} e^{(1-\alpha/2)y} \left(\frac{3}{2}e^{\alpha y/2} - 2v_k + \frac{1}{2}v_{k-1} \right) y dx \\ = \frac{\sigma}{\alpha\tau} \int_{\{y < 0\}} (3e^y y - 4e^{(1-\alpha/2)y} v_k y + e^{(1-\alpha/2)y} v_{k-1} y) dx \\ + \frac{\sigma}{\alpha\tau} \int_{\{y \geq 0\}} (3e^y y - 4e^{(1-\alpha/2)y} v_k y + e^{(1-\alpha/2)y} v_{k-1} y) dx. \end{aligned}$$

The first integral on the right-hand side is estimated by using the Young inequalities $-4e^{(1-\alpha/2)y} v_k y \geq -2e^{(2-\alpha)y} y^2 - 2v_k^2$ and $e^{(1-\alpha/2)y} v_{k-1} y \geq -\frac{1}{2}e^{(2-\alpha)y} y^2 - \frac{1}{2}v_{k-1}^2$:

$$\begin{aligned} \frac{\sigma}{\alpha\tau} \int_{\{y < 0\}} (3e^y y - 4e^{(1-\alpha/2)y} v_k y + e^{(1-\alpha/2)y} v_{k-1} y) dx \\ \geq \frac{\sigma}{\alpha\tau} \int_{\{y < 0\}} \left(3e^y y - \frac{5}{2}e^{(2-\alpha)y} y^2 - 2v_k^2 - \frac{1}{2}v_{k-1}^2 \right) dx \\ = \frac{\sigma}{\alpha\tau} \int_{\{y < 0\}} \left(e^y (y - 1) + 1 + (1 + 2y) e^y - \frac{5}{2}e^{(2-\alpha)y} y^2 - 1 - 2v_k^2 - \frac{1}{2}v_{k-1}^2 \right) dx. \end{aligned}$$

Since $y \mapsto (1 + 2y)e^y - \frac{5}{2}e^{(2-\alpha)y}y^2 - 1$, $y < 0$, is bounded from below (remember that $\alpha < 2$), we find that

$$\begin{aligned} & \frac{\sigma}{\alpha\tau} \int_{\{y < 0\}} (3e^y y - 4e^{(1-\alpha/2)y} v_k y + e^{(1-\alpha/2)y} v_{k-1} y) dx \\ & \geq \frac{\sigma}{\alpha\tau} \int_{\{y < 0\}} (e^y(y-1) + 1) dx - \frac{\sigma}{\alpha\tau} c_1 - \frac{\sigma}{\alpha\tau} \int_{\{y < 0\}} \left(2v_k^2 + \frac{1}{2}v_{k-1}^2 \right) dx, \end{aligned}$$

where $c_1 > 0$ depends only on the lower bound of $y \mapsto (1 + 2y)e^y - \frac{5}{2}e^{(2-\alpha)y}y^2 - 1$, $y < 0$, and $\text{meas}(\mathbb{T}^d)$. For the remaining integral over $\{y \geq 0\}$, we employ the Young inequalities $-4e^{(1-\alpha/2)y} v_k y \geq -2e^{(2-\alpha)y} - y^4 - v_k^4$ and $e^{(1-\alpha/2)y} v_{k-1} y \geq -\frac{1}{2}e^{(2-\alpha)y} - \frac{1}{4}y^4 - \frac{1}{4}v_{k-1}^4$:

$$\begin{aligned} & \frac{\sigma}{\alpha\tau} \int_{\{y \geq 0\}} (3e^y y - 4e^{(1-\alpha/2)y} v_k y + e^{(1-\alpha/2)y} v_{k-1} y) dx \\ & \geq \frac{\sigma}{\alpha\tau} \int_{\{y \geq 0\}} \left(3e^y y - \frac{5}{2}e^{(2-\alpha)y} - \frac{5}{4}y^4 - v_k^4 - \frac{1}{4}v_{k-1}^4 \right) dx \\ & = \frac{\sigma}{\alpha\tau} \int_{\{y \geq 0\}} \left(e^y(y-1) + 1 + \left((1+2y)e^y - \frac{5}{2}e^{(2-\alpha)y} - \frac{5}{4}y^4 - 1 \right) \right. \\ & \quad \left. - v_k^4 - \frac{1}{4}v_{k-1}^4 \right) dx. \end{aligned}$$

The mapping $y \mapsto (1 + 2y)e^y - \frac{5}{2}e^{(2-\alpha)y} - \frac{5}{4}y^4 - 1$, $y \geq 0$, is bounded from below which implies the existence of a constant $c_2 > 0$ such that

$$\begin{aligned} & \frac{\sigma}{\alpha\tau} \int_{\{y \geq 0\}} (3e^y y - 4e^{(1-\alpha/2)y} v_k y + e^{(1-\alpha/2)y} v_{k-1} y) dx \\ & \geq \frac{\sigma}{\alpha\tau} \int_{\{y \geq 0\}} (e^y(y-1) + 1) dx - \frac{\sigma}{\alpha\tau} c_2 - \frac{\sigma}{\alpha\tau} \int_{\{y \geq 0\}} \left(v_k^4 + \frac{1}{4}v_{k-1}^4 \right) dx. \end{aligned}$$

Summarizing the estimates for both integrals over $\{y > 0\}$ and $\{y \geq 0\}$, it follows that

$$\begin{aligned} (22) \quad & \frac{2\sigma}{\alpha\tau} \int_{\mathbb{T}^d} e^{(1-\alpha/2)y} \left(\frac{3}{2}e^{\alpha y/2} - 2v_k + \frac{1}{2}v_{k-1} \right) y dx \geq \frac{\sigma}{\alpha\tau} \int_{\mathbb{T}^d} (e^y(y-1) + 1) dx \\ & - \frac{\sigma}{\alpha\tau} \int_{\mathbb{T}^d} \left(2v_k^2 + v_k^4 + \frac{1}{2}v_{k-1}^2 + \frac{1}{4}v_{k-1}^4 \right) dx - \frac{\sigma}{\alpha\tau} (c_1 + c_2). \end{aligned}$$

For the second integral in (21), we use Lemma 6:

$$\frac{1}{2} \int_{\mathbb{T}^d} e^y (\partial_{ij}^2 y)^2 dx \geq 2\kappa_1 \int_{\mathbb{T}^d} (\Delta e^{y/2})^2 dx,$$

where $\kappa_1 > 0$ depends only on the space dimension d . With this estimate and (22), equation (21) implies that

$$\begin{aligned} & \frac{\sigma}{\alpha\tau} \int_{\mathbb{T}^d} (e^y(y-1) + 1) dx + 2\kappa_1 \int_{\mathbb{T}^d} (\Delta e^{y/2})^2 dx + \varepsilon \int_{\mathbb{T}^d} ((\Delta y)^2 + |\nabla y|^4 + y^2) dx \\ & \leq \frac{\sigma}{\alpha\tau} \int_{\mathbb{T}^d} \left(2v_k^2 + v_k^4 + \frac{1}{2}v_{k-1}^2 + \frac{1}{4}v_{k-1}^4 \right) dx + \frac{\sigma}{\alpha\tau} (c_1 + c_2). \end{aligned}$$

By the definition of the entropy, this inequality can be written as

$$\begin{aligned} (23) \quad E_1[n] + \frac{2\alpha\tau\kappa_1}{\sigma} \int_{\mathbb{T}^d} (\Delta e^{y/2})^2 dx + \frac{\varepsilon\alpha\tau}{\sigma} \int_{\mathbb{T}^d} ((\Delta y)^2 + |\nabla y|^4 + y^2) dx \\ \leq \int_{\mathbb{T}^d} \left(2v_k^2 + v_k^4 + \frac{1}{2}v_{k-1}^2 + \frac{1}{4}v_{k-1}^4 \right) dx + c_1 + c_2. \end{aligned}$$

The right-hand side gives a uniform (with respect to σ) bound since $v_{k-1}, v_k \in W^{1,4}(\mathbb{T}^d)$. Hence, by the Poincaré inequality we obtain the H^2 -bound

$$\|y\|_{H^2(\mathbb{T}^d)}^2 \leq C \int_{\mathbb{T}^d} ((\Delta y)^2 + y^2) dx \leq C,$$

where the constant $C > 0$ depends on $\alpha, \varepsilon, \tau, v_k$, and v_{k-1} but not on σ . The continuous embedding $H^2(\mathbb{T}^d) \hookrightarrow W^{1,4}(\mathbb{T}^d)$ then implies the desired uniform bound, $\|y\|_{W^{1,4}(\mathbb{T}^d)} \leq C$. Leray-Schauder's fixed-point theorem provides the existence of a fixed point y_ε of $S(y, 1) = y$, i.e. of a solution to (20).

Step 3: Limit $\varepsilon \rightarrow 0$. Let y_ε be a solution to (20), constructed in the previous steps. Set $v_\varepsilon := e^{\alpha y_\varepsilon/2}$ and $n_\varepsilon := e^{y_\varepsilon}$. Then v_ε solves

$$(24) \quad \frac{2}{\alpha\tau} v_\varepsilon^{2/\alpha-1} \left(\frac{3}{2}v_\varepsilon - 2v_k + \frac{1}{2}v_{k-1} \right) + \partial_{ij}^2 \left(\frac{1}{\alpha} v_\varepsilon^{2/\alpha-1} \partial_{ij}^2 v_\varepsilon - \alpha \partial_i (v_\varepsilon^{1/\alpha}) \partial_j (v_\varepsilon^{1/\alpha}) \right) + \varepsilon L(y_\varepsilon) = 0.$$

The goal is to pass to the limit $\varepsilon \rightarrow 0$ in this equation.

Let $\alpha > 1$. We employ the test function $e^{(\alpha-1)y_\varepsilon}/(\alpha-1) \in H^2(\mathbb{T}^d)$ in (20) and find that

$$\begin{aligned} 0 &= \frac{2}{\alpha(\alpha-1)} \int_{\mathbb{T}^d} \left(\frac{3}{2}v_\varepsilon - 2v_k + \frac{1}{2}v_{k-1} \right) v_\varepsilon dx + \frac{\tau}{2(\alpha-1)} \int_{\mathbb{T}^d} e^{y_\varepsilon} \partial_{ij}^2 y_\varepsilon \partial_{ij}^2 (e^{(\alpha-1)y_\varepsilon}) dx \\ & \quad + \frac{\varepsilon\tau}{\alpha-1} \langle L(y_\varepsilon), e^{(\alpha-1)y_\varepsilon} \rangle_{H^{-2}, H^2}. \end{aligned}$$

Inequality (18) shows that

$$\begin{aligned} \frac{2}{\alpha(\alpha-1)} \int_{\mathbb{T}^d} \left(\frac{3}{2}v_\varepsilon - 2v_k + \frac{1}{2}v_{k-1} \right) v_\varepsilon dx &\geq \frac{1}{\alpha(\alpha-1)} \int_{\mathbb{T}^d} \left(\frac{3}{2}v_\varepsilon^2 - 2v_k^2 + \frac{1}{2}v_{k-1}^2 \right) dx \\ & \quad + \frac{1}{\alpha(\alpha-1)} \int_{\mathbb{T}^d} ((v_\varepsilon - v_k)^2 - (v_k - v_{k-1})^2) dx. \end{aligned}$$

The integral involving the second derivatives is again estimated by using Lemma 6:

$$\frac{\tau}{2(\alpha-1)} \int_{\mathbb{T}^d} e^{y_\varepsilon} \partial_{ij}^2 y_\varepsilon \partial_{ij}^2 (e^{(\alpha-1)y_\varepsilon}) dx \geq 2\kappa_\alpha \tau \int_{\mathbb{T}^d} (\Delta e^{\alpha y_\varepsilon/2})^2 dx = 2\kappa_\alpha \tau \int_{\mathbb{T}^d} (\Delta v_\varepsilon)^2 dx.$$

Now let us consider the ε -term and show that $\langle L(y_\varepsilon), e^{(\alpha-1)y_\varepsilon} \rangle_{H^{-2}, H^2}$ is bounded from below uniformly in ε . By construction, v_ε and n_ε are strictly positive since $y_\varepsilon \in H^2(\mathbb{T}^d) \hookrightarrow L^\infty(\mathbb{T}^d)$. Therefore, we can write (cf. [22, Section 4.1])

$$\begin{aligned} \langle L(y_\varepsilon), e^{(\alpha-1)y_\varepsilon} \rangle_{H^{-2}, H^2} &= 4(\alpha-1) \int_{\mathbb{T}^d} \left(e^{(\alpha-1)y_\varepsilon} \left(\frac{\Delta e^{y_\varepsilon/2}}{e^{y_\varepsilon/2}} - (2-\alpha) \left| \frac{\nabla e^{y_\varepsilon/2}}{e^{y_\varepsilon/2}} \right|^2 \right)^2 \right. \\ &\quad \left. + 4(\alpha^2-1)(3-\alpha) \int_{\mathbb{T}^d} e^{(\alpha-1)y_\varepsilon} \left| \frac{\nabla e^{y_\varepsilon/2}}{e^{y_\varepsilon/2}} \right|^4 dx + \int_{\mathbb{T}^d} y_\varepsilon e^{(\alpha-1)y_\varepsilon} dx \right) \geq -C, \end{aligned}$$

where $C > 0$ depends only on α . We have used the fact that $xe^{(\alpha-1)x} \geq -1/((\alpha-1)e)$ for all $x \in \mathbb{R}$.

Summarizing the above inequalities, we obtain

$$\begin{aligned} &\frac{1}{\alpha(\alpha-1)} \int_{\mathbb{T}^d} \left(\frac{3}{2}v_\varepsilon^2 - 2v_k^2 + \frac{1}{2}v_{k-1}^2 \right) dx + \frac{1}{\alpha(\alpha-1)} \int_{\mathbb{T}^d} ((v_\varepsilon - v_k)^2 - (v_k - v_{k-1})^2) dx \\ (25) \quad &+ 2\tau\kappa_\alpha \int_{\mathbb{T}^d} (\Delta v_\varepsilon)^2 dx \leq C\varepsilon. \end{aligned}$$

Inequality (25) provides the estimate for (v_ε) in $H^2(\mathbb{T}^d)$ uniformly in ε . Therefore, there exists a limit function $v \in H^2(\mathbb{T}^d)$ such that, up to a subsequence, as $\varepsilon \rightarrow 0$,

$$\begin{aligned} v_\varepsilon &\rightharpoonup v \quad \text{weakly in } H^2(\mathbb{T}^d), \\ v_\varepsilon &\rightarrow v \quad \text{strongly in } W^{1,4}(\mathbb{T}^d) \text{ and } L^\infty(\mathbb{T}^d). \end{aligned}$$

Consequently, since $2/\alpha - 1 > 0$,

$$(26) \quad v_\varepsilon^{2/\alpha-1} \partial_{ij}^2 v_\varepsilon \rightharpoonup v^{2/\alpha-1} \partial_{ij}^2 v \quad \text{weakly in } L^2(\mathbb{T}^d), \quad i, j = 1, \dots, d.$$

According to the Lions-Villani lemma on the regularity of the square root of Sobolev functions (see the version in [3, Lemma 26]), there exists $C > 0$ independent of ε such that

$$\|\sqrt{v_\varepsilon}\|_{W^{1,4}(\mathbb{T}^d)}^2 \leq C \|v_\varepsilon\|_{H^2(\mathbb{T}^d)} \leq C.$$

Since $1/2 < 1/\alpha < 1$, Proposition A.1 in [23] shows that the strong convergence $v_\varepsilon \rightarrow v$ in $H^1(\mathbb{T}^d)$ and the boundedness of $(\sqrt{v_\varepsilon})$ in $W^{1,4}(\mathbb{T}^d)$ imply that

$$v_\varepsilon^{1/\alpha} \rightarrow v^{1/\alpha} \quad \text{strongly in } W^{1,2\alpha}(\mathbb{T}^d).$$

Hence, we have

$$(27) \quad \partial_i(v_\varepsilon^{1/\alpha}) \partial_j(v_\varepsilon^{1/\alpha}) \rightarrow \partial_i(v^{1/\alpha}) \partial_j(v^{1/\alpha}) \quad \text{strongly in } L^\alpha(\mathbb{T}^d), \quad i, j = 1, \dots, d.$$

Estimate (23) and $E_1[n] \geq 0$ provide the uniform bound

$$\sqrt{\varepsilon} \|y_\varepsilon\|_{H^2(\mathbb{T}^d)} + \sqrt[4]{\varepsilon} \|\nabla y_\varepsilon\|_{L^4(\mathbb{T}^d)} \leq C,$$

which shows that

$$(28) \quad \varepsilon L(y_\varepsilon) \rightharpoonup 0 \quad \text{weakly in } H^{-2}(\mathbb{T}^d).$$

Using $\phi \in W^{2,\infty}(\Omega)$ as a test function in the weak formulation of (24), the convergence results (26)-(28) allow us to pass to the limit $\varepsilon \rightarrow 0$ in the resulting equation, which yields (11) for $v_{k+1} := v$. In fact, it is sufficient to use test functions $\phi \in W^{2,\alpha/(\alpha-1)}(\mathbb{T}^d)$.

If $\alpha = 1$, the convergence result follows similarly as above based on the uniform bound $\|e^{y\varepsilon/2}\|_{H^2} \leq C$, which is obtained from a priori estimate (23), using the elementary inequality $s \leq s(\log s - 1) + e$ for all $s \geq 0$, which gives a uniform L^2 -bound for $e^{y\varepsilon}$. In that case, the test functions $\phi \in H^2(\mathbb{T}^d)$ can be used in (24).

Step 4: Entropy stability. Let $\alpha > 1$. Using the test function $v_1^{2-2/\alpha}/(\alpha-1)$ in (10), it follows that

$$\frac{1}{\tau\alpha(\alpha-1)} \int_{\mathbb{T}^d} (v_1^2 - v_0^2 + (v_1 - v_0)^2) dx + \frac{1}{2(\alpha-1)} \int_{\mathbb{T}^d} v_1^{2/\alpha} \partial_{ij}^2 (\log v_1^{2/\alpha}) \partial_{ij}^2 (v_1^{2-2/\alpha}) dx = 0.$$

By Lemma 6, we infer that

$$(29) \quad \frac{1}{\alpha(\alpha-1)} \int_{\mathbb{T}^d} (v_1^2 + (v_1 - v_0)^2) dx + 2\tau\kappa_\alpha \int_{\mathbb{T}^d} (\Delta v_1)^2 dx \leq \frac{1}{\alpha(\alpha-1)} \int_{\mathbb{T}^d} v_0^2 dx.$$

This gives an H^2 -bound for v_1 .

Next, let $k \geq 1$ and let y_ε be a weak solution to (20). Set $v_\varepsilon = e^{\alpha y_\varepsilon/2}$. The convergence results of Step 3 allow us to pass to the limit $\varepsilon \rightarrow 0$ in (25). Using the weakly lower semi-continuity of $u \mapsto \|\Delta u\|_{L^2(\mathbb{T}^d)}^2$ on $H^2(\mathbb{T}^d)$, it follows that

$$(30) \quad \frac{1}{\alpha(\alpha-1)} \int_{\mathbb{T}^d} \left(\frac{3}{2} v_{k+1}^2 - 2v_k^2 + \frac{1}{2} v_{k-1}^2 \right) dx + \frac{1}{\alpha(\alpha-1)} \int_{\mathbb{T}^d} ((v_{k+1} - v_k)^2 - (v_k - v_{k-1})^2) dx + 2\kappa_\alpha \tau \int_{\mathbb{T}^d} (\Delta v_{k+1})^2 dx \leq 0,$$

where, as before, $v_{k+1} = \lim_{\varepsilon \rightarrow 0} v_\varepsilon$. Summing (29) and (30) over $k = 1, \dots, m-1$, some terms cancel and we end up with

$$\frac{3}{2\alpha(\alpha-1)} \int_{\mathbb{T}^d} v_m^2 dx + 2\kappa_\alpha \tau \sum_{k=0}^{m-1} \int_{\mathbb{T}^d} (\Delta v_{k+1})^2 dx \leq \frac{1}{2\alpha(\alpha-1)} \int_{\mathbb{T}^d} (v_{m-1}^2 + v_1^2 + v_0^2) dx.$$

Set $a_m = \|v_m\|_{L^2(\Omega)}^2$ for $m \geq 0$. By (29), $a_1 \leq a_0$. Then, the above estimate shows that $a_m \leq \frac{1}{3}a_{m-1} + \frac{2}{3}a_0$. A simple induction argument gives $a_m \leq a_0$ for all $m \geq 1$. Therefore,

$$\frac{1}{\alpha(\alpha-1)} \int_{\mathbb{T}^d} v_m^2 dx + \frac{4}{3}\kappa_\alpha \tau \sum_{k=1}^m \int_{\mathbb{T}^d} (\Delta v_k)^2 dx \leq \frac{1}{\alpha(\alpha-1)} \int_{\mathbb{T}^d} v_0^2 dx.$$

This implies the entropy stability estimate (12). \square

The proof of Corollary 2 is a consequence of the above proof. Indeed, employing inequality (19) instead of (18), we can replace (30) by

$$\begin{aligned} & \frac{1}{2\alpha(\alpha-1)} \int_{\mathbb{T}^d} (v_{k+1}^2 + (2v_{k+1} - v_k)^2) dx + 2\kappa_\alpha \tau \int_{\mathbb{T}^d} (\Delta v_{k+1})^2 dx \\ & \leq \frac{1}{2\alpha(\alpha-1)} \int_{\mathbb{T}^d} (v_k^2 + (2v_k - v_{k-1})^2) dx, \end{aligned}$$

which equals (13).

Next, we prove that, if $\alpha = 1$, the solutions v_k are smooth as long as they are strictly positive.

Lemma 7. *Let $\alpha = 1$ and let (v_k) be the sequence of weak solutions constructed in Theorem 1 satisfying $v_k \geq \mu_k > 0$ in \mathbb{T}^d for $k \geq 1$ and some $\mu_k > 0$. Then $v_k \in C^\infty(\mathbb{T}^d)$.*

Proof. We recall that the weak form (11) for $\alpha = 1$ reads as

$$\int_{\mathbb{T}^d} v_{k+1} \left(\frac{3}{2} v_{k+1} - 2v_k + \frac{1}{2} v_{k-1} \right) \phi dx + \frac{\tau}{2} \int_{\mathbb{T}^d} (v_{k+1} \partial_{ij}^2 v_{k+1} - \partial_i v_{k+1} \partial_j v_{k+1}) \partial_{ij}^2 \phi dx = 0$$

for $\phi \in H^2(\mathbb{T}^d)$. Since v_k is assumed to be strictly positive, we can write

$$v_{k+1} \partial_{ij}^2 v_{k+1} - \partial_i v_{k+1} \partial_j v_{k+1} = \frac{1}{2} n_{k+1} \partial_{ij}^2 \log n_{k+1},$$

where $n_{k+1} = v_{k+1}^2$ and consequently,

$$(31) \quad v_{k+1} \left(\frac{3}{2} v_{k+1} - 2v_k + \frac{1}{2} v_{k-1} \right) + \frac{\tau}{4} \partial_{ij}^2 (n_{k+1} \partial_{ij}^2 \log n_{k+1}) = 0 \quad \text{in } H^{-2}(\mathbb{T}^d).$$

With the identity

$$\partial_{ij}^2 (n_{k+1} \partial_{ij}^2 \log n_{k+1}) = \Delta^2 n_{k+1} - \partial_i \left(2 \frac{\partial_{ij}^2 n_{k+1} \partial_j n_{k+1}}{n_{k+1}} - \frac{(\partial_j n_{k+1})^2 \partial_i n_{k+1}}{n_{k+1}^2} \right),$$

it follows that n_{k+1} solves

$$(32) \quad \Delta^2 n_{k+1} = \partial_i \left(2 \frac{\partial_{ij}^2 n_{k+1} \partial_j n_{k+1}}{n_{k+1}} - \frac{(\partial_j n_{k+1})^2 \partial_i n_{k+1}}{n_{k+1}^2} \right) - \frac{4}{\tau} v_{k+1} \left(\frac{3}{2} v_{k+1} - 2v_k + \frac{1}{2} v_{k-1} \right)$$

in the sense of $H^{-2}(\mathbb{T}^d)$. The second term on the right-hand side is an element of $H^2(\mathbb{T}^d)$. The continuity of the Sobolev embedding $H^2(\mathbb{T}^d) \hookrightarrow W^{1,6}(\mathbb{T}^d)$ (for $d \leq 3$) implies that $(\partial_j n_{k+1})^2 \partial_i n_{k+1} / n_{k+1} \in L^2(\mathbb{T}^d)$ and $\partial_{ij}^2 n_{k+1} \partial_j n_{k+1} / n_{k+1} \in L^{3/2}(\mathbb{T}^d) \hookrightarrow H^{-1/2}(\mathbb{T}^d)$ for all $i, j = 1, \dots, d$. This proves that

$$\Delta^2 n_{k+1} \in H^{-3/2}(\mathbb{T}^d).$$

The regularity theory for elliptic operator on \mathbb{T}^d (e.g., using Fourier transforms on the torus) yields $n_{k+1} \in H^{5/2}(\mathbb{T}^d)$ which improves the previous regularity $n_{k+1} \in H^2(\mathbb{T}^d)$. Taking into account the improved regularity and the embedding $H^{5/2}(\mathbb{T}^d) \hookrightarrow W^{2,3}(\mathbb{T}^d)$, we infer that the right-hand side of (32) lies in $H^{-1}(\mathbb{T}^d)$, i.e.

$$\Delta^2 n_{k+1} \in H^{-1}(\mathbb{T}^d),$$

which implies that $n_{k+1} \in H^3(\mathbb{T}^d)$. By bootstrapping, we conclude that $n_{k+1} \in H^m(\mathbb{T}^d)$ for all $m \in \mathbb{N}$. \square

Now, we are in the position to prove Theorem 3.

Proof of Theorem 3. Let (v_k) be a sequence of weak solutions to (11). Since we have assumed that v_k is strictly positive, Lemma 7 shows that v_k is smooth. As a consequence, v_k solves (see (31))

$$\frac{3}{2}v_{k+1} - 2v_k + \frac{1}{2}v_{k-1} + \frac{1}{v_{k+1}}\partial_{ij}^2(v_{k+1}^2\partial_{ij}^2\log v_{k+1}) = 0 \quad \text{in } \mathbb{T}^d.$$

Let $n = v^2$ be a solution to (2) with the regularity indicated in the theorem. By Taylor expansion,

$$v_t(t_{k+1}) = \frac{1}{\tau} \left(\frac{3}{2}v(t_{k+1}) - 2v(t_k) + \frac{1}{2}v(t_{k-1}) \right) + \frac{f_k}{\tau}, \quad k \geq 1,$$

where

$$f_k = - \int_{t_k}^{t_{k+1}} v_{ttt}(s)(t_k - s)^2 ds + \frac{1}{4} \int_{t_{k-1}}^{t_{k+1}} v_{ttt}(s)(t_{k-1} - s)^2 ds$$

can be interpreted as the local truncation error. We estimate f_k as follows:

$$(33) \quad \sum_{k=1}^{m-1} \|f_k\|_{L^2(\mathbb{T}^d)}^2 \leq C_R \|v_{ttt}\|_{L^2(0,T;L^2(\mathbb{T}^d))}^2 \tau^5,$$

where $C_R > 0$ does not depend on τ or m . Similarly, we have

$$v_t(t_1) = \frac{1}{\tau}(v(t_1) - v(t_0)) + \frac{f_0}{\tau}, \quad \text{where } f_0 = \int_0^\tau v_{tt}(s) ds,$$

and

$$(34) \quad \|f_0\|_{L^2(\mathbb{T}^d)} \leq \int_0^\tau \|v_{tt}(s)\|_{L^2(\mathbb{T}^d)} ds \leq \frac{\tau^2}{2} \|v_{tt}\|_{L^\infty(0,T;L^2(\mathbb{T}^d))}.$$

Replacing the time derivative v_t in (2), written as $v_t + v^{-1}\partial_{ij}^2(v^2\partial_{ij}^2\log v) = 0$, by the above expansions, it follows that

$$(35) \quad v(t_1) - v(t_0) + \frac{\tau}{v(t_1)}\partial_{ij}^2(v(t_1)^2\partial_{ij}^2\log v(t_1)) = -f_0,$$

$$(36) \quad \frac{3}{2}v(t_{k+1}) - 2v(t_k) + \frac{1}{2}v(t_{k-1}) + \frac{\tau}{v(t_{k+1})}\partial_{ij}^2(v(t_{k+1})^2\partial_{ij}^2\log v(t_{k+1})) = -f_k,$$

for $k \geq 1$. Taking the difference of (10), multiplied by v_1^{-1} , and (35), and the difference of (9), multiplied by v_{k+1}^{-1} , and (36), we obtain the error equations for $e_k := v_k - v(t_k)$:

$$e_1 - e_0 + \tau(A(v_1) - A(v(t_1))) = f_0,$$

$$\frac{3}{2}e_{k+1} - 2e_k + \frac{1}{2}e_{k-1} + \tau(A(v_{k+1}) - A(v(t_{k+1}))) = f_k, \quad k \geq 1,$$

where we have introduced the operator

$$A : D(A) \rightarrow H^{-2}(\mathbb{T}^d), \quad A(v) = \frac{1}{v} \partial_{ij}^2 (v^2 \partial_{ij}^2 \log v),$$

with domain $D(A) = \{v \in H^2(\mathbb{T}^d) : v > 0 \text{ in } \mathbb{T}^d\}$.

We multiply the error equations by e_1 and e_{k+1} , respectively, integrate over \mathbb{T}^d , and sum over $k = 0, \dots, m-1$:

$$(37) \quad \int_{\mathbb{T}^d} (e_1 - e_0) e_1 dx + \sum_{k=1}^{m-1} \int_{\mathbb{T}^d} \left(\frac{3}{2} e_{k+1} - 2e_k + \frac{1}{2} e_{k-1} \right) e_{k+1} dx \\ + \tau \sum_{k=0}^{m-1} \int_{\mathbb{T}^d} (A(v_{k+1}) - A(v(t_{k+1}))) (v_{k+1} - v(t_{k+1})) dx = \sum_{k=0}^{m-1} f_k e_{k+1} dx.$$

Using $e_0 = 0$ and inequality (18), the first two integrands can be estimated by

$$(e_1 - e_0) e_1 + \sum_{k=1}^{m-1} \left(\frac{3}{2} e_{k+1} - 2e_k + \frac{1}{2} e_{k-1} \right) e_{k+1} \\ \geq e_1^2 + \sum_{k=1}^{m-1} \left(\frac{3}{4} e_{k+1}^2 - e_k^2 + \frac{1}{4} e_{k-1}^2 + \frac{1}{2} (e_{k+1} - e_k)^2 - \frac{1}{2} (e_k - e_{k-1})^2 \right) dx \\ = e_1^2 + \frac{3}{4} e_m^2 - \frac{3}{4} e_1^2 - \frac{1}{4} e_{m-1}^2 + \frac{1}{4} e_0^2 + \frac{1}{2} (e_m - e_{m-1})^2 - \frac{1}{2} (e_1 - e_0)^2 \\ = \frac{3}{4} e_m^2 - \frac{1}{4} e_{m-1}^2 - \frac{1}{4} e_1^2 + \frac{1}{2} (e_m - e_{m-1})^2 \\ \geq \frac{3}{4} e_m^2 - \frac{1}{4} e_{m-1}^2 - \frac{1}{4} e_1^2.$$

For the third integral in (37), we employ the monotonicity of the operator A . In fact, it is proved in [26, Lemma 3.5] that for positive functions $w_1, w_2 \in H^4(\mathbb{T}^d)$,

$$\int_{\mathbb{T}^d} (A(w_1) - A(w_2))(w_1 - w_2) dx = \int_{\mathbb{T}^d} \frac{1}{w_1 w_2} \left| \operatorname{div} \left(w_1^2 \nabla \left(\frac{w_1 - w_2}{w_1} \right) \right) \right|^2 dx \geq 0.$$

The right-hand side of (37) is estimated by Young's inequality:

$$\int_{\mathbb{T}^d} f_0 e_1 dx \leq 2 \|f_0\|_{L^2(\mathbb{T}^d)}^2 + \frac{1}{8} \|e_1\|_{L^2(\mathbb{T}^d)}^2, \\ \int_{\mathbb{T}^d} f_k e_{k+1} dx \leq \frac{1}{2\tau} \|f_k\|_{L^2(\mathbb{T}^d)}^2 + \frac{\tau}{2} \|e_{k+1}\|_{L^2(\mathbb{T}^d)}^2, \quad k \geq 1.$$

Summarizing the above estimates and taking into account (33) and (34), we find that

$$\begin{aligned} \frac{3}{4} \|e_m\|_{L^2(\mathbb{T}^d)}^2 &\leq \frac{1}{4} \|e_{m-1}\|_{L^2(\mathbb{T}^d)}^2 + \frac{1}{4} \|e_1\|_{L^2(\mathbb{T}^d)}^2 + 2 \|f_0\|_{L^2(\mathbb{T}^d)}^2 + \frac{1}{8} \|e_1\|_{L^2(\mathbb{T}^d)}^2 \\ &\quad + \frac{1}{2\tau} \sum_{k=1}^{m-1} \|f_k\|_{L^2(\mathbb{T}^d)}^2 + \frac{\tau}{2} \sum_{k=1}^{m-1} \|e_{k+1}\|_{L^2(\mathbb{T}^d)}^2 \\ &\leq \frac{1}{4} \|e_{m-1}\|_{L^2(\mathbb{T}^d)}^2 + \frac{3}{8} \|e_1\|_{L^2(\mathbb{T}^d)}^2 + C\tau^4 + \frac{\tau}{2} \sum_{k=2}^m \|e_k\|_{L^2(\mathbb{T}^d)}^2, \end{aligned}$$

where $C > 0$ depends on the $L^2(0, T; L^2(\mathbb{T}^d))$ norm of v_{ttt} and the $L^\infty(0, T; L^2(\mathbb{T}^d))$ norm of v_{tt} but not on τ . Taking the maximum over $m = 1, \dots, M$, we infer that

$$\frac{3}{4} \max_{m=1, \dots, M} \|e_m\|_{L^2(\mathbb{T}^d)}^2 \leq \frac{5}{8} \max_{m=1, \dots, M} \|e_{m-1}\|_{L^2(\mathbb{T}^d)}^2 + C\tau^4 + \frac{\tau}{2} \sum_{k=2}^M \|e_k\|_{L^2(\mathbb{T}^d)}^2.$$

The first term on the right-hand side is controlled by the left-hand side, leading to

$$\|e_M\|_{L^2(\mathbb{T}^d)}^2 \leq \max_{m=1, \dots, M} \|e_m\|_{L^2(\mathbb{T}^d)}^2 \leq 8C\tau^4 + 4\tau \sum_{k=2}^M \|e_k\|_{L^2(\mathbb{T}^d)}^2.$$

We separate the last summand in the sum,

$$(1 - 4\tau) \|e_M\|_{L^2(\mathbb{T}^d)}^2 \leq 8C\tau^4 + 4\tau \sum_{k=2}^{M-1} \|e_k\|_{L^2(\mathbb{T}^d)}^2,$$

and apply the inequality $1 + x \leq e^x$ for all $x \geq 0$ and the discrete Gronwall lemma (see, e.g., [30, Theorem 4]):

$$\|e_M\|_{L^2(\mathbb{T}^d)}^2 \leq \frac{8C\tau^4}{1 - 4\tau} \left(1 + \frac{4\tau}{1 - 4\tau}\right)^{M-2} \leq \frac{8C\tau^4}{1 - 4\tau} \exp\left(\frac{4t_{M-2}}{1 - 4\tau}\right) \leq 16C\tau^4 \exp(8t_{M-2}).$$

The result follows for all $0 < \tau < 1/8$ with the constant $4\sqrt{C} \exp(4T)$, where $T > 0$ is the terminal time. \square

3. FULLY DISCRETE VARIATIONAL DERIVATIVE METHOD

In this section, we explore the variational structure of the DLSS equation on a discrete level, using the discrete variational derivative method of [13]. In order to explain the idea, we consider first the implicit Euler discretization.

Let $x_i = ih$, $i = 0, \dots, N - 1$, be an equidistant grid on the one-dimensional torus $\mathbb{T} \cong [0, 1)$, let $t_k = k\tau$ with $\tau > 0$, and let U_i^k approximate $n(t_k, x_i)$. Set $U^k = (U_0^k, \dots, U_{N-1}^k) \in \mathbb{R}^N$ and $U_\ell = U_{\ell \bmod N}$ for all $\ell \in \mathbb{Z}$. We introduce the following difference operators for $U = (U_i) \in \mathbb{R}^N$:

$$\begin{aligned}
\text{forward difference:} & \quad \delta_i^+ U = h^{-1}(U_{i+1} - U_i), \\
\text{backward difference:} & \quad \delta_i^- U = h^{-1}(U_i - U_{i-1}), \\
\text{central difference:} & \quad \delta_i^{(1)} U = (2h)^{-1}(U_{i+1} - U_{i-1}), \\
\text{second-order central difference:} & \quad \delta_i^{(2)} U = \delta_i^+ \delta_i^- U = \delta_i^- \delta_i^+ U.
\end{aligned}$$

The first step is to define the discrete Fisher information. We choose a symmetric form for the derivative, $v_x^2(x_i) \approx \frac{1}{2}((\delta_i^+ V)^2 + (\delta_i^- V)^2)$, where $V = (V_i) = (\sqrt{U_i}) \in \mathbb{R}^N$. The Fisher information $F[v^2] = \int_{\mathbb{T}} v_x^2 dx$ is approximated by using the first-order quadrature rule $\int_{\mathbb{T}} w(x) dx \approx \sum_{i=0}^{N-1} w(x_i)h$. Actually, this rule is of second order $O(h^2)$ here, since due to the periodic boundary conditions, it coincides with the trapezoidal rule, $(w(x_0) + w(x_N))h/2 + \sum_{i=1}^{N-1} w(x_i)h$. Therefore, the discrete Fisher information reads as

$$F_d[U] = \frac{1}{2} \sum_{i=0}^{N-1} ((\delta_i^+ V)^2 + (\delta_i^- V)^2)h, \quad U = (U_i) \in \mathbb{R}^N.$$

The second step is the definition of the discrete variational derivative. Applying the discrete variation procedure and using summation by parts (see [13, Prop. 3.2]), we calculate

$$\begin{aligned}
(38) \quad F_d[U^{k+1}] - F_d[U^k] &= \frac{1}{2} \sum_{i=0}^{N-1} ((\delta_i^+ V^{k+1})^2 - (\delta_i^+ V^k)^2 + (\delta_i^- V^{k+1})^2 - (\delta_i^- V^k)^2) h \\
&= \frac{1}{2} \sum_{i=0}^{N-1} [\delta_i^+ (V^{k+1} + V^k) \delta_i^+ (V^{k+1} - V^k) \\
&\quad + \delta_i^- (V^{k+1} + V^k) \delta_i^- (V^{k+1} - V^k)] h \\
&= - \sum_{i=0}^{N-1} \delta_i^{(2)} (V^{k+1} + V^k) (V_i^{k+1} - V_i^k) h \\
&= - \sum_{i=0}^{N-1} \frac{\delta_i^{(2)} (V^{k+1} + V^k)}{V_i^{k+1} + V_i^k} (U_i^{k+1} - U_i^k) h, \quad k \geq 0.
\end{aligned}$$

This motivates the definition of the discrete variational derivative

$$(39) \quad \frac{\delta F_d}{\delta(U^{k+1}, U^k)_i} = - \frac{\delta_i^{(2)} (V^{k+1} + V^k)}{V_i^{k+1} + V_i^k}, \quad i = 0, \dots, N-1,$$

since this implies the discrete chain rule

$$F_d[U^{k+1}] - F_d[U^k] = \sum_{i=0}^{N-1} \frac{\delta F_d}{\delta(U^{k+1}, U^k)_i} (U_i^{k+1} - U_i^k) h.$$

Observe that (39) is a Crank-Nicolson type approximation of the variational derivative $\delta F[n]/\delta n = -(\sqrt{n})_{xx}/\sqrt{n} = -v_{xx}/v$, where $n = v^2$. The implicit Euler discrete variational derivative (DVD) method for the DLSS equation is then given by the nonlinear system

with unknowns $U^{k+1} = (V^{k+1})^2$:

$$(40) \quad \frac{1}{\tau}(U_i^{k+1} - U_i^k) = \delta_i^{(1)} \left(U^{k+1} \delta_i^{(1)} \left(\frac{\delta F_d}{\delta(U^{k+1}, U^k)} \right) \right), \quad i = 0, \dots, N-1, \quad k \geq 0.$$

The initial condition n_0 is approximated by its projection on the discrete grid, defining the starting vector $U^0 \in \mathbb{R}^N$. Multiplying the above scheme by $\delta F_d / \delta(U^{k+1}, U^k)_i$, summing over $i = 0, \dots, N-1$, and employing the discrete chain rule (38), we infer the discrete dissipation property

$$(41) \quad \frac{1}{\tau}(F_d[U^{k+1}] - F_d[U^k]) + \sum_{i=0}^{N-1} U_i^{k+1} \left(\delta_i^{(1)} \left(\frac{\delta F_d}{\delta(U^{k+1}, U^k)} \right) \right)^2 h = 0.$$

In fact, this proves the monotonicity of the discrete Fisher information for $q = 1$.

Remark 8. Observe that we could have taken a different approximation for the discrete Fisher information, e.g. $\tilde{F}_d[U] = \sum_{i=0}^{N-1} (\delta_i^{(1)} V)^2 h$. This would lead to a different variational derivative $\delta \tilde{F}_d / \delta(U^{k+1}, U^k)$ and eventually to a another scheme (40), with F_d replaced by \tilde{F}_d , which dissipates \tilde{F}_d instead. Besides the symmetry, which brings the second-order consistency in space, the above choice of the discrete Fisher information is motivated by the fact that $\delta_i^+ \delta_i^- = \delta_i^{(2)}$, used in the discrete variation procedure. \square

In the following, we consider temporally higher-order discretizations. There are several ways to generalize the above DVD method. In order to stay in the spirit of Section 2, we derive higher-order DVD methods, which are based on backward differentiation formulas. The function $f(\xi, \eta) = (\xi^2 + \eta^2)/2$ represents both the Fisher information $F[n] = \int_{\mathbb{T}} f(v_x, v_x) dx$ and the discrete Fisher information $F_d[U] = \sum_{i=0}^{N-1} f(\delta_i^+ V, \delta_i^- V) h$. The definition of f is motivated by the following formal representation of the variational derivative,

$$\frac{\delta F[n]}{\delta n} = -\frac{v_{xx}}{v} = -\frac{1}{2v} \left(\partial_x \partial_\xi f|_{\xi=v_x} + \partial_x \partial_\eta f|_{\eta=v_x} \right).$$

This formula gives an idea how to approximate the variational derivative in general. We denote by $\delta_k^{1,q}$ the q -th step BDF operator at time t_k . For instance, the formulas for $q = 1$ and $q = 2$ are given in (15) and (16), respectively. The discrete variational derivative of order q is defined componentwise by

$$(42) \quad \frac{\delta F_d}{\delta(U^{k+1}, \dots, U^{k-q+1})_i} = -\frac{1}{2V_i^{k+1}} \left(\delta_i^- (\partial_\xi^d f) + \delta_i^+ (\partial_\eta^d f) \right), \quad k \geq q-1,$$

where the discrete operators $\partial_\xi^d f$ and $\partial_\eta^d f$ are given by

$$\begin{aligned} (\partial_\xi^d f)_i &= \partial_\xi f|_{\xi=\delta_i^+ V^{k+1}} + r_{\text{corr}} \delta_{k+1}^{1,q} (\delta_i^+ U^{k+1}) = \delta_i^+ V^{k+1} + r_{\text{corr}} \delta_{k+1}^{1,q} (\delta_i^+ U^{k+1}), \\ (\partial_\eta^d f)_i &= \partial_\eta f|_{\eta=\delta_i^- V^{k+1}} + r_{\text{corr}} \delta_{k+1}^{1,q} (\delta_i^- U^{k+1}) = \delta_i^- V^{k+1} + r_{\text{corr}} \delta_{k+1}^{1,q} (\delta_i^- U^{k+1}), \end{aligned}$$

and r_{corr} is a correction term, which has to be determined in such a way that the discrete chain rule

$$\delta_{k+1}^{1,q} F_d[U^{k+1}] = \sum_{i=0}^{N-1} \frac{\delta F_d}{\delta(U^{k+1}, \dots, U^{k-q+1})_i} \delta_{k+1}^{1,q} U_i^{k+1} h$$

holds. The role of the correction term is not only to satisfy the discrete chain rule but also to increase the temporal accuracy of the discrete variational derivative. Straightforward computations with the above expressions using summation by parts formulas and periodic boundary conditions yield

$$(43) \quad \frac{\delta F_d}{\delta(U^{k+1}, \dots, U^{k-q+1})_i} = -\frac{\delta_i^{(2)} V^{k+1}}{V_i^{k+1}} - r_{\text{corr}} \frac{\delta_{k+1}^{1,q} \delta_i^{(2)} U^{k+1}}{V_i^{k+1}}, \quad k \geq q-1,$$

$$(44) \quad r_{\text{corr}} = \frac{\delta_{k+1}^{1,q} F_d[U^{k+1}] - \sum_{i=0}^{N-1} \delta_i^+ V^{k+1} \delta_i^+ \left(\frac{\delta_{k+1}^{1,q} U^{k+1}}{V^{k+1}} \right) h}{\sum_{i=0}^{N-1} (\delta_i^+ \delta_{k+1}^{1,q} U^{k+1}) \delta_i^+ \left(\frac{\delta_{k+1}^{1,q} U^{k+1}}{V^{k+1}} \right) h}.$$

We note that for $q = 1$, this definition generally does not coincide with the discrete variational derivative (39). The temporally BDF q discrete variational derivative (BDF q DVD) method is then defined by the following nonlinear system in the unknowns $U^{k+1} = (V^{k+1})^2$:

$$(45) \quad \delta_{k+1}^{1,q} U_i^{k+1} = \delta_i^{(1)} \left(U^{k+1} \delta_i^{(1)} \left(\frac{\delta F_d}{\delta(U^{k+1}, \dots, U^{k-q+1})} \right) \right), \quad i = 0, \dots, N-1, \quad k \geq q-1.$$

In particular, for $q = 1$, we obtain two methods: the BDF1 DVD scheme (45) and the DVD scheme (40).

Proof of Theorem 4. Let $n = v^2$ be a smooth positive solution to (1) with $d = 1$. According to [2], such a solution exists at least in a small time interval if the initial datum is smooth and positive. Furthermore, let $q \in \mathbb{N}$, $q \geq 2$ (and typically $q \leq 6$), be the order of the backward differentiation formula.

First, we consider the discrete variational derivative (39). A Taylor expansion around (t_{k+1}, x_i) yields

$$\begin{aligned} \frac{\delta F_d}{\delta(n(t_{k+1}), n(t_k))} \Big|_{x=x_i} &= -\frac{\delta_i^{(2)} (v(t_{k+1}, x_i) + v(t_k, x_i))}{v(t_{k+1}, x_i) + v(t_k, x_i)} = \frac{v_{xx}}{v}(t_{k+1}, x_i) + O(\tau) + O(h^2) \\ &= \frac{\delta F}{\delta n}[n](t_{k+1}, x_i) + O(\tau) + O(h^2), \end{aligned}$$

where $i = 0, \dots, N-1$, $k \geq 0$. Similarly,

$$\delta_i^{(1)} \left(n(t_{k+1}) \delta_i^{(1)} \left(\frac{\delta F_d}{\delta(n(t_{k+1}), n(t_k))} \right) \right) \Big|_{x=x_i} = \left(n \left(\frac{\delta F[n]}{\delta n} \right) \right)_x (t_{k+1}, x_i) + O(\tau) + O(h^2).$$

Thus, the local truncation error of the right-hand side in (39) is of order $O(\tau) + O(h^2)$. Since the left-hand side is of order $O(\tau)$ in time and exact at spatial grid points x_i , the local truncation error of scheme (39) is of order $O(\tau) + O(h^2)$. The monotonicity of the discrete Fisher information is shown in (41).

The mass conservation is an obvious consequence of the scheme. To prove the uniform boundedness, we observe that, by the discrete H^1 -seminorm,

$$\sum_{i=0}^{N-1} (\delta_i^+ V^k)^2 h \leq F_d[U^0] < \infty \quad \text{for all } k \geq 1.$$

Then, according to the discrete Poincaré-Wirtinger inequality, for $i = 0, \dots, N-1$, $k \geq 1$, [13, Lemma 3.3],

$$|V_i^k - M_k|^2 \leq \sum_{i=0}^{N-1} (\delta_i^+ V^k)^2 h \leq F_d[U^0]$$

with $M_k = \sum_{i=0}^{N-1} V_i^k h$. Jensen's inequality for the quadratic function and the mass conservation property of the method give $M_k \leq 1$ for all $k \geq 0$. Finally, by the triangle inequality, $|V_i^k| \leq F_d[U^0]^{1/2} + 1$ and thus, $|U_i^k| \leq 2F_d[U^0] + 2$.

Next, we consider scheme (45) with the discrete variational derivative (43). By construction, the left-hand side of (43) is of order q in time and exact at the spatial grid points x_i . Thus, it remains to prove that the right-hand side is of order $(q, 2)$ with respect to time-space discretization.

Taylor expansions show, with a slight abuse of notation, that

$$(46) \quad \delta_i^\pm v(t_{k+1}, x_i) = v_x(t_{k+1}, x_i) \pm \frac{h}{2} v_{xx}(t_{k+1}, x_i) + O(h^2),$$

$$(47) \quad -\frac{\delta_i^{(2)} v(t_{k+1}, x_i)}{v(t_{k+1}, x_i)} = -\frac{v_{xx}}{v}(t_{k+1}, x_i) + O(h^2),$$

$$(48) \quad \frac{\delta_{k+1}^{1,q} \delta_i^{(2)} n(t_{k+1}, x_i)}{v(t_{k+1}, x_i)} = \frac{n_{txx}}{v}(t_{k+1}, x_i) + O(\tau^q) + O(h^2),$$

$$(49) \quad \delta_i^\pm \delta_{k+1}^{1,q} n(t_{k+1}, x_i) = n_{tx}(t_{k+1}, x_i) \pm \frac{h}{2} n_{txx}(t_{k+1}, x_i) + O(\tau^q) + O(h^2),$$

$$(50) \quad \delta_i^\pm \left(\frac{\delta_{k+1}^{1,q} n(t_{k+1}, x_i)}{v(t_{k+1}, x_i)} \right) = 2v_{tx}(t_{k+1}, x_i) \pm hv_{txx}(t_{k+1}, x_i) + O(\tau^q) + O(h^2).$$

We prove that r_{corr} is of order $(q, 2)$. Let r_n and r_d denote the numerator and denominator of r_{corr} , respectively, replacing V_i^{k+1} by $v(t_{k+1}, x_i)$ and U_i^{k+1} by $n(t_{k+1}, x_i)$. Taking into account the periodic boundary conditions, we find that

$$\begin{aligned} & \sum_{i=0}^{N-1} (\delta_i^+ \delta_{k+1}^{1,q} n(t_{k+1}, x_i)) \delta_i^+ \left(\frac{\delta_{k+1}^{1,q} n(t_{k+1}, x_i)}{v(t_{k+1}, x_i)} \right) h \\ &= \sum_{i=0}^{N-1} (\delta_i^- \delta_{k+1}^{1,q} n(t_{k+1}, x_i)) \delta_i^- \left(\frac{\delta_{k+1}^{1,q} n(t_{k+1}, x_i)}{v(t_{k+1}, x_i)} \right) h. \end{aligned}$$

Therefore, we can split r_d into two parts:

$$\begin{aligned} r_d &= \frac{1}{2} \sum_{i=0}^{N-1} \left[(\delta_i^+ \delta_{k+1}^{1,q} n(t_{k+1}, x_i)) \delta_i^+ \left(\frac{\delta_{k+1}^{1,q} n(t_{k+1}, x_i)}{v(t_{k+1}, x_i)} \right) \right. \\ &\quad \left. + (\delta_i^- \delta_{k+1}^{1,q} n(t_{k+1}, x_i)) \delta_i^- \left(\frac{\delta_{k+1}^{1,q} n(t_{k+1}, x_i)}{v(t_{k+1}, x_i)} \right) \right] h. \end{aligned}$$

In view of (49)-(50), it follows that

$$r_d = 2 \sum_{i=0}^{N-1} (n_{tx} v_{tx})(t_{k+1}, x_i) h + O(\tau^q) + O(h^2).$$

The numerator r_n is treated in a similar way. Using (46), the first term in r_n can be written as

$$\begin{aligned} \delta_{k+1}^{1,q} F_d[n(t_{k+1})] &= \frac{1}{2} \frac{d}{dt} \sum_{i=0}^{N-1} ((\delta_i^+ v(t, x_i))^2 + (\delta_i^- v(t, x_i))^2) h \Big|_{t=t_{k+1}} + O(\tau^q) \\ &= \sum_{i=0}^{N-1} (v_x v_{xt})(t_{k+1}, x_i) h + O(\tau^q) + O(h^2). \end{aligned}$$

For the second term in r_n , we observe that, because of the periodic boundary conditions,

$$\sum_{i=0}^{N-1} \delta_i^+ v(t_{k+1}, x_i) \delta_i^+ \left(\frac{\delta_{k+1}^{1,q} n(t_{k+1}, x_i)}{v(t_{k+1}, x_i)} \right) h = \sum_{i=0}^{N-1} \delta_i^- v(t_{k+1}, x_i) \delta_i^- \left(\frac{\delta_{k+1}^{1,q} n(t_{k+1}, x_i)}{v(t_{k+1}, x_i)} \right) h,$$

and hence, employing (46) and (50),

$$\begin{aligned} \sum_{i=0}^{N-1} \delta_i^+ v(t_{k+1}, x_i) \delta_i^+ \left(\frac{\delta_{k+1}^{1,q} n(t_{k+1}, x_i)}{v(t_{k+1}, x_i)} \right) h &= \frac{1}{2} \sum_{i=0}^{N-1} \left[\delta_i^+ v(t_{k+1}, x_i) \delta_i^+ \left(\frac{\delta_{k+1}^{1,q} n(t_{k+1}, x_i)}{v(t_{k+1}, x_i)} \right) \right. \\ &\quad \left. + \delta_i^- v(t_{k+1}, x_i) \delta_i^- \left(\frac{\delta_{k+1}^{1,q} n(t_{k+1}, x_i)}{v(t_{k+1}, x_i)} \right) \right] h \\ &= 2 \sum_{i=0}^{N-1} (v_x v_{xt})(t_{k+1}, x_i) h + O(\tau^q) + O(h^2). \end{aligned}$$

Summarizing these identities yields $r_{\text{corr}} = O(\tau^q) + O(h^2)$. Finally, (47)-(48) imply that

$$\begin{aligned} \frac{\delta F_d}{\delta(n(t_{k+1}), \dots, n(t_{k+1-q}))} \Big|_{x=x_i} &= -\frac{\delta_i^{(2)} v(t_{k+1}, x_i)}{v(t_{k+1}, x_i)} - r_{\text{corr}} \frac{\delta_{k+1}^{1,q} \delta_i^{(2)} n(t_{k+1}, x_i)}{v(t_{k+1}, x_i)} \\ &= \frac{\delta F[n]}{\delta n}(t_{k+1}, x_i) + O(\tau^q) + O(h^2). \end{aligned}$$

This shows that the discrete variational derivative (43) is of order q in time, finishing the proof. \square

4. NUMERICAL EXAMPLES

In this section, we present some numerical examples which illustrate the decay properties of the entropy functionals and Fisher information as well as the convergence properties of the schemes presented in the previous sections.

4.1. BDF2 finite-difference scheme. The DLSS equation (2) is approximated by the BDF2 method in time and central finite differences in space. The scheme is given by the following nonlinear system with unknowns $V_i^k = (U_i^k)^{\alpha/2}$: For $i = 0, \dots, N-1$ and $k = 1$,

$$(V_i^1)^{2/\alpha-1}(V_i^1 - V_i^0) + \tau \delta_i^{(2)} \left((V_i^1)^{2/\alpha} \delta_i^{(2)} \log V_i^1 \right) = 0$$

and for $i = 0, \dots, N-1$, $k \geq 2$,

$$(V_i^{k+1})^{2/\alpha-1} \left(\frac{3}{2} V_i^{k+1} - 2V_i^k + \frac{1}{2} V_i^{k-1} \right) + \tau \delta_i^{(2)} \left((V_i^{k+1})^{2/\alpha} \delta_i^{(2)} \log V_i^{k+1} \right) = 0.$$

The initial datum (V_i^0) is given by $(n_0(x_i)^{\alpha/2})$. For $k = 1$, the scheme corresponds to the implicit Euler discretization, needed to initialize the BDF2 scheme for $k \geq 2$. The above nonlinear system, with periodic boundary conditions, is solved using the Newton method.

We choose the initial datum $n_0(x) = 0.001 + \cos^{16}(\pi x)$, $x \in [0, 1]$. The spatial mesh size is $h = 0.005$ ($N = 200$) and the time step $\tau = 10^{-6}$. The (continuous) entropies $E_\alpha[n]$ are dissipated for $1 \leq \alpha < 3/2$. Figure 1 (a) illustrates the stability and, in fact, decay of the discrete entropies $E_{\alpha,d}$, defined below, for various values of α . Although Theorem 1 does not provide a stability estimate for $\alpha = 1$, the numerical results indicate that the discrete entropy $E_{1,d}[U] = \sum_{i=0}^{N-1} (U_i(\log U_i - 1) + 1)h$ is decreasing. Figure 1 (b) shows that the decay of the discrete relative entropy is exponential, and even the discrete Fisher information converges exponentially fast to zero. Here, the discrete relative entropy is defined by

$$E_{\alpha,d}^{rel}[U^k] = E_{\alpha,d}[U^k] - E_{\alpha,d}[\bar{U}], \quad \text{where } E_{\alpha,d}[U^k] = \sum_{i=0}^{N-1} (U_i^k)^\alpha h, \quad \bar{U} = \sum_{i=0}^{N-1} U_i^k h.$$

According to Theorem 3, the semi-discrete BDF2 scheme converges in second order if $\alpha = 1$. This may be not the case for the fully discrete scheme, since the discretization may destroy the monotonicity structure of the spatial operator. However, Figure 2 shows that the numerical convergence rate is close to 2, even for $\alpha \neq 1$. The numerical convergence rates cr have been obtained by the linear regression method. The convergence of the method is measured in the discrete ℓ^2 -norm

$$\|e_m\|_2 := \left(\sum_{i=0}^{N-1} (V_{\text{ex},i}^m - V_i^m)^2 h \right)^{1/2},$$

and the numerical solutions are compared at time $t = 5 \cdot 10^{-5}$. Here, the ‘‘exact’’ solution $V_{\text{ex},i}^m$ is computed by the above scheme using the very small time step $\tau = 10^{-10}$.

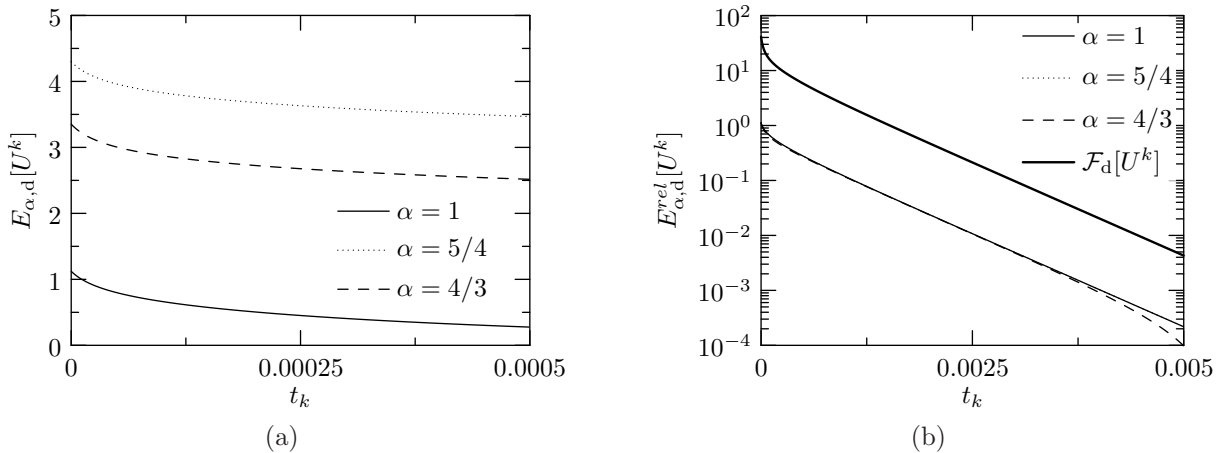


FIGURE 1. (a) Entropy stability (decay) for the BDF2 finite-difference scheme. (b) Exponential decay of the discrete relative entropy and the discrete Fisher information for the BDF2 finite-difference scheme.

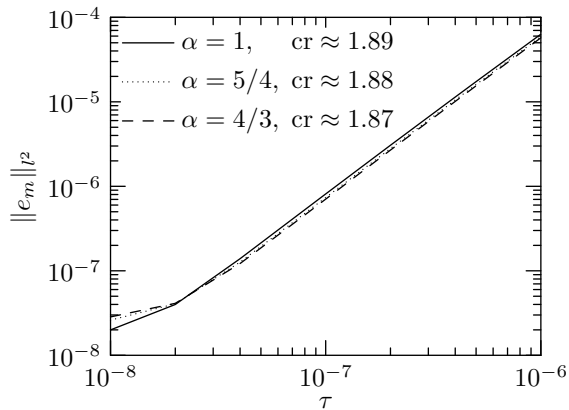


FIGURE 2. Temporal convergence of the BDF2 finite-difference scheme for various values of α ; the convergence rate is denoted by cr .

4.2. Discrete variational derivative method. We present some numerical results obtained from the DVD and BDF q DVD schemes derived in Section 3. The initial datum and the numerical parameters are chosen as in previous subsection. In order to solve the discrete nonlinear systems, we employed here the NAG toolbox routine `c05nb`, which is based on a modification of the Powell hybrid method. It turned out that this routine is at least three times faster than the standard MATLAB routine `fsolve`.

In Figure 3, the temporal evolution of the discrete relative entropies $E_{\alpha}^{\text{rel}}[U^k]$ and the discrete Fisher information $F_d[U^k]$ are depicted for (a) the implicit Euler scheme (40) and (b) the BDF2 scheme (45). We observe that the decay is in all cases exponential. This holds also true for the BDF3 scheme (results not shown).

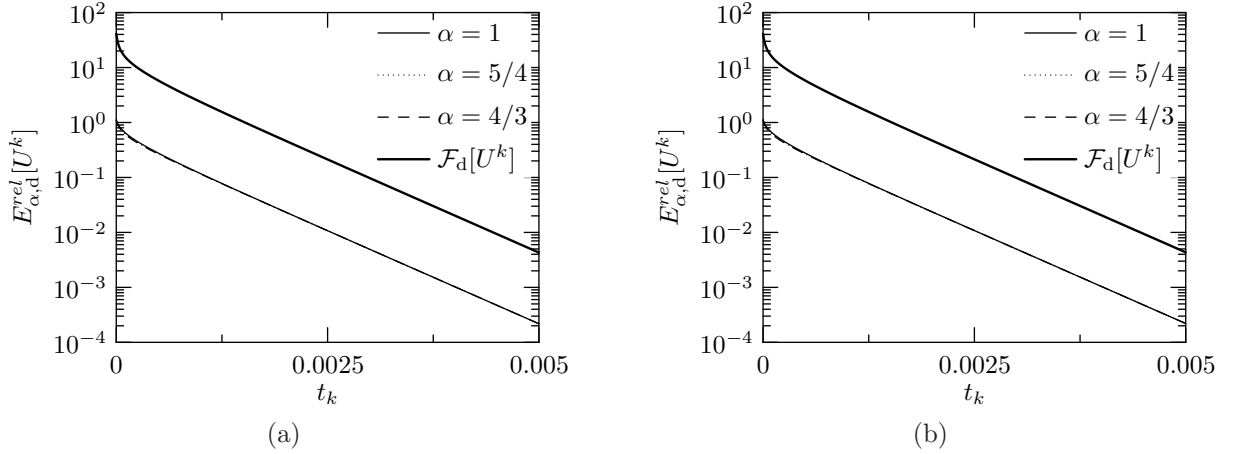


FIGURE 3. Exponential decay of the discrete Fisher information and relative entropies using (a) the DVD scheme and (b) the BDF2 DVD scheme.

Next, we test numerically the convergence in time of the DVD scheme. Figure 4 illustrates the ℓ^2 -errors of the methods. We have chosen the mesh size $h = 0.01$, and we compared the numerical solutions at time $t_m = 5 \cdot 10^{-5}$. The “exact” solutions are computed by the respective method taking the time step $\tau = 10^{-9}$. The numerical convergence rates, computed by the linear regression method, are given in Table 1. We note that the BDF3 DVD scheme gives only slightly better results than the BDF2 DVD scheme. The reason is that the first step is initialized by the first-order scheme (40), and this initialization error cannot be compensated by the higher-order accuracy of the local approximation. In order to obtain a third-order scheme, we need to initialize the scheme with a second-order discretization.

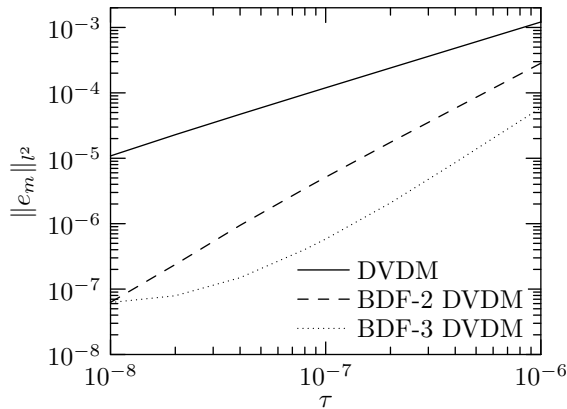


FIGURE 4. Temporal convergence of the DVD, BDF2 DVD, and BDF3 DVD schemes.

Scheme	Convergence rate
DVD	1.020
BDF2 DVD	1.824
BDF3 DVD	1.977

TABLE 1. Numerical temporal convergence rates for the discrete variational derivative methods.

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