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Complex pattern formation governed by a Cahn–Hilliard–Swift–Hohenberg system: Analysis and numerical simulations

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Abstract

This paper investigates a Cahn–Hilliard–Swift–Hohenberg system, focusing on a three-species chemical mixture subject to physical constraints on volume fractions. The resulting system leads to complex patterns involving a separation into phases as typical of the Cahn–Hilliard equation and small scale stripes and dots as seen in the Swift–Hohenberg equation. We introduce singular potentials of logarithmic type to enhance the model's accuracy in adhering to essential physical constraints. The paper establishes the existence and uniqueness of weak solutions within this extended framework. The insights gained contribute to a deeper understanding of phase separation in complex systems, with potential applications in materials science and related fields. We introduce a stable finite element approximation based on an obstacle formulation. Subsequent numerical simulations demonstrate that the model allows for complex structures as seen in pigment patterns of animals and in porous polymeric materials.

Keywords: Cahn–Hilliard–Swift–Hohenberg equation, phase separation, pattern formation, materials science, singular potentials, well-posedness, numerical simulations.

AMS (MOS) Subject Classification: 35K55, 35K61, 74N05, 82D25.

1 Introduction

Pattern formation, particularly in biological systems, often arises through complex interactions between various processes occurring at multiple length and time scales. The seminal works of Turing [30], Meinhardt and co-workers [13, 18] provided a methodology to study pattern formation via reaction-diffusion systems. In a multitude of subsequent works, see, e.g., [19, 22, 23, 24, 25, 26] and the references cited therein, inclusion of chemical and mechanical effects through coupling with nonlinear systems permits more accurate descriptions of the chemical-physical processes driving skin pigmentation.

In this work we are interested in a model proposed by Martínez-Agustín et al. [17] that couples a Cahn–Hilliard equation [5] with a Swift–Hohenberg equation [29]. The former is a well-known model in the theory of phase separation and the latter arises as a model in the study of patterns driven by Rayleigh–Bénard convection in fluid thermodynamics. While

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differing in origin from the reaction-diffusion systems mentioned above, the solution dynamics to both the Cahn–Hilliard and Swift–Hohenberg models generate spatial-temporal patterns under appropriate conditions. The intended application for this coupled model in [17] is directed towards capturing the spinodal decomposition of a (charged) polymer-polymer-solvent mixture for the purpose of designing porous polymeric materials with specialized morphologies and pore sizes. In particular, by leveraging the competition between the Cahn–Hilliard and Swift–Hohenberg dynamics, a number of complex morphologies ranging from labyrinth-like patterns, mixtures of dotted and striped phases, to well-packed laminate sheets, as well as tubular hexagonal structures can be realized.

The development of these hierarchically porous structures, with their high surface areas, high pore volume ratios, and high storage capacities, serves to enable new designs for energy storage [31], catalysis [28], sensors [1], separation [16] and adsorption processes [20], see also [32] for an overview. With recent advances in additive manufacturing and 3D printing technologies, such complex and hierarchically structured designs can be rapidly prototyped and deployed in areas such as bone engineering tissues [8], fiber-reinforced composites [9] and organic solar cells [15]. We remark that the the Cahn–Hilliard–Swift–Hohenberg model studied here can also be used for pattern formation in the biological context and our numerical simulations produced configurations similar to those in [23] resembling complex patterns on fish skins.

Let us introduce the model to be studied. In a bounded domain $\Omega \subset \mathbb{R}^d$, $d \in \{2, 3\}$, with boundary $\partial\Omega$, we consider a mixture of two chemical species and a solvent, whose volume fractions are denoted by ϕ_1, ϕ_2, and ψ, respectively. In accordance with their role as volume fractions, we expect the following physically relevant constraints

$$0 \le \phi_1,\ \phi_2,\ \psi \le 1, \quad \phi_1 + \phi_2 + \psi = 1 \quad \text{ for a.e. } (x,t) \in \Omega \times [0,T], \tag{1.1}$$

where $T > 0$ denote a fixed but arbitrary terminal time. It is more convenient to introduce the auxiliary variable $\phi := \phi_1 - \phi_2$, which in turn allows us to express ϕ_1 and ϕ_2 as linear combinations of ψ and ϕ as

$$\phi_1 = \tfrac{1}{2}(1 - \psi + \phi), \quad \phi_2 = \tfrac{1}{2}(1 - \psi - \phi).$$

Then, the physically relevant constraints in (1.1) can be equivalently expressed as $(\phi, \psi) \in \mathcal{K}$ for a.e. $(x,t) \in \Omega \times [0,T]$, with the convex admissible set

$$\mathcal{K} := \{(r,s) \in \mathbb{R}^2 \,:\, r \in [-1,1],\, r + s \le 1,\, s - r \le 1\} \tag{1.2}$$

consisting of the triangular region of $\mathbb{R}^2$ enclosed by the vertices at $(-1,0)$, $(1,0)$ and $(0,1)$ (see Figure 1).

The total *free energy* of the system is given by

$$E(\phi,\psi) = \int_\Omega \frac{\varepsilon}{2}|\nabla\phi|^2 + \frac{\lambda}{2}|(\Delta + \omega^2)(\psi - \tfrac{1}{2})|^2 + F(\phi,\psi) + \sigma\phi\Delta\psi \, dx, \tag{1.3}$$

where $\varepsilon > 0$, $\omega \in \mathbb{R}$, $\lambda > 0$ and $\sigma \in \mathbb{R}$ are fixed constants, Δ denotes the Neumann-Laplacian operator and F denotes a potential function. It will be convenient to split F into a sum of a convex part F_0 and a non-convex part F_1. One example used in previous contributions [17, 22, 23] is

$$\begin{aligned} F_0(\phi,\psi) &= \frac{1}{4}\phi^4 + \frac{1}{4}(\psi - \tfrac{1}{2})^4, \\ F_1(\phi,\psi) &= -\frac{\alpha}{2}\phi^2 - \frac{g}{3}(\psi - \tfrac{1}{2})^3 - \frac{\gamma}{2}(\psi - \tfrac{1}{2})^2 + \frac{\delta}{2}\phi^2(\psi - \tfrac{1}{2}), \end{aligned} \tag{1.4}$$

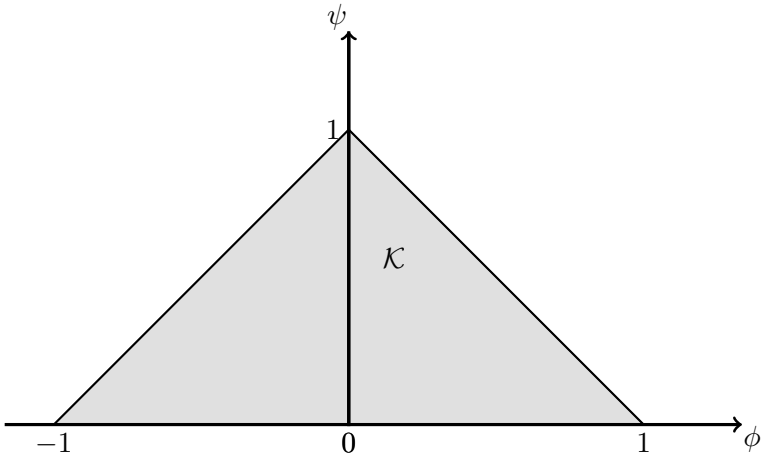

Figure 1: Schematics for the set $\mathcal{K}$ of admissible pairs.

with constants $\alpha \geq 0$, $g \in \mathbb{R}$, $\gamma \geq 0$ and $\delta \in \mathbb{R}$. In contrast to other papers, we use $|(\Delta + \omega^2)(\psi - \frac{1}{2})|^2$ instead of $|(\Delta + \omega^2)\psi|^2$ because we take $\psi = \frac{1}{2}$ as the center for the Swift–Hohenberg variable ψ, instead of $\psi = 0$ in other papers.

Setting $Q := \Omega \times (0, T)$ and $\Sigma := \partial\Omega \times (0, T)$, we consider the following Cahn–Hilliard–Swift–Hohenberg system that was proposed in [17]:

$$\partial_t \phi = \Delta \mu \qquad \text{in } Q, \tag{1.5a}$$

$$\mu = -\varepsilon \Delta \phi + F_{,\phi}(\phi, \psi) + \sigma \Delta \psi \qquad \text{in } Q, \tag{1.5b}$$

$$\partial_t \psi = -z \qquad \text{in } Q, \tag{1.5c}$$

$$z = \lambda(\Delta + \omega^2)^2(\psi - \tfrac{1}{2}) + F_{,\psi}(\phi, \psi) + \sigma \Delta \phi \qquad \text{in } Q, \tag{1.5d}$$

$$\partial_{\boldsymbol{n}} \phi = \partial_{\boldsymbol{n}} \mu = \partial_{\boldsymbol{n}} \psi = \partial_{\boldsymbol{n}} \Delta \psi = 0 \qquad \text{on } \Sigma, \tag{1.5e}$$

$$\phi(0) = \phi_0, \quad \psi(0) = \psi_0 \qquad \text{in } \Omega, \tag{1.5f}$$

where $\partial_{\boldsymbol{n}} f = \nabla f \cdot \boldsymbol{n}$ denotes the normal derivative of the function f at the boundary $\partial\Omega$ with outer unit normal $\boldsymbol{n}$, and $F_{,\phi} := \frac{\partial F}{\partial \phi}$ and $F_{,\psi} := \frac{\partial F}{\partial \psi}$ indicate the partial derivatives of F. We remark that (1.5) as presented here slightly differs from the model in [17] and can be recovered by performing a shift of $\psi - \frac{1}{2} \mapsto \psi$ and setting $\omega = 1$.

We now present some modeling aspects to compare our work with the existing literature. The free energy E can be viewed as a sum of three energetic contributions: the first energetic contribution is a Ginzburg–Landau functional encoding short-range interactions and phase separation of the polymers and one example is

$$E_{\mathrm{GL}}(\phi) = \int_\Omega \frac{\varepsilon}{2} |\nabla \phi|^2 + \frac{1}{4} |\phi|^4 - \frac{\alpha}{2} |\phi|^2 \, dx,$$

the second energetic contribution is a solvent free energy functional accounting for short-range interactions and Coulomb's electrostatic interactions between small charged particles:

$$\begin{aligned} E_{\mathrm{Solvent}}(\phi, \psi) = \int_\Omega & -\frac{\lambda_0}{2} |\nabla(\psi - \tfrac{1}{2})|^2 + \frac{\delta}{2} \phi^2 (\psi - \tfrac{1}{2}) \\ & + \Big(\frac{\lambda \omega^4}{2} (\psi - \tfrac{1}{2})^2 - \frac{g}{3} (\psi - \tfrac{1}{2})^3 - \frac{\gamma}{2} (\psi - \tfrac{1}{2})^2 + \frac{1}{4} (\psi - \tfrac{1}{2})^4 \Big) \, dx, \end{aligned}$$

where the second term represents a coupling between the two scalar fields ϕ and ψ and the last term is a fourth order series expansion of the electrostatic interactions. The

third energetic contribution accounts for the immiscibility between the polymers and the solvent, as well as superficial deformations like bending and stretching:

$$E_{\mathrm{Stretch}}(\phi,\psi) = \int_\Omega \frac{\Lambda}{2}|\nabla(\psi-\tfrac{1}{2})|^2 + \frac{\lambda}{2}|\Delta(\psi-\tfrac{1}{2})|^2 + \sigma\phi\Delta(\psi-\tfrac{1}{2})\,dx$$

with the last term providing a coupling between the polymer order parameter ϕ and a measure of the local curvature $\Delta\psi$, see [17, 22] for further details. Depending on the phase given by the value parameter ϕ, a different sign of the "spontaneous curvature" is preferred. We consider setting $\lambda_0 = \Lambda + 2\lambda$ to obtain the energy functional (2.1) used for the subsequent mathematical analysis, as well as to recover the setting considered in [17, 22]. A significant drawback of smooth potentials such as (1.4) is their inability to ensure that the solutions adhere to the essential physical constraint $(\phi,\psi) \in \mathcal{K}$. One main aim of this work is to address this limitation through the use of suitable singular potentials ensuring the physical validity of the solutions. In particular, instead of the quartic polynomial function F_0 in (1.4), we suggest the singular form

$$F_0(\phi,\psi) = \frac{\theta}{2}\Big[\Pi\Big(\tfrac{1}{2}(1-\psi+\phi)\Big) + \Pi\Big(\tfrac{1}{2}(1-\psi-\phi)\Big) + \Pi(\psi)\Big], \tag{1.6}$$

where $\Pi(s) := s\ln s$ and θ plays the role of the absolute temperature, so that finite values are attained when

$$1-\psi+\phi \geq 0, \quad 1-\psi-\phi \geq 0, \quad \psi \geq 0 \quad \Longleftrightarrow \quad (\phi,\psi) \in \mathcal{K}.$$

In the formal deep quench limit $\theta \to 0$, we arrive at

$$F_0(\phi,\psi) = \mathbb{I}_{\mathcal{K}}(\phi,\psi) = \begin{cases} 0 & \text{if } (\phi,\psi) \in \mathcal{K}, \\ +\infty & \text{otherwise,} \end{cases} \tag{1.7}$$

where $\mathbb{I}_X$ denotes the indicator function of the set X. Our theoretical investigations address potentials $F = F_0 + F_1$ where the convex part F_0 is taken either as the logarithmic function (1.6) or the indicator function (1.7), while the non-convex perturbation F_1 can be taken as in (1.4). We shall henceforth refer to F as the logarithmic potential if F_0 is of the form (1.6) and as the obstacle potential if F_0 is of the form (1.7).

Despite both the Cahn–Hilliard and Swift–Hohenberg are fourth order equations, the former is a H^{-1}-gradient flow while the latter is a L^2-gradient flow of their respective energy functionals. Hence, (1.5) can be interpreted as a $H^{-1} \times L^2$ gradient flow of a suitable energy functional as shown in Section 2.2. In particular, this differs from the conventional multicomponent Cahn–Hilliard systems [10, 11], and it turns out that the situation when considering Swift–Hohenberg equation with singular terms is more involved compared to the second order case with the Allen–Cahn equation. Similarly observed in [6], a weak solution to (1.5) is defined based on a variational inequality for (1.5d). While this is natural if F_0 is the indicator function (1.7), for the logarithmic function (1.6) it is weaker than the conventional variational solutions for similar systems. Nevertheless, our chief result ensures well-posedness to the coupled system (1.5) with either (1.6) or (1.7).

The rest of the paper is organized as follows: in Section 2 we provide a derivation of (1.5) and list the main results, whose proofs can be found in Section 3. We introduce a fully discrete and unconditionally stable numerical scheme in Section 4 and present various numerical simulations showing that the Cahn–Hilliard–Swift–Hohenberg system models complex pattern formation scenarios.

2 Model derivation, main assumptions and results

2.1 Notation

Let Ω be a bounded domain in $\mathbb{R}^d$, where $d \in \{2, 3\}$. The Lebesgue measure of Ω and the Hausdorff measure of $\partial\Omega$ are denoted by $|\Omega|$ and $|\partial\Omega|$, respectively.

For any Banach space X, the norm of X is represented as $\|\cdot\|_X$, its dual space is denoted as X^*, and the duality pairing between X^* and X is given by $\langle\cdot,\cdot\rangle_X$. In the case where X is a Hilbert space, the inner product is denoted by $(\cdot,\cdot)_X$.

For each $1 \le p \le \infty$, $k \ge 0$, and $s > 0$, the standard Lebesgue and Sobolev spaces defined on Ω are denoted as $L^p(\Omega)$, and $W^{k,p}(\Omega)$, with their respective norms $\|\cdot\|_{L^p(\Omega)}$, and $\|\cdot\|_{W^{k,p}(\Omega)}$, respectively. In some instances, we use $\|\cdot\|_{L^p}$ instead of $\|\cdot\|_{L^p(\Omega)}$, and employ a similar shorthand for other norms. We adopt the standard convention $H^k(\Omega) := W^{k,2}(\Omega)$ for all $k \in \mathbb{N}$, and denote the mean value of a function $f \in L^1(\Omega)$ and a functional $h \in H^1(\Omega)^*$ as

$$\langle f\rangle_\Omega := \frac{1}{|\Omega|}\int_\Omega f\,dx, \quad \langle h\rangle_\Omega := \frac{1}{|\Omega|}\langle h, 1\rangle_{H^1}.$$

2.2 Model derivation

As previously mentioned, we consider the following energy functional

$$E(\phi,\psi) = \int_\Omega \frac{\varepsilon}{2}|\nabla\phi|^2 + \frac{\lambda}{2}|(\Delta+\omega^2)(\psi-\tfrac{1}{2})|^2 + F(\phi,\psi) - \sigma\nabla\phi\cdot\nabla\psi\,dx \tag{2.1}$$

with fixed constants $\omega \in \mathbb{R}$, $\lambda > 0$ and $\sigma \in \mathbb{R}$, and in the subsection we take a potential function F which is differentiable. For $m \in \mathbb{R}$, we define

$$H^1(\Omega)_m := \{f \in H^1(\Omega) \,:\, \langle f\rangle_\Omega = m\}, \quad H^1(\Omega)_0^* := \{h \in H^1(\Omega)^* \,:\, \langle h\rangle_\Omega = 0\}$$

and the operator $\mathcal{N} : H^1(\Omega)_0^* \to H^1(\Omega)_0$ defined as the map $h \mapsto \mathcal{N}(h)$ with $\mathcal{N}(h)$ as the solution to the variational equality

$$\int_\Omega \nabla\mathcal{N}(h)\cdot\nabla\zeta\,dx = \langle h,\zeta\rangle_{H^1} \quad \forall\zeta \in H^1(\Omega),$$

which can be interpreted as the inverse Neumann–Laplacian operator. Based on this operator, we consider the inner product

$$\langle (f,h),(\gamma,v)\rangle_{H^1(\Omega)_0^*\times L^2(\Omega)} := \int_\Omega \nabla\mathcal{N}(f)\cdot\nabla\mathcal{N}(\gamma) + hv\,dx \tag{2.2}$$

for $f,\gamma \in H^1(\Omega)_0^*$ and $h,v \in L^2(\Omega)$. We now consider E to be defined on $H^1(\Omega)_m \times H^2_{\boldsymbol{n}}(\Omega)$ with $H^2_{\boldsymbol{n}}(\Omega) := \{f \in H^2(\Omega) \,:\, \partial_{\boldsymbol{n}} f = 0 \text{ on } \partial\Omega\}$. Then, for arbitrary $\zeta \in H^1(\Omega)_0$ and $\eta \in H^2_{\boldsymbol{n}}(\Omega)$, we compute the first variation of E with respect to (ϕ,ψ) in the direction (ζ,η) as

$$\begin{aligned}\frac{\delta E}{\delta(\phi,\psi)}((\phi,\psi))[(\zeta,\eta)] = &\int_\Omega \varepsilon\nabla\phi\cdot\nabla\zeta + F_{,\phi}(\phi,\psi)\zeta - \sigma\nabla\zeta\cdot\nabla\psi\,dx \\ &+ \int_\Omega \lambda(\Delta+\omega^2)(\psi-\tfrac{1}{2})\,(\Delta+\omega^2)\eta - \sigma\nabla\phi\cdot\nabla\eta + F_{,\psi}(\phi,\psi)\eta\,dx.\end{aligned}$$

We aim to identify the gradient of E, expressed as the pair (p,q), with respect to the inner product (2.2). Namely, we are looking for the pair $(p,q) \in H^1(\Omega)_0^* \times L^2(\Omega)$ fulfilling

$$\langle (p,q),(\zeta,\eta)\rangle_{H^1(\Omega)_0^*\times L^2(\Omega)} = \frac{\delta E}{\delta(\phi,\psi)}(\phi,\psi)[(\zeta,\eta)] \quad \text{for every } \zeta \in H^1(\Omega)_0, \eta \in H^2_{\boldsymbol{n}}(\Omega).$$

Then, from the definition of $\mathcal{N}$, we find that

$$\int_\Omega \mathcal{N}(p)\zeta + q\eta\,dx = \int_\Omega \varepsilon\nabla\phi\cdot\nabla\zeta + F_{,\phi}(\phi,\psi)\zeta - \sigma\nabla\psi\cdot\nabla\zeta\,dx \\ + \int_\Omega \lambda(\Delta+\omega^2)(\psi-\tfrac{1}{2})\,(\Delta+\omega^2)\eta - \sigma\nabla\phi\cdot\nabla\eta + F_{,\psi}(\phi,\psi)\eta\,dx.$$

For arbitrary $\widetilde{\zeta}\in H^1(\Omega)$ we insert $\zeta = \widetilde{\zeta} - \langle\widetilde{\zeta}\rangle_\Omega \in H^1(\Omega)_0$ into the above identity, and then performing integration by parts on the right-hand side yields

$$\begin{aligned}&\int_\Omega (\mathcal{N}(p) + \langle F_{,\phi}(\phi,\psi)\rangle_\Omega)\widetilde{\zeta} + q\eta\,dx \\ &\quad= \int_\Omega \Big(-\varepsilon\Delta\phi + F_{,\phi}(\phi,\psi) + \sigma\Delta\psi\Big)\widetilde{\zeta}\,dx + \int_{\partial\Omega}(\varepsilon\partial_{\boldsymbol{n}}\phi - \sigma\partial_{\boldsymbol{n}}\psi)\widetilde{\zeta}\,ds \\ &\qquad+ \int_\Omega \Big(\lambda(\Delta+\omega^2)^2(\psi-\tfrac{1}{2}) + \sigma\Delta\phi + F_{,\psi}(\phi,\psi)\Big)\eta\,dx \\ &\qquad- \int_{\partial\Omega}\Big(\lambda\partial_{\boldsymbol{n}}((\Delta+\omega^2)\psi + \sigma\partial_{\boldsymbol{n}}\phi\Big)\eta\,dS,\end{aligned}$$

for arbitrary $\widetilde{\zeta}\in H^1(\Omega)$, and $\eta\in H^2_{\boldsymbol{n}}(\Omega)$, and we noted that a boundary term of the form $\lambda(\Delta+\omega^2)(\psi-\frac{1}{2})\partial_{\boldsymbol{n}}\eta$ vanished due to the fact that $\eta\in H^2_{\boldsymbol{n}}(\Omega)$. By the fundamental theorem of calculus of variations we have the identifications

$$\begin{aligned}\mu &:= \mathcal{N}(p) + \langle F_{,\phi}(\phi,\psi)\rangle_\Omega = -\varepsilon\Delta\phi + F_{,\phi}(\phi,\psi) + \sigma\Delta\psi,\\ z &:= q = \lambda(\Delta+\omega^2)^2(\psi-\tfrac{1}{2}) + F_{,\psi}(\phi,\psi) + \sigma\Delta\phi,\end{aligned}$$

along with the boundary conditions

$$\partial_{\boldsymbol{n}}\phi = 0,\quad \partial_{\boldsymbol{n}}\psi = 0,\quad \partial_{\boldsymbol{n}}\Delta\psi = 0.$$

Thus, the gradient flow

$$\langle(\partial_t\phi,\partial_t\psi),(\zeta,\eta)\rangle_{H^1(\Omega)_0^*\times L^2(\Omega)} = -\frac{\delta E}{\delta(\phi,\psi)}(\phi,\psi)[(\zeta,\eta)],$$

for arbitrary $\zeta\in H^1(\Omega)_0$ and $\eta\in H^2_{\boldsymbol{n}}(\Omega)$ can be expressed as

$$\begin{aligned}&\int_\Omega \nabla\mathcal{N}(\partial_t\phi)\cdot\nabla\mathcal{N}(\zeta) + \partial_t\psi\eta\,dx \\ &\quad= \int_\Omega \mathcal{N}(\partial_t\phi)\zeta + \partial_t\psi\eta\,dx = \int_\Omega -(\mu - \langle F_{,\phi}(\phi,\psi)\rangle_\Omega)\zeta - z\eta\,dx.\end{aligned}$$

Substituting $\eta = \widetilde{\eta} - \langle\widetilde{\eta}\rangle_\Omega$ for arbitrary $\widetilde{\eta}\in H^1(\Omega)$ then leads to the identification

$$\mathcal{N}(\partial_t\phi) = -\mu + \langle\mu\rangle_\Omega,\quad \partial_t\psi = -z,$$

where by the definition of $\mathcal{N}$ we infer from the first equation:

$$\partial_t\phi = \Delta\mu \quad \text{in } \Omega,\qquad \partial_{\boldsymbol{n}}\mu = 0 \quad \text{on } \partial\Omega.$$

Remark 2.1. *Alternate choices of boundary conditions to* (1.5e) *for similar types of equations can be found in [12, Sec. 9].*

2.3 Assumptions and main results

We make the following assumptions:

(A1) $\Omega \subset \mathbb{R}^d$, $d \in \{2,3\}$, is a bounded domain which is either convex or has $C^{1,1}$ boundary $\partial\Omega$.

(A2) The potential function $F = F_0 + F_1$ is a sum of $F_0 : \mathbb{R}^2 \to [0,\infty)$ taking the form (1.6) or (1.7), while $F_1 \in C^1(\mathcal{K})$.

(A3) The initial conditions satisfy $\phi_0 \in H^1(\Omega)$, $\psi_0 \in H^2_{\boldsymbol{n}}(\Omega)$, with $(\phi_0,\psi_0) \in \mathcal{K}$ for a.e. $x \in \Omega$ and $\langle\phi_0\rangle_\Omega \in (-1,1)$.

In order to introduce an appropriate notion of solution to (1.5) with singular potentials, we first make the following definition.

Definition 2.1 (Admissible function pair)**.**

- *For the logarithmic potential* (1.6)*, we say that a pair of functions* (ζ,η) *is log-admissible if*
$$\pi(\eta)\in L^1(Q), \quad \pi\big(\tfrac{1}{2}(1+\zeta-\eta)\big)\in L^1(Q), \quad \pi\big(\tfrac{1}{2}(1-\zeta-\eta)\big) \in L^1(Q),$$
where $\pi(s) = 1 + \ln s$.
- *For the obstacle potential* (1.7)*, we say that a pair of functions* (ζ,η) *is obstacle-admissible if*
$$(\zeta,\eta) \in \mathcal{K} \quad \text{for a.e. } (x,t) \in Q.$$

Definition 2.2 (Variational solution)**.** *A quadruple of functions* (ϕ,ψ,μ,z) *is a variational solution to* (1.5) *if*

(i) they satisfy the regularities
$$\begin{aligned}
\phi &\in L^\infty(0,T;H^1(\Omega)) \cap L^2(0,T;H^2_{\boldsymbol{n}}(\Omega)) \cap H^1(0,T;(H^1(\Omega))^*),\\
\psi &\in L^\infty(0,T;H^2_{\boldsymbol{n}}(\Omega)) \cap H^1(0,T;L^2(\Omega)),\\
\Delta\psi &\in L^2(0,T;H^1(\Omega)),\\
\mu &\in L^2(0,T;H^1(\Omega)),\\
z &\in L^2(0,T;L^2(\Omega)).
\end{aligned}$$

(ii) The initial conditions are attained: $\phi(0) = \phi_0$ *and* $\psi(0) = \psi_0$ *a.e. in* Ω.

(iii) For a.e. $t \in (0,T)$*, arbitrary* $v \in L^2(Q)$ *and* $u \in L^2(0,T;H^1(\Omega))$*, it holds that*
$$0 = \langle\partial_t\phi, u\rangle_{H^1} + \int_\Omega \nabla\mu\cdot\nabla u\,dx, \tag{2.3a}$$
$$0 = \int_\Omega \partial_t\psi v + zv\,dx. \tag{2.3b}$$

(iv-a) If F_0 *is the logarithmic potential* (1.6)*, then* (ϕ,ψ) *is log-admissible in the sense of Definition 2.1 and for a.e.* $t \in (0,T)$ *and arbitrary log-admissible pair* $(\zeta,\eta) \in (L^2(0,T;H^1(\Omega)))^2$*:*
$$\begin{aligned}
0 \le{}& \int_\Omega \big(F_{0,\phi}(\phi,\psi) + F_{1,\phi}(\phi,\psi) - \mu\big)(\zeta-\phi) + \nabla(\varepsilon\phi - \sigma\psi)\cdot\nabla(\zeta-\phi)\,dx\\
&+ \int_\Omega \big(F_{0,\psi}(\phi,\psi) + F_{1,\psi}(\phi,\psi) - z\big)(\eta-\psi) - \sigma\nabla\psi\cdot\nabla(\eta-\psi)\,dx\\
&+ \int_\Omega \big(2\lambda\omega^2\Delta\psi + \lambda\omega^4(\psi - \tfrac{1}{2})\big)(\eta-\psi) - \lambda\nabla\Delta\psi\cdot\nabla(\eta-\psi)\,dx.
\end{aligned} \tag{2.4}$$

(iv-b) If F_0 is the obstacle potential (1.7)*, then (ϕ,ψ) is obstacle-admissible in the sense of Definition 2.1 and for a.e. $t\in(0,T)$ and arbitrary obstacle-admissible pair $(\zeta,\eta)\in(L^2(0,T;H^1(\Omega))^2$:*

$$\begin{aligned}0\le&\int_\Omega \big(F_{1,\phi}(\phi,\psi)-\mu\big)(\zeta-\phi)+\nabla(\varepsilon\phi-\sigma\psi)\cdot\nabla(\zeta-\phi)\,dx\\&+\int_\Omega \big(F_{1,\psi}(\phi,\psi)-z\big)(\eta-\psi)-\sigma\nabla\psi\cdot\nabla(\eta-\psi)\,dx\\&+\int_\Omega \big(2\lambda\omega^2\Delta\psi+\lambda\omega^4(\psi-\tfrac12)\big)(\eta-\psi)-\lambda\nabla\Delta\psi\cdot\nabla(\eta-\psi)\,dx.\end{aligned}\tag{2.5}$$

Remark 2.2. *The equations* (1.5b) *and* (1.5d) *are formulated together as a variational inequality. For the logarithmic potential* (1.6)*, it turns out that we can show $F_{0,\phi}(\phi,\psi)\in L^2(Q)$ and hence item (iv-a) in Definition 2.2 can be replaced by the requirement that (ϕ,ψ) is log-admissible and satisfies*

$$\mu=-\varepsilon\Delta\phi+F_{0,\phi}(\phi,\psi)+F_{1,\phi}(\phi,\psi)+\sigma\Delta\psi\qquad\text{a.e. in } Q,\tag{2.6}$$

and

$$\begin{aligned}0\le&\int_\Omega \big(F_{0,\psi}(\phi,\psi)+F_{1,\psi}(\phi,\psi)-z\big)(\eta-\psi)-\sigma\nabla\psi\cdot\nabla(\eta-\psi)\,dx\\&+\int_\Omega \big(2\lambda\omega^2\Delta\psi+\lambda\omega^4(\psi-\tfrac12)\big)(\eta-\psi)-\lambda\nabla\Delta\psi\cdot\nabla(\eta-\psi)\,dx\end{aligned}\tag{2.7}$$

holding for a.e. $t\in(0,T)$ and arbitrary $\eta\in L^2(0,T;H^1(\Omega))$ such that (ϕ,η) is log-admissible, i.e., $\pi(\frac12(1+\phi-\eta))\in L^1(Q)$ and $\pi(\frac12(1-\phi-\eta))\in L^1(Q)$.

Our main result is formulated as follows.

Theorem 2.1 (Well-posedness of variational solutions)**.** *Under assumptions* (A1)-(A3)*, there exists a unique variational solution (ϕ,ψ,μ,z) to the system* (1.5) *in the sense of Definition 2.2, and for any pair of variational solutions $\{(\phi_i,\psi_i,\mu_i,z_i)\}_{i=1,2}$ with initial data $\{(\phi_{0,i},\psi_{0,i})\}_{i=1,2}$ fulfilling* (A3)*, there exist a positive constant C independent of their differences $\widehat\phi:=\phi_1-\phi_2$, $\widehat\psi:=\psi_1-\psi_2$, $\widehat\mu:=\mu_1-\mu_2$, $\widehat z=z_1-z_2$, such that*

$$\begin{aligned}&\sup_{t\in(0,T]}\Big(\|\nabla\mathcal{N}\big(\widehat\phi-\langle\widehat\phi\rangle_\Omega\big)(t)\|^2+\|\widehat\psi(t)\|^2\Big)+\int_0^T\|\widehat\phi\|_{H^1}^2+\|\widehat\psi\|_{H^2}^2\,dt\\&\quad\le C\Big(\|\nabla\mathcal{N}\big(\widehat\phi_0-\langle\widehat\phi_0\rangle_\Omega\big)\|^2+\|\widehat\psi_0\|^2\Big).\end{aligned}\tag{2.8}$$

We have the following connection between the logarithmic potential and the obstacle potential.

Theorem 2.2 (Deep quench limit)**.** *For $\theta\in(0,1]$ we denote by $(\phi_\theta,\psi_\theta,\mu_\theta,z_\theta)$ to be a variational solution to* (1.5) *for the logarithmic potential* (1.6) *originating from the initial conditions (ϕ_0,ψ_0) fulfilling* (A3)*. Then, as $\theta\to0$,*

$$\begin{aligned}\phi_\theta&\to\phi_*\quad&&\text{weakly* in } L^\infty(0,T;H^1(\Omega))\cap H^1(0,T;(H^1(\Omega))^*),\\\psi_\theta&\to\psi_*\quad&&\text{weakly* in } L^\infty(0,T;H^2_{\boldsymbol n}(\Omega))\cap H^1(0,T;L^2(\Omega)),\\\mu_\theta&\to\mu_*\quad&&\text{weakly in } L^2(0,T;H^1(\Omega)),\\z_\theta&\to z_*\quad&&\text{weakly in } L^2(0,T;L^2(\Omega)),\end{aligned}$$

where $(\phi_*, \psi_*, \mu_*, z_*)$ *is the unique variational solution to* (1.5) *with obstacle potential* (1.7) *originating from the same initial data. Furthermore, there exists a positive constant* C*, independent of* θ*, such that*

$$\begin{aligned}\sup_{t\in(0,T]} \Big(\|\nabla \mathcal{N}(\phi_*(t) - \phi_\theta(t))\|^2 + \|\psi_*(t) - \psi_\theta(t)\|^2 \Big) \\ + \int_0^T \|\phi_* - \phi_\theta\|_{H^1}^2 + \|\psi_* - \psi_\theta\|_{H^2}^2 \, dt \leq C\theta.\end{aligned} \tag{2.9}$$

3 Mathematical analysis

3.1 Existence of variational solutions

We first treat the case of the logarithmic potential (1.6) and defer the case of the obstacle potential (1.7) to Section 3.3. The first step is to regularize the nonlinearity by formulating an appropriate approximation scheme.

3.1.1 Approximation scheme

For $N \in \mathbb{N}$ we consider the fourth-order Taylor approximation Π_N of Π given by:

$$\Pi_N(s) = \begin{cases} \Pi(s) = s\ln(s) & \text{for } s \geq \frac{1}{N}, \\ \sum_{j=0}^4 \frac{1}{j!}\Pi^{(j)}(\frac{1}{N})(s - \frac{1}{N})^j & \text{for } s \leq \frac{1}{N}. \end{cases} \tag{3.1}$$

We note that there exist a constant $d_1 \geq 0$ such that

$$\Pi_N(s) \geq -d_1 \quad \forall s \in \mathbb{R}. \tag{3.2}$$

Let us now show another useful property that will be used later on.

Lemma 3.1. *Setting* $\pi_N(s) = \Pi_N'(s)$*, for any* $u \in (0,1)$ *there exist constants* $d_2 > 0$*,* $d_3 \geq 0$ *dependent on* u *but independent of* N *such that for* N *sufficiently large,*

$$|\pi_N(s)| \leq d_2 \pi_N(s)(s-u) + d_3 \quad \forall s \in \mathbb{R}. \tag{3.3}$$

Proof. For fixed $u \in (0,1)$ and for all $N > \frac{2}{u}$, we can choose $d_2 = \frac{2}{u}$ so that $d_2(s-u) \leq -1$ for all $s \leq \frac{1}{N}$ and

$$d_2 \pi_N(s)(s-u) \geq |\pi_N(s)|. \tag{3.4}$$

For the remaining case we first note that the solvability of the nonlinear equation $s(2 + \ln(s)) = y$ for any $y \in (0, \frac{3}{2})$ holds with positive solutions. Then, setting $d_2 = \frac{2}{u}$ we notice that for $\frac{1}{N} \leq s \leq e^{-1}$ we have $|1 + \ln(s)| = -1 - \ln(s)$ and the function $f(s) = \frac{2}{u}(1 + \ln(s))(s-u) - |1+\ln(s)|$ admits a minimum at $s_* \in (0,1)$ which also solves $s_*(2+\ln(s_*)) = \frac{u}{2}$. Hence, there exists a constant $d \geq 0$ such that

$$\frac{2}{u}\pi_N(s)(s-u) - |\pi_N(s)| \geq -d. \tag{3.5}$$

Lastly for $s \geq e^{-1}$, we have $|1+\ln(s)| = 1+\ln(s)$ and analogously the function $g(s) = \frac{2}{u}(1+\ln(s))(s-u) - 1 - \ln(s)$ admits a minimum at $s^* \in (0,1)$ which also solves $s^*(2+\ln(s^*)) = \frac{3u}{2}$. Likewise, we can find a constant $d \geq 0$ such that (3.5) is fulfilled. Hence, (3.3) holds for the approximation π_N. □

We then define

$$F_0^N(r,s) := \theta\Big[\Pi_N\big(\tfrac{1}{2}(1+r-s)\big) + \Pi_N\big(\tfrac{1}{2}(1-r-s)\big) + \Pi_N(s)\Big] \quad \forall r,s \in \mathbb{R},$$

and from the above definition of Π_N we deduce via Young's inequality and the fact $\Pi^{(4)}(\frac{1}{N}) = 2N^3 > 0$ that there exist constants $d_4 > 0$ and $d_5 \geq 0$ independent of $N \in \mathbb{N}$ such that

$$F_0^N(r,s) \geq d_4(|r|^4 + |s|^4) - d_5 \quad \forall r,s \in \mathbb{R}. \tag{3.6}$$

In Theorem 2.1, the solution (ϕ,ψ) only take values in the admissible set $\mathcal{K}$. Hence, only $F_{1,\phi}$ and $F_{1,\psi}$ restricted to $\mathcal{K}$ enter into the definition of a variational solution. We can therefore extend F_1 from $\mathcal{K}$ to the whole of $\mathbb{R}^2$ such that F_1, $F_{1,\phi}$ and $F_{1,\psi}$ are bounded. Then, replacing F_0 with F_0^N leads to the following approximate problem expressed in strong form:

$$\begin{aligned}
\partial_t\phi_N &= \Delta\mu_N && \text{in } Q, && \text{(3.7a)}\\
\mu_N &= -\varepsilon\Delta\phi_N + F_{0,\phi}^N(\phi_N,\psi_N) + F_{1,\phi}(\phi_N,\psi_N) + \sigma\Delta\psi_N && \text{in } Q, && \text{(3.7b)}\\
\partial_t\psi_N &= -z_N && \text{in } Q, && \text{(3.7c)}\\
z_N &= \lambda(\Delta+\omega^2)^2(\psi_N - \tfrac{1}{2}) + F_{0,\psi}^N(\phi_N,\psi_N) + F_{1,\psi}(\phi_N,\psi_N) + \sigma\Delta\phi_N && \text{in } Q, && \text{(3.7d)}\\
\partial_{\boldsymbol{n}}\phi_N &= \partial_{\boldsymbol{n}}\mu_N = \partial_{\boldsymbol{n}}\psi_N = \partial_{\boldsymbol{n}}\Delta\psi_N = 0 && \text{on } \Sigma, && \text{(3.7e)}\\
\phi_N(0) &= \phi_0, \quad \psi_N(0) = \psi_0 && \text{in } \Omega. && \text{(3.7f)}
\end{aligned}$$

The existence of a weak solution tuple $(\phi_N,\psi_N,\mu_N,z_N)$ can be established by a standard Galerkin approximation. We omit the details here as in the next section we will derive uniform estimates that can also be used as a foundation for the existence proof of (3.7) via a Galerkin approximation.

3.1.2 Uniform estimates

In the sequel the symbol C denotes nonnegative constants independent of N whose value may change from line to line and also within the same line. We test (3.7a) with μ_N, (3.7b) with $\partial_t\phi_N$, (3.7c) with z_N and (3.7d) with $\partial_t\psi_N$, respectively. Without entering the details, let us highlight that all the mentioned testing procedures can be justified within a rigorous framework as mentioned above. Then, upon summing, we arrive at the energy identity

$$\frac{d}{dt}E_N(\phi_N,\psi_N) + \|\nabla\mu_N\|^2 + \|z_N\|^2 = 0,$$

where E_N is the energy functional

$$\begin{aligned}
E_N(\phi_N,\psi_N) = &\int_\Omega \frac{\varepsilon}{2}|\nabla\phi_N|^2 + \frac{\lambda}{2}|(\Delta+\omega^2)(\psi_N - \tfrac{1}{2})|^2\,dx\\
&+ \int_\Omega F_0^N(\phi_N,\psi_N) + F_1(\phi_N,\psi_N) - \sigma\nabla\phi_N\cdot\nabla\psi_N\,dx.
\end{aligned}$$

Upon integrating in time, for arbitrary $t \in (0,T]$, the above identity gives

$$E_N(\phi_N(t),\psi_N(t)) + \int_0^t \|\nabla\mu_N\|^2 + \|z_N\|^2\,dt = E_N(\phi_0,\psi_0). \tag{3.8}$$

Note that by assumption (A3) for the initial conditions in (3.7e), it holds that

$$E_N(\phi_0,\psi_0) \le C\big(\|\phi_0\|_{H^1},\|\psi_0\|_{H^2}\big).$$

Thanks to the Neumann boundary conditions, we have the interpolation inequality and elliptic regularity estimates, see, e.g., [14, Thm. 2.4.2.7] for $C^{1,1}$-domains or [14, Thm. 3.2.1.3] for convex domains:

$$\|\nabla\psi_N\|^2 \le \|\Delta\psi_N\|\|\psi_N\|, \quad \|\psi_N\|_{H^2} \le C(\Omega)\big(\|\Delta\psi_N\| + \|\psi_N\|\big), \tag{3.9}$$

which leads to the lower bound

$$\begin{aligned}\|(\Delta+\omega^2)(\psi_N-\tfrac12)\|^2 &\ge \|\Delta\psi_N\|^2 + \omega^4\|\psi_N-\tfrac12\|^2 - 2\omega^2\|\Delta\psi_N\|\|\psi_N-\tfrac12\| \\ &\ge \frac14\|\Delta\psi_N\|^2 - 3\omega^4\|\psi_N-\tfrac12\|^2.\end{aligned}$$

Furthermore, for the term with indefinite sign $-\sigma\nabla\phi_N\cdot\nabla\psi_N$ in E_N, we compute a lower bound:

$$\begin{aligned}-\sigma\int_\Omega \nabla\phi_N\cdot\nabla(\psi_N-\tfrac12)\,dx &\ge -|\sigma|\|\nabla\phi_N\|\|\Delta\psi_N\|^{1/2}\|\psi_N-\tfrac12\|^{1/2} \\ &\ge -\frac{\varepsilon}{4}\|\nabla\phi_N\|^2 - \frac{\lambda}{4}\|\Delta\psi_N\|^2 - \frac{|\sigma|^4}{\lambda\varepsilon^2}\|\psi_N-\tfrac12\|^2.\end{aligned} \tag{3.10}$$

Using the lower bound in (3.6) for F_0^N, by Young's inequality we see that

$$\frac12\int_\Omega F_0^N(\phi_N,\psi_N)\,dx \ge \frac{d_4}{4}\|\psi_N-\tfrac12\|_{L^4}^4 - C \ge \Big(\frac{|\sigma|^4}{\lambda\varepsilon^2}+3\omega^4\Big)\|\psi_N-\tfrac12\|^2 - C,$$

and hence we deduce the lower bound for E_N:

$$\begin{aligned}E_N(\phi_N,\psi_N) \ge{}& \frac{\varepsilon}{4}\|\nabla\phi_N\|^2 + \frac{\lambda}{4}\|\Delta\psi_N\|^2 \\ &+ \frac12\int_\Omega F_0^N(\phi_N,\psi_N)\,dx + \int_\Omega F_1(\phi_N,\psi_N)\,dx - C,\end{aligned} \tag{3.11}$$

where C is a positive constant independent of N, ϕ_N and ψ_N. Next, we test (3.7a) with $1/|\Omega|$ and (3.7c) with ψ_N to obtain

$$\langle\phi_N(t)\rangle_\Omega = \langle\phi_0\rangle_\Omega \quad \forall t\in(0,T], \tag{3.12}$$

and

$$\frac12\|\psi_N(t)\|^2 \le \frac12\|\psi_0\|^2 + \frac12\int_0^t \|z_N\|^2\,dt + \frac12\int_0^t\|\psi_N\|^2\,dt. \tag{3.13}$$

Adding this to (3.8), applying Gronwall's inequality and the lower bound (3.11) in conjunction with Poincaré's inequality for ϕ_N and the elliptic regularity estimate (3.9) for ψ_N, as well as comparison argument in (3.7c), we deduce the uniform estimates

$$\begin{aligned}&\|\phi_N\|_{L^\infty(0,T;H^1)} + \|\psi_N\|_{L^\infty(0,T;H^2)} + \|\partial_t\psi_N\|_{L^2(Q)} \\ &\quad + \|\nabla\mu_N\|_{L^2(Q)} + \|z_N\|_{L^2(Q)} + \|F_0^N(\phi_N,\psi_N)\|_{L^\infty(0,T;L^1(\Omega))} \le C.\end{aligned} \tag{3.14}$$

Since $\langle\phi_N\rangle_\Omega = \langle\phi_0\rangle_\Omega \in (-1,1)$, we see that the constant $\nu := \frac12(1-|\langle\phi_0\rangle_\Omega|)$ satisfies the properties

$$\nu\in(0,1) \quad \text{and} \quad \frac12(1-\nu\pm\langle\phi_0\rangle_\Omega)\in(0,1).$$

Then, we consider testing (3.7b) with $\phi_N - \langle\phi_N\rangle_\Omega$ and (3.7d) with $\psi_N - \nu$, which leads to

$$\begin{aligned}
&\int_\Omega \varepsilon|\nabla\phi_N|^2 + F^N_{0,\phi}(\phi_N,\psi_N)(\phi_N - \langle\phi_N\rangle_\Omega)\,dx\\
&\quad= \int_\Omega (\mu_N - \langle\mu_N\rangle_\Omega)(\phi_N - \langle\phi_N\rangle_\Omega) - \big(F_{1,\phi}(\phi_N,\psi_N) + \sigma\Delta\psi_N\big)(\phi_N - \langle\phi_N\rangle_\Omega)\,dx\\
&\quad\le C\big(\|\nabla\mu_N\| + \|F_{1,\phi}(\phi_N,\psi_N)\| + \sigma\|\Delta\psi_N\|\big)\|\nabla\phi_N\|\\
&\quad\le C(1 + \|\nabla\mu_N\|),
\end{aligned}$$

and

$$\begin{aligned}
&\int_\Omega \lambda|(\Delta+\omega^2)\psi_N|^2 + F^N_{0,\psi}(\phi_N,\psi_N)(\psi_N - \nu)\,dx\\
&\quad= \int_\Omega \sigma\nabla\phi_N\cdot\nabla\psi_N + (z_N - F_{1,\psi}(\phi_N,\psi_N))(\psi_N-\nu)\,dx\\
&\qquad+ \int_\Omega \tfrac{1}{2}\lambda\omega^2(\Delta+\omega^2)(\psi_N-\nu) + \lambda\nu(\Delta+\omega^2)\psi_N + \tfrac{1}{2}\lambda\nu\,dx\\
&\quad\le C(1+\|z_N\|),
\end{aligned}$$

where we have used the uniform estimates (3.14), as well as the boundedness of F_1, $F_{1,\phi}$ and $F_{1,\psi}$ to deduce that $F_{1,\phi}(\phi_N,\psi_N)$ and $F_{1,\psi}(\phi_N,\psi_N)$ are uniformly bounded in $L^\infty(0,T;L^2(\Omega))$. Using (3.12) and adding these inequalities, we find that

$$\begin{aligned}
&\int_\Omega F^N_{0,\phi}(\phi_N,\psi_N)(\phi_N - \langle\phi_0\rangle_\Omega) + F^N_{0,\psi}(\phi_N,\psi_N)(\psi_N-\nu)\,dx\\
&\qquad\le C(1+\|\nabla\mu_N\| + \|z_N\|).
\end{aligned}\tag{3.15}$$

A direct computation shows the left-hand side can be expressed as

$$\begin{aligned}
&\int_\Omega \frac{\theta}{2}\big(\pi_N\big(\tfrac{1}{2}(1-\psi_N+\phi_N)\big) - \pi_N\big(\tfrac{1}{2}(1-\psi_N-\phi_N)\big)\big)(\phi_N - \langle\phi_0\rangle_\Omega)\,dx\\
&\quad+\int_\Omega \frac{\theta}{2}\big(\pi_N\big(\tfrac{1}{2}(1-\psi_N+\phi_N)\big) + \pi_N\big(\tfrac{1}{2}(1-\psi_N-\phi_N)\big) - \pi_N(\psi_N)\big)\\
&\qquad\times\big((1-\psi_N)-(1-\nu)\big)\,dx\\
&=\int_\Omega \theta\big(\pi_N\big(\tfrac{1}{2}(1-\psi_N+\phi_N)\big)\big[\tfrac{1}{2}(1-\psi_N+\phi_N) - \tfrac{1}{2}(1-\nu+\langle\phi_0\rangle_\Omega)\big]\,dx\\
&\quad+\int_\Omega \theta\pi_N\big(\tfrac{1}{2}(1-\psi_N-\phi_N)\big)\big[\tfrac{1}{2}(1-\psi_N-\phi_N) - \tfrac{1}{2}(1-\nu-\langle\phi_0\rangle_\Omega)\big]\,dx\\
&\quad+\int_\Omega \theta\pi_N(\psi_N)(\psi_N-\nu)\,dx.
\end{aligned}$$

As $\frac{1}{2}(1-\nu\pm\langle\phi_0\rangle_\Omega)\in(0,1)$ and $\nu\in(0,1)$, by invoking (3.3) we deduce that

$$\begin{aligned}
&\|\pi_N\big(\tfrac{1}{2}(1+\phi_N-\psi_N)\big)\|_{L^1} + \|\pi_N\big(\tfrac{1}{2}(1-\phi_N-\psi_N)\big)\|_{L^1} + \|\pi_N(\psi_N)\|_{L^1}\\
&\qquad\le C(1+\|\nabla\mu_N\| + \|z_N\|),
\end{aligned}$$

which implies

$$\|F^N_{0,\phi}(\phi_N,\psi_N)\|_{L^2(0,T;L^1)} + \|F^N_{0,\psi}(\phi_N,\psi_N)\|_{L^2(0,T;L^1)} \le C.\tag{3.16}$$

Consequently, integrating (3.7b) yields the estimate on the mean value of μ_N:

$$\|\langle\mu_N\rangle_\Omega\|_{L^2(0,T)} \le \|F^N_{0,\phi}(\phi_N,\psi_N)\|_{L^2(0,T;L^1)} + \|F_{1,\phi}(\phi_N,\psi_N)\|_{L^2(0,T;L^1)} \le C,$$

and by the Poincaré inequality we obtain

$$\|\mu_N\|_{L^2(Q)} \leq C. \tag{3.17}$$

Then, testing (3.7b) with $-\Delta\phi_N$ and (3.7d) with $-\Delta\psi_N$, upon summing we obtain

$$\begin{aligned}
&\int_\Omega F^N_{0,\phi\phi}(\phi_N,\psi_N)\nabla\phi_N\cdot\nabla\phi_N + \nabla F^N_{0,\phi\psi}(\phi_N,\psi_N)\nabla\psi_N\cdot\nabla\phi_N\,dx \\
&\quad + \int_\Omega F^N_{0,\psi\phi}(\phi_N,\psi_N)\nabla\phi_N\cdot\nabla\psi_N + F^N_{0,\psi\psi}(\phi_N,\psi_N)\nabla\psi_N\cdot\nabla\psi_N\,dx \\
&\quad + \varepsilon\|\Delta\phi_N\|^2 + \lambda\|\nabla\Delta\psi_N\|^2 \\
&= \int_\Omega \Big(F_{1,\phi}(\phi_N,\psi_N) - \mu_N + \sigma\Delta\psi_N\Big)\Delta\phi_N\,dx \\
&\quad + \int_\Omega \Big(F_{1,\psi}(\phi_N,\psi_N) + \sigma\Delta\phi_N - z_N + 2\lambda\omega^2\Delta\psi_N + \lambda\omega^4(\psi_N - \tfrac{1}{2})\Big)\Delta\psi_N\,dx \\
&\leq \frac{1}{2}\|\Delta\phi_N\|^2 + C\big(1 + \|\mu_N\|^2 + \|z_N\|^2 + \|\nabla F_1(\phi_N,\psi_N)\|^2\big).
\end{aligned}$$

Using the convexity of F_0^N the sum of the first and second lines on the left-hand side is non-negative. Recalling that $F_{1,\phi}(\phi_N,\psi_N)$ and $F_{1,\psi}(\phi_N,\psi_N)$ are bounded in $L^\infty(0,T;L^2(\Omega))$, we then infer the estimate

$$\|\Delta\phi_N\|^2_{L^2(0,T;L^2)} + \|\nabla\Delta\psi_N\|^2_{L^2(0,T;L^2)} \leq C,$$

and by invoking elliptic regularity estimate (3.9) we obtain

$$\|\phi_N\|_{L^2(0,T;H^2)} \leq C. \tag{3.18}$$

Through a comparison of terms in (3.7b) we deduce also that

$$\|F^N_{0,\phi}(\phi_N,\psi_N)\|_{L^2(Q)} \leq C. \tag{3.19}$$

Lastly, testing (3.7a) with an arbitrary test function $\zeta \in L^2(0,T;H^1(\Omega))$ yields

$$\|\partial_t\phi_N\|_{L^2(0,T;(H^1)^*)} \leq C, \tag{3.20}$$

while from the uniform estimate (3.14) for $\partial_t\psi_N$ we readily see that

$$\|\partial_t\Delta\psi_N\|_{L^2(0,T;H^2_{\boldsymbol{n}}(\Omega)^*)} \leq \|\partial_t\psi_N\|_{L^2(Q)} \leq C. \tag{3.21}$$

Remark 3.1. *With a more regular domain boundary $\partial\Omega$, it is possible to obtain a uniform boundedness of ψ_N in $L^2(0,T;H^3(\Omega))$.*

3.1.3 Passing to the limit

From the uniform estimates (3.14), (3.16)–(3.20) and (3.21), we deduce the existence of limit functions ϕ, ψ, μ and z, as well as a non-relabelled subsequence $N \to \infty$, such that

as $N \to \infty$,

$$\begin{aligned}
\phi_N &\to \phi \quad \text{weakly* in } L^\infty(0,T;H^1(\Omega)) \cap L^2(0,T;H^2_{\boldsymbol{n}}(\Omega)) \cap H^1(0,T;H^1(\Omega)^*),\\
\phi_N &\to \phi \quad \text{strongly in } C^0([0,T];L^s(\Omega)) \cap L^2(0,T;W^{1,s}(\Omega)) \text{ and a.e. in } Q,\\
\psi_N &\to \psi \quad \text{weakly* in } L^\infty(0,T;H^2_{\boldsymbol{n}}(\Omega)) \cap H^1(0,T;L^2(\Omega)),\\
\psi_N &\to \psi \quad \text{strongly in } C^0([0,T];W^{1,s}(\Omega)) \text{ and a.e. in } Q,\\
\Delta\psi_N &\to \Delta\psi \quad \text{weakly in } L^2(0,T;H^1(\Omega)) \cap H^1(0,T;H^2_{\boldsymbol{n}}(\Omega)^*),\\
\Delta\psi_N &\to \Delta\psi \quad \text{strongly in } L^2(0,T;L^s(\Omega)),\\
\mu_N &\to \mu \quad \text{weakly in } L^2(0,T;H^1(\Omega)),\\
z_N &\to z \quad \text{weakly in } L^2(Q),
\end{aligned} \tag{3.22}$$

for any $s < \infty$ in two dimensions and any $s \in [2,6)$ in three dimensions. Note that the initial conditions are attained by virtue of the continuity properties $\phi \in C^0([0,T];L^2(\Omega))$ and $\psi \in C^0([0,T];H^1(\Omega))$. By the generalized dominated convergence theorem and the boundedness of F_1, $F_{1,\phi}$ and $F_{1,\psi}$ we deduce as $N \to \infty$

$$F_{1,\phi}(\phi_N,\psi_N) \to F_{1,\phi}(\phi,\psi) \ \text{ and } \ F_{1,\psi}(\phi_N,\psi_N) \to F_{1,\psi}(\phi,\psi) \ \text{ strongly in } L^2(Q).$$

From the a.e. convergence of ϕ_N and ψ_N, we deduce that $F^N_{0,\phi}(\phi_N,\psi_N) \to F_{0,\phi}(\phi,\psi)$ a.e. in Q. Together with the uniform estimate (3.19), invoking Vitali's convergence theorem yields the strong convergence of $F^N_{0,\phi}(\phi_N,\psi_N)$ to $F_{0,\phi}(\phi,\psi)$ in $L^q(Q)$ for $q \in [1,2)$. This allows us to identify the weak limit of $F^N_{0,\phi}(\phi_N,\psi_N)$ in $L^2(Q)$ as $F_{0,\phi}(\phi,\psi)$ and obtain

$$F^N_{0,\phi}(\phi_N,\psi_N) \to F_{0,\phi}(\phi,\psi) \text{ weakly in } L^2(Q). \tag{3.23}$$

However, as we only have a uniform estimate of $F^N_{0,\psi}(\phi_N,\psi_N)$ in $L^2(0,T;L^1(\Omega))$, this is insufficient to identify the limit of $F^N_{0,\psi}(\phi_N,\psi_N)$ as $N \to \infty$. This primarily explains why, in the limit, we can just achieve a variational inequality rather than an equality. Nevertheless, we can show that the limit functions satisfy the physical property $(\phi,\psi) \in \mathcal{K}$ for a.e. $(x,t) \in Q$. Owning to the explicit expression for Π_N, recall that $d_1 \geq 0$, we have for $s \leq \frac{1}{N}$,

$$\Pi_N(s) = \frac{2N^3}{4!}\Big(s-\frac{1}{N}\Big)^4 - \frac{N^2}{3!}\Big(s-\frac{1}{N}\Big)^3 + \frac{N}{2}\Big(s-\frac{1}{N}\Big)^2 + \Big(\ln\frac{1}{N}+1\Big)\Big(s-\frac{1}{N}\Big) + \frac{1}{N}\ln\frac{1}{N}.$$

By Young's inequality we deduce that

$$\frac{2N^3}{4!}\Big(s-\frac{1}{N}\Big)^4 - \frac{N^2}{3!}\Big(s-\frac{1}{N}\Big)^3 + \frac{N}{2}\Big(s-\frac{1}{N}\Big)^2 \geq 0 \quad \forall s \in \mathbb{R},$$

and hence, due to the lower bound in (3.2), for N sufficiently large we obtain

$$\begin{aligned}
\int_Q (\Pi_N(\psi_N)+d_1)\,dx\,dt &\geq \int_{\{(x,t)\in Q\,:\,\psi_N(x,t)<0\}} (\Pi_N(\psi_N)+d_1)\,dx\,dt\\
&\geq \Big(\ln\frac{1}{N}+1\Big)\int_{\{(x,t)\in Q\,:\,\psi_N(x,t)<0\}} \psi_N\,dx\,dt - \frac{1}{N}|\Omega|T\\
&= \Big|\ln\frac{1}{N}+1\Big|\int_Q (-\psi_N)_+\,dx\,dt - \frac{1}{N}|\Omega|T,
\end{aligned}$$

where, for a given scalar function f, $(f)_+ = \max(f,0)$ denotes the positive part of f, and $(-f)_+ = \max(-f,0) = -\min(f,0)$ is the negative part of f. Combining this with the uniform estimate (3.14) for F_0^N, we infer that

$$\begin{aligned} C &\geq \int_Q F_0^N(\phi_N,\psi_N)\,dx\,dt \\ &\geq \theta\left|\ln\frac{1}{N}+1\right|\int_Q (-\psi_N)_+ + \big(-\tfrac{1}{2}(1+\phi_N-\psi_N)\big)_+ + \big(-\tfrac{1}{2}(1-\phi_N-\psi_N)\big)_+\,dx\,dt \\ &\quad - 3\theta\frac{1}{N}|\Omega|T. \end{aligned}$$

Since $3\theta\frac{1}{N}|\Omega|T \leq C$, we obtain

$$\begin{aligned} &\|(-\psi_N)_+\|_{L^1(0,T;L^1)} + \|\big(-\tfrac{1}{2}(1+\phi_N-\psi_N)\big)_+\|_{L^1(0,T;L^1)} \\ &\qquad + \|\big(-\tfrac{1}{2}(1-\phi_N-\psi_N)\big)_+\|_{L^1(0,T;L^1)} \leq \frac{C}{\theta|\ln\frac{1}{N}+1|}, \end{aligned} \tag{3.24}$$

where the right-hand side vanishes as $N\to\infty$. By Fatou's lemma we deduce that the limit functions ϕ and ψ satisfy

$$(-\psi)_+ = 0, \quad \big(-\tfrac{1}{2}(1+\phi-\psi)\big)_+ = 0, \quad \big(-\tfrac{1}{2}(1-\phi-\psi)\big)_+ = 0 \quad \text{ a.e. in } Q,$$

which in turn implies

$$\psi \geq 0, \quad \frac{1}{2}(1+\phi-\psi)\geq 0, \quad \frac{1}{2}(1-\phi-\psi)\geq 0 \quad \text{ a.e. in } Q, \tag{3.25}$$

meaning that $(\phi,\psi)\in\mathcal{K}$ a.e. in Q as claimed.

Lastly, for arbitrary test functions $v\in L^2(Q)$, $u\in L^2(0,T;H^1(\Omega))$ and arbitrary log-admissible test function pair $(\zeta,\eta)\in (L^2(0,T;H^1(\Omega))^2$, we test (3.7a) with u, (3.7c) with v, (3.7b) with $\zeta-\phi$ and (3.7d) with $\eta-\psi$. Then, integrating by parts and upon adding the resulting equalities involving (3.7b) and (3.7d) we obtain

$$0 = \int_Q \partial_t\phi_N u + \nabla\mu_N\cdot\nabla u\,dx\,dt, \tag{3.26a}$$

$$0 = \int_Q \partial_t\psi_N v + z_N v\,dx\,dt, \tag{3.26b}$$

$$\begin{aligned} 0 &= \int_Q \big(F_{0,\phi}^N(\phi_N,\psi_N) + F_{1,\phi}(\phi_N,\psi_N) - \mu_N\big)(\zeta-\phi_N)\,dx\,dt \\ &\quad + \int_Q \nabla(\varepsilon\phi_N+\sigma\psi_N)\cdot\nabla(\zeta-\phi_N)\,dx\,dt \\ &\quad + \int_Q -(\lambda\nabla\Delta\psi_N+\sigma\nabla\phi_N)\cdot\nabla(\eta-\psi_N) + \big(F_{1,\psi}(\phi_N,\psi_N)-z_N\big)(\eta-\psi_N)\,dx\,dt \\ &\quad + \int_Q \big(2\lambda\omega^2\Delta\psi_N + \lambda\omega^4(\psi_N-\tfrac{1}{2}) + F_{0,\psi}^N(\phi_N,\psi_N)\big)(\eta-\psi_N)\,dx\,dt. \end{aligned} \tag{3.26c}$$

Monotonicity of π_N yields

$$(\pi_N(r)-\pi_N(s))(r-s)\geq 0 \quad \forall r,s\in\mathbb{R},$$

and a short calculation reveals that for log-admissible test function pair (ζ,η) it holds that

$$(F_{0,\phi}^N(\zeta,\eta)-F_{0,\phi}^N(\phi_N,\psi_N))(\zeta-\phi_N) + (F_{0,\psi}^N(\zeta,\eta)-F_{0,\psi}^N(\phi_N,\psi_N)(\eta-\psi_N)\geq 0. \tag{3.27}$$

Hence, we replace (3.26c) with the inequality

$$\begin{aligned}0 \le &\int_Q \big(F^N_{0,\phi}(\zeta,\eta) + F_{1,\phi}(\phi_N,\psi_N) - \mu_N\big)(\zeta-\phi_N)\,dx\,dt \\ &+ \int_Q \nabla(\varepsilon\phi_N - \sigma\psi_N)\cdot\nabla(\zeta-\phi_N)\,dx\,dt \\ &+ \int_Q -(\lambda\nabla\Delta\psi_N + \sigma\nabla\phi_N)\cdot\nabla(\eta-\psi_N) + \big(F_{1,\psi}(\phi_N,\psi_N) - z_N\big)(\eta-\psi_N)\,dx\,dt \\ &+ \int_Q \big(2\lambda\omega^2\Delta\psi_N + \lambda\omega^4(\psi_N - \tfrac12) + F^N_{0,\psi}(\zeta,\eta)\big)(\eta-\psi_N)\,dx\,dt.\end{aligned} \tag{3.28}$$

Passing to the limit $N\to\infty$ with the compactness assertions (3.22) yields that the limit functions ϕ, ψ, μ and z satisfy

$$0 = \int_0^T \langle \partial_t\phi, u\rangle_{H^1}\,dt + \int_Q \nabla\mu\cdot\nabla u\,dx\,dt, \tag{3.29a}$$

$$0 = \int_Q \partial_t\psi v + zv\,dx\,dt, \tag{3.29b}$$

$$\begin{aligned}0 \le &\int_Q \big(F_{0,\phi}(\zeta,\eta) + F_{1,\phi}(\phi,\psi) - \mu\big)(\zeta-\phi) + \nabla(\varepsilon\phi - \sigma\psi)\cdot\nabla(\zeta-\phi)\,dx\,dt \\ &+ \int_Q -(\lambda\nabla\Delta\psi + \sigma\nabla\phi)\cdot\nabla(\eta-\psi) + \big(F_{1,\psi}(\phi,\psi) - z\big)(\eta-\psi)\,dx\,dt \\ &+ \int_Q \big(2\lambda\omega^2\Delta\psi + \lambda\omega^4(\psi - \tfrac12) + F_{0,\psi}(\zeta,\eta)\big)(\eta-\psi)\,dx\,dt,\end{aligned} \tag{3.29c}$$

for arbitrary $v\in L^2(Q)$, $u\in L^2(0,T;H^1(\Omega))$ and log-admissible test function pair $(\zeta,\eta)\in (L^2(0,T;H^1(\Omega))^2$. In the above we also used that

$$|\pi_N(s)| \le |\pi(s)| + 1 \quad \text{for } s\in(0,1),$$

so that for an arbitrary log-admissible test function pair (ζ,η) we have

$$\begin{aligned}|F^N_{0,\phi}(\zeta,\eta)| &\le 2 + |\pi\big(\tfrac12(1+\zeta-\eta)\big)| + |\pi\big(\tfrac12(1-\zeta-\eta)\big)|,\\ |F^N_{0,\psi}(\zeta,\eta)| &\le 3 + |\pi(\eta)| + |\pi\big(\tfrac12(1+\zeta-\eta)\big)| + |\pi\big(\tfrac12(1-\zeta-\eta)\big)|,\end{aligned}$$

whence by the generalized Lebesgue dominated convergence theorem we obtain

$$F^N_{0,\phi}(\zeta,\eta)\to F_{0,\phi}(\zeta,\eta) \quad \text{and} \quad F^N_{0,\psi}(\zeta,\eta)\to F_{0,\psi}(\zeta,\eta) \quad \text{strongly in } L^1(Q).$$

Note that (3.29c) is an alternate variational inequality where we evaluated $F_{0,\phi}$ and $F_{0,\psi}$ at the log-admissible test function pair (ζ,η) instead at the solution pair (ϕ,ψ). To recover (2.4) we argue similar to the ideas of [6]. Let $(\alpha,\beta)\in(L^2(0,T;H^1(\Omega))^2$ be an arbitrary log-admissible test function pair, and we consider, for $\kappa\in(0,1]$,

$$\zeta_\kappa = (1-\kappa)\phi + \kappa\alpha \quad \text{and} \quad \eta_\kappa = (1-\kappa)\psi + \kappa\beta.$$

Then, it is clear that $(\zeta_\kappa,\eta_\kappa)\in\mathcal{K}$ a.e. in Q, and by the convexity of $h: s\mapsto|\ln(s)|$ we can deduce that

$$\begin{aligned}&\big|\pi\big(\tfrac12((1-\kappa)(1\pm\phi-\psi)+\kappa(1\pm\alpha-\beta))\big)\big| \\ &\quad\le 1 + h\big(\tfrac12((1-\kappa)(1\pm\phi-\psi)+\kappa(1\pm\alpha-\beta))\big) \\ &\quad\le 1 + (1-\kappa)h\big(\tfrac12(1\pm\phi-\psi)\big) + \kappa h\big(\tfrac12(1\pm\alpha-\beta)\big) \\ &\quad\le 2 + |\pi\big(\tfrac12(1\pm\phi-\psi)\big)| + |\pi\big(\tfrac12(1\pm\alpha-\beta)\big)| \in L^1(Q),\end{aligned} \tag{3.30}$$

so that by a similar argument,

$$|\pi((1-\kappa)\psi+\kappa\beta)| \le 2+|\pi(\psi)|+|\pi(\beta)| \in L^1(Q). \tag{3.31}$$

Hence, $(\zeta_\kappa,\eta_\kappa)$ is a log-admissible test function pair in the sense of Definition 2.1. Substituting this choice of ζ_κ and η_κ into (2.4) and dividing by κ we find that

$$\begin{aligned}0 \le &\int_Q \big(F_{0,\phi}(\zeta_\kappa,\eta_\kappa)+F_{1,\phi}(\phi,\psi)-\mu\big)(\alpha-\phi)+\nabla(\varepsilon\phi-\sigma\psi)\cdot\nabla(\alpha-\phi)\,dx\,dt\\ &+\int_Q \big(-\lambda\nabla\Delta\psi-\sigma\nabla\phi\big)\cdot\nabla(\eta-\psi)+\big(F_{1,\psi}(\phi,\psi)-z\big)(\beta-\psi)\,dx\,dt\\ &+\int_Q \big(2\lambda\omega^2\Delta\psi+\lambda\omega^4(\psi-\tfrac12)+F_{0,\psi}(\zeta_\kappa,\eta_\kappa)\big)(\alpha-\psi)\,dx\,dt.\end{aligned} \tag{3.32}$$

By virtue of (3.30) and (3.31), we infer that

$$\begin{aligned}&|F_{0,\phi}(\zeta_\kappa,\eta_\kappa)|+|F_{0,\psi}(\zeta_\kappa,\eta_\kappa)|\\ &\quad\le C\big(1+|\pi(\psi)|+|\pi(\beta)|+|\pi\big(\tfrac12(1\pm\phi-\psi)\big)|+|\pi\big(\tfrac12(1\pm\alpha-\beta)\big)|\big)\end{aligned}$$

uniformly in $\kappa\in(0,1]$. Hence, by the dominated convergence theorem we obtain, as $\kappa\to0$,

$$F_{0,\phi}(\zeta_\kappa,\eta_\kappa)\to F_{0,\phi}(\phi,\psi) \quad\text{and}\quad F_{0,\psi}(\zeta_\kappa,\eta_\kappa)\to F_{0,\psi}(\phi,\psi) \quad\text{strongly in } L^1(Q),$$

and by passing to the limit $\kappa\to0$ in (3.32) we obtain (2.4). This shows that (ϕ,ψ,μ,z) is a variational solution to (1.5) with logarithmic potential in the sense of Definition 2.2.

Remark 3.2. *By utilizing* (3.22) *and* (3.23)*, we can pass to the limit in* (3.7b) *to deduce that the limit functions* (ϕ,ψ,μ) *satisfy* (2.6)*. On the other hand,* (2.7) *can be derived by choosing* $\zeta=\phi$ *in* (2.4) *whilst keeping* η *arbitrary.*

Remark 3.3. *We mention that a weaker variational inequality than* (2.4) *or* (3.28) *can also be derived. Let us use the notation* $F_{\log}=F_0$ *as there is no ambiguity. We start with* (3.26c) *with arbitrary test function* $(\zeta,\eta)\in(L^2(0,T;H^1(\Omega))^2$ *such that* $F_{\log}(\zeta,\eta)\in L^1(Q)$*. For instance, an obstacle-admission test function pair satisfies the requirement due to the continuity of* $F_{\log}$ *over* $\mathcal{K}$*. Using the convexity of* $F^N_{\log}$ *we have instead of* (3.27) *the following relation*

$$\int_\Omega F^N_{\log}(\zeta,\eta)-F^N_{\log}(\phi_N,\psi_N)\,dx \ge \int_\Omega (F^N_{\log,\phi}(\phi_N,\psi_N)(\zeta-\phi_N)+F^N_{\log,\psi}(\phi_N,\psi_N)(\eta-\psi_N)\,dx.$$

Then, instead of (3.28) *we obtain the variational inequality*

$$\begin{aligned}0 \le &\int_Q \big(F_{1,\phi}(\phi_N,\psi_N)-\mu_N\big)(\zeta-\phi_N)+\nabla(\varepsilon\phi_N-\sigma\psi_N)\cdot\nabla(\zeta-\phi_N)\,dx\,dt\\ &+\int_Q -(\lambda\nabla\Delta\psi_N+\sigma\nabla\phi_N)\cdot\nabla(\eta-\psi_N)+\big(F_{1,\psi}(\phi_N,\psi_N)-z_N\big)(\eta-\psi_N)\,dx\,dt\\ &+\int_Q \big(2\lambda\omega^2\Delta\psi_N+\lambda\omega^4(\psi_N-\tfrac12)\big)(\eta-\psi_N)+F^N_{\log}(\zeta,\eta)-F^N_{\log}(\phi_N,\psi_N)\,dx\,dt,\end{aligned} \tag{3.33}$$

holding for arbitrary $(\zeta,\eta)\in (L^2(0,T;H^1(\Omega))^2$ *such that* $F_{\log}(\zeta,\eta)\in L^1(Q)$*. Passing to the limit* $N\to\infty$ *yields*

$$\begin{aligned}0\le{}&\int_\Omega \big(F_{1,\phi}(\phi,\psi)-\mu\big)(\zeta-\phi)+\nabla(\varepsilon\phi-\sigma\psi)\cdot\nabla(\zeta-\phi)\,dx\\&+\int_\Omega -(\lambda\nabla\Delta\psi+\sigma\nabla\phi)\cdot\nabla(\eta-\psi)+\big(F_{1,\psi}(\phi,\psi)-z\big)(\eta-\psi)\,dx\\&+\int_\Omega \big(2\lambda\omega^2\Delta\psi+\lambda\omega^4(\psi-\tfrac12)\big)(\eta-\psi)+F_{\log}(\zeta,\eta)-F_{\log}(\phi,\psi)\,dx,\end{aligned}\tag{3.34}$$

holding for a.e. $t\in(0,T)$ *and arbitrary* $(\zeta,\eta)\in(L^2(0,T;H^1(\Omega))^2$ *such that* $F_{\log}(\zeta,\eta)\in L^1(Q)$*.*

3.2 Continuous dependence and uniqueness

Let now $(\phi_1,\psi_1,\mu_1,z_1)$ and $(\phi_2,\psi_2,\mu_2,z_2)$ be two variational solutions to (1.5) with logarithmic potential corresponding to initial data $(\phi_{0,1},\psi_{0,1})$ and $(\phi_{0,2},\psi_{0,2})$, respectively. Consider (2.4) for (ϕ_1,ψ_1) with $\zeta=\phi_2$ and $\eta=\psi_2$, and likewise with the alternate variational inequality (3.29c) for (ϕ_2,ψ_2) with $\zeta=\phi_1$ and $\eta=\psi_1$. Upon summing the resulting inequalities we obtain for the differences $\widehat\phi:=\phi_1-\phi_2$, $\widehat\psi:=\psi_1-\psi_2$, $\widehat\mu:=\mu_1-\mu_2$ and $\widehat z:=z_1-z_2$ that

$$\begin{aligned}0\ge{}&\int_\Omega \big(F_{1,\phi}(\phi_1,\psi_1)-F_{1,\phi}(\phi_2,\psi_2)-\widehat\mu\big)\widehat\phi+\nabla(\varepsilon\widehat\phi-\sigma\widehat\psi)\cdot\nabla\widehat\phi\,dx\\&+\int_\Omega -\lambda\nabla\Delta\widehat\psi\cdot\nabla\widehat\psi+\big(F_{1,\psi}(\phi_1,\psi_1)-F_{1,\psi}(\phi_2,\psi_2)-\widehat z\big)\widehat\psi-\sigma\nabla\widehat\phi\cdot\nabla\widehat\psi\,dx\\&+\int_\Omega(2\lambda\omega^2\Delta\widehat\psi+\lambda\omega^4\widehat\psi)\widehat\psi\,dx,\end{aligned}\tag{3.35}$$

where we had a cancellation of terms involving F_0.

Next, we consider the difference between (2.3a) and (2.3b) for the two solutions $(\phi_1,\psi_1,\mu_1,z_1)$ and $(\phi_2,\psi_2,\mu_2,z_2)$ to derive that

$$0=\langle\partial_t\widehat\phi,u\rangle_{H^1}+\int_\Omega\nabla\widehat\mu\cdot\nabla u\,dx,\quad 0=\int_\Omega\partial_t\widehat\psi v+\widehat z v\,dx,$$

for any $u\in H^1(\Omega)$, and $v\in L^2(\Omega)$. From the first equality, it readily follows that, for every $t\in[0,T]$, $\langle\widehat\phi(t)\rangle_\Omega=\langle\phi_{0,1}-\phi_{0,2}\rangle_\Omega$. Next, we can consider the choices $u=\mathcal N(\widehat\phi-\widehat\phi_\Omega)$ and $v=\widehat\psi$ to infer

$$\begin{aligned}&0=\langle\partial_t\widehat\phi,\mathcal N(\widehat\phi-\widehat\phi_\Omega)\rangle_{H^1}+\int_\Omega\widehat\mu(\widehat\phi-\widehat\phi_\Omega)\,dx=\frac12\frac{d}{dt}\|\nabla\mathcal N(\widehat\phi-\widehat\phi_\Omega)\|^2+\int_\Omega\widehat\mu(\widehat\phi-\widehat\phi_\Omega)\,dx,\\&0=\frac12\frac{d}{dt}\|\widehat\psi\|^2+\int_\Omega\widehat z\widehat\psi\,dx.\end{aligned}$$

Adding these to (3.35) and using the local Lipschitz continuity of $F_{1,\phi}$, $F_{1,\psi}$, as well as the

boundedness of ϕ_i and ψ_i, $i = 1, 2$, leads to

$$\begin{aligned}
&\frac{1}{2}\frac{d}{dt}\Big(\|\nabla\mathcal{N}(\widehat{\phi}-\widehat{\phi}_\Omega)\|^2+\|\widehat{\psi}\|^2\Big)+\varepsilon\|\nabla\widehat{\phi}\|^2+\lambda\|\Delta\widehat{\psi}\|^2+\lambda\omega^4\|\widehat{\psi}\|^2\\
&\quad\le\int_\Omega |F_{1,\phi}(\phi_1,\psi_1)-F_{1,\phi}(\phi_2,\psi_2)||\widehat{\phi}-\widehat{\phi}_\Omega|+|F_{1,\psi}(\phi_1,\psi_1)-F_{1,\psi}(\phi_2,\psi_2)||\widehat{\psi}|\,dx\\
&\qquad+2|\sigma|\|\nabla\widehat{\psi}\|\|\nabla\widehat{\phi}\|+2\lambda\omega^2\|\nabla\widehat{\psi}\|^2 \qquad (3.36)\\
&\quad\le C\big(\|\widehat{\phi}-\widehat{\phi}_\Omega\|^2+\|\widehat{\psi}\|^2\big)+\frac{\lambda}{2}\|\Delta\widehat{\psi}\|^2+\frac{\varepsilon}{4}\|\nabla\widehat{\phi}\|^2+C\|\widehat{\psi}\|^2\\
&\quad\le C\Big(\|\nabla\mathcal{N}(\widehat{\phi}-\widehat{\phi}_\Omega)\|^2+\|\widehat{\psi}\|^2\Big)+\frac{\lambda}{2}\|\Delta\widehat{\psi}\|^2+\frac{\varepsilon}{2}\|\nabla\widehat{\phi}\|^2,
\end{aligned}$$

where we have used Young's inequality and the following:

$$\|\widehat{\phi}-\widehat{\phi}_\Omega\|^2=\int_\Omega\nabla\mathcal{N}(\widehat{\phi}-\widehat{\phi}_\Omega)\cdot\nabla\widehat{\phi}\,dx\le\|\nabla\mathcal{N}(\widehat{\phi}-\widehat{\phi}_\Omega)\|\|\nabla\widehat{\phi}\|.$$

Applying the elliptic regularity estimate (3.9) and the Gronwall inequality leads to (2.8).

3.3 Obstacle potential

The well-posedness of (1.5) with the obstacle potential (1.7) follows along similar lines of argument as in the proof for the logarithmic potential (1.6). Thus, let us just outline the essential modifications. In place of (3.1), we set

$$\Pi_N(s)=\begin{cases}0 & \text{if } s\ge 0,\\ \frac{N}{4!}s^4 & \text{if } s\le 0.\end{cases} \qquad (3.37)$$

Then, it is clear that the lower bound (3.2) is fulfilled, and by setting

$$F_0^N(r,s)=\Pi_N\big(\tfrac{1}{2}(1+r-s)\big)+\Pi_N\big(\tfrac{1}{2}(1-r-s)\big)+\Pi_N(s)\quad\forall r,s\in\mathbb{R},$$

we see that (3.6) is also fulfilled with constants independent of $N\in\mathbb{N}$. Furthermore, for fixed $u\in(0,1)$ we can find a constant $C_u>0$ such that $C_u u>1$. Then, for any $s\le 0$ we deduce that the function $f(s)=C_u s^3(s-u)-|s|^3$ is non-negative and consequently we find an analogue to (3.3)

$$|\pi_N(s)|\le C\pi_N(s)(s-u)\quad\forall s\in\mathbb{R}, \qquad (3.38)$$

where the positive constant C is independent of N.

Analogous to the proof for the logarithmic potential, we obtain from the approximate system (3.7), now with F_0^N defined as above, the uniform estimates (3.12) and (3.14). Then, testing (3.7b) with $\phi_N-\langle\phi_0\rangle_\Omega$ and (3.7d) with $\psi_N-\nu$ we obtain from (3.15) and (3.38) that

$$\begin{aligned}
&\|\pi_N\big(\tfrac{1}{2}(1+\phi_N-\psi_N)\big)\|_{L^1}+\|\pi_N\big(\tfrac{1}{2}(1-\phi_N-\psi_N)\big)\|_{L^1}+\|\pi_N\big(\psi_N\big)\|_{L^1}\\
&\quad\le C\int_\Omega F_{0,\phi}^N(\phi_N,\psi_N)(\phi_N-\langle\phi_0\rangle_\Omega)+F_{0,\psi}^N(\phi_N,\psi_N)(\psi_N-\nu)\,dx\\
&\quad\le C\big(1+\|\nabla\mu_N\|+\|z_N\|\big),
\end{aligned}$$

which in turn leads to the uniform estimates (3.16) and (3.17). Similarly, by the convexity of F_0^N we obtain the regularity estimate (3.18), as well as the remaining uniform estimates

(3.19) and (3.20). It remains to show that the limit (ϕ, ψ) of (ϕ_N, ψ_N), along a non-relabelled subsequence, satisfies $(\phi, \psi) \in \mathcal{K}$ for a.e. $(x,t) \in Q$. From the explicit formula in (3.37) we infer that

$$\int_Q \Pi_N(\psi_N)\,dx\,dt \geq \int_{\{(x,t)\in Q\,:\,\psi_N(x,t)<0\}} \frac{N}{4!}|\psi_N|^4\,dx\,dt = \frac{N}{4!}\int_Q (-\psi_N)_+^4\,dx\,dt,$$

and so by (3.14) we have, similar to (3.24),

$$\begin{aligned}&\|(-\psi_N)_+\|_{L^4(Q)} + \|(-\tfrac{1}{2}(1+\phi_N-\psi_N))_+\|_{L^4(Q)} + \|(-\tfrac{1}{2}(1-\phi_N-\psi_N))_+\|_{L^4(Q)}\\ &\quad\leq CN^{-\frac{1}{4}},\end{aligned}$$

where the right-hand side vanishes as $N \to \infty$. Fatou's lemma then implies that the limit functions ϕ and ψ satisfy (3.25), that is $(\phi, \psi) \in \mathcal{K}$ a.e. in Q.

Lastly, for an obstacle-admissible test function pair $(\zeta, \eta) \in L^2(0,T; H^1(\Omega))^2$, notice that from the definition (3.37) it holds that

$$\pi_N(\eta) = 0, \quad \pi_N\big(\tfrac{1}{2}(1+\zeta-\eta)\big) = 0, \quad \pi_N\big(\tfrac{1}{2}(1-\zeta-\eta)\big) = 0,$$

and hence

$$F^N_{0,\phi}(\zeta,\eta) = 0, \quad F^N_{0,\psi}(\zeta,\eta) = 0.$$

This leads the following analogue of (3.28):

$$\begin{aligned}0 \leq &\int_Q \big(F_{1,\phi}(\phi_N,\psi_N) - \mu_N\big)(\zeta-\phi_N) + \nabla(\varepsilon\phi_N - \sigma\psi_N)\cdot\nabla(\zeta-\phi_N)\,dx\,dt\\ &+ \int_Q -\lambda\nabla\Delta\psi_N\cdot\nabla(\eta-\psi_N) + \big(F_{1,\psi}(\phi_N,\psi_N) - z_N\big)(\eta-\psi_N)\,dx\,dt\\ &+ \int_Q -\sigma\nabla\psi_N\cdot\nabla(\eta-\psi_N) + \big(2\lambda\omega^2\Delta\psi_N + \lambda\omega^4(\psi_N - \tfrac{1}{2})\big)(\eta-\psi_N)\,dx\,dt,\end{aligned}$$

and with the compactness assertions (3.22) we find that in the limit $N \to \infty$ the limit solution pair (ϕ, ψ) satisfy the variational inequality (2.5). This completes the proof of existence. For continuous dependence and uniqueness of variational solution, the proof proceeds exactly as in Section 3.2 and so we omit the details.

3.4 Deep quench limit

3.4.1 Weak convergence

For $\theta \in (0,1]$, we denote by $(\phi_\theta, \psi_\theta, \mu_\theta, z_\theta)$ as the variational solution to (1.5) with logarithmic potential $F_0 = F_{\log}$ obtained through Theorem 2.1. From (3.22) we see that $\phi_N\Delta\psi_N \to \phi_\theta\Delta\psi_\theta$ strongly in $L^1(0,T;L^1(\Omega))$, and hence it holds that for a.e. $t \in (0,T)$,

$$\int_\Omega \phi_N(t)\Delta\psi_N(t)\,dx \to \int_\Omega \phi_\theta(t)\Delta\psi_\theta(t)\,dx.$$

Then, we revisit (3.8) and find that after neglecting the non-negative $F^N_{\log}$, employing the boundedness of F_1, and performing an integration by parts, where for arbitrary $t \in (0,T]$,

$$\begin{aligned}&\int_\Omega \frac{\varepsilon}{2}|\nabla\phi_N(t)|^2 + \frac{\lambda}{2}|(\Delta+\omega^2)(\psi_N(t)-\tfrac{1}{2})|^2 + \sigma\phi_N(t)\Delta\psi_N(t)\,dx\\ &\quad+\int_0^t \|\nabla\mu_N\|^2 + \|z_N\|^2\,dt \leq C\big(\|\phi_0\|_{H^1}, \|\psi_0\|_{H^2}\big)\end{aligned} \tag{3.39}$$

with a positive constant C independent of $\theta \in (0,1]$. Invoking the compactness properties listed in (3.22) and the weak lower semicontinuity of the norms we deduce from (3.39) that for a.e. $t \in (0,T)$,

$$\begin{aligned}\int_\Omega \frac{\varepsilon}{2}|\nabla\phi_\theta(t)|^2 + \frac{\lambda}{2}|(\Delta+\omega^2)(\psi_\theta(t)-\tfrac{1}{2})|^2 + \sigma\phi_\theta(t)\Delta\psi_\theta(t)\,dx \\ + \int_0^t \|\nabla\mu_\theta\|^2 + \|z_\theta\|^2\,dt \le C\big(\|\phi_0\|_{H^1}, \|\psi_0\|_{H^2}\big).\end{aligned} \tag{3.40}$$

Together with Young's inequality and the property $(\phi_\theta,\psi_\theta)\in\mathcal{K}$ a.e. in Q, we infer from (3.40) that

$$\begin{aligned}\|\phi_\theta\|^2_{L^\infty(0,T;H^1)} + \|\psi_\theta\|^2_{L^\infty(0,T;H^2)} + \|\nabla\mu_\theta\|^2_{L^2(Q)} \\ + \|z_\theta\|^2_{L^2(Q)} + \|\partial_t\psi_\theta\|^2_{L^2(Q)} + \|\partial_t\phi_\theta\|^2_{L^2(0,T;(H^1)^*)} \le C,\end{aligned} \tag{3.41}$$

with a positive constant C independent of $\theta\in(0,1]$, where the uniform estimates on the time derivatives are inferred from a comparison of terms in (2.3a) and (2.3b).

Next, in (2.4) for $(\phi_\theta,\psi_\theta,\mu_\theta,z_\theta)$ we consider $\zeta = \langle\phi_\theta\rangle_\Omega = \langle\phi_0\rangle_\Omega$ and $\eta = \nu = \frac{1}{2}(1-|\langle\phi_0\rangle_\Omega|)$, integrating by parts and employing the boundedness property for $(\phi_\theta,\psi_\theta)$, $F_{1,\phi}(\phi_\theta,\psi_\theta)$ and $F_{1,\psi}(\phi_\theta,\psi_\theta)$ leads to

$$\begin{aligned}&\int_\Omega F_{\log,\phi}(\phi_\theta,\psi_\theta)(\phi_\theta-\langle\phi_\theta\rangle_\Omega) + F_{\log,\psi}(\phi_\theta,\psi_\theta)(\psi_\theta-\nu)\,dx \\ &\quad\le C\big(1+\|\nabla\mu_\theta\|\|\nabla\phi_\theta\| + \|z_\theta\| + \|\nabla\psi_\theta\|^2 + \|\Delta\psi_\theta\|^2 + \|\nabla\phi_\theta\|\|\nabla\psi_\theta\|\big) \\ &\quad\le C\big(1+\|\nabla\mu_\theta\| + \|z_\theta\|\big).\end{aligned} \tag{3.42}$$

Invoking the analogue of (3.3) for $\Pi(s) = s\ln s$ and $\pi(s) = \Pi'(s) = 1+\ln(s)$, cf. [21, Prop. A.1]: there exist constants $C_1>0$ and $C_2\ge 0$ depending on $u\in(0,1)$ such that

$$|\Pi(s)| + |\pi(s)| \le C_1\pi(s)(s-u) + C_2 \quad \forall s\in(0,1),$$

we may deduce from (3.42) that

$$\begin{aligned}\|F_{\log}(\phi_\theta,\psi_\theta)\|_{L^2(0,T;L^1)} \\ + \|F_{\log,\phi}(\phi_\theta,\psi_\theta)\|_{L^2(0,T;L^1)} + \|F_{\log,\psi}(\phi_\theta,\psi_\theta)\|_{L^2(0,T;L^1)} \le C.\end{aligned} \tag{3.43}$$

Then, integrating (2.6) over Ω yields

$$|\langle\mu_\theta\rangle_\Omega| \le C\|F_{\log,\phi}(\phi_\theta,\psi_\theta)\|_{L^1} + C\|F_{1,\phi}(\phi_\theta,\psi_\theta)\|_{L^1},$$

and by (3.43) we deduce that $\langle\mu_\theta\rangle_\Omega$ is uniformly bounded in $L^2(0,T)$. Hence, by the Poincaré inequality we obtain

$$\|\mu_\theta\|_{L^2(Q)} \le C. \tag{3.44}$$

The uniform estimates (3.41) and (3.44) allows us to deduce, along a non-relabelled subsequence $\theta\to 0$, the existence of limit functions $(\phi_*,\psi_*,\mu_*,z_*)$ such that

$$\begin{aligned}&\phi_\theta \to \phi_* \text{ weakly* in } L^\infty(0,T;H^1(\Omega))\cap H^1(0,T;H^1(\Omega)^*),\\ &\phi_\theta \to \phi_* \text{ strongly in } C^0([0,T];L^s(\Omega)) \text{ and a.e. in } Q,\\ &\psi_\theta \to \psi_* \text{ weakly* in } L^\infty(0,T;H^2_{\boldsymbol{n}}(\Omega))\cap H^1(0,T;L^2(\Omega)),\\ &\psi_\theta \to \psi_* \text{ strongly in } C^0([0,T];W^{1,s}(\Omega)) \text{ and a.e. in } Q,\\ &\mu_\theta \to \mu_* \text{ weakly in } L^2(0,T;H^1(\Omega)),\\ &z_\theta \to z_* \text{ weakly in } L^2(Q),\end{aligned} \tag{3.45}$$

for any $s < \infty$ in two dimensions and any $s \in [2,6)$ in three dimensions, along with $(\phi_*, \psi_*) \in \mathcal{K}$ for a.e. $(x,t) \in Q$ as well as attainment of the initial conditions $\phi_*(0) = \phi_0$ and $\psi_*(0) = \psi_0$. Passing to the limit in (2.3a)-(2.3b) for $(\phi_\theta, \psi_\theta, \mu_\theta, z_\theta)$ yields the analogous identities for $(\phi_*, \psi_*, \mu_*, z_*)$. Next, we consider an arbitrary obstacle-admissible test function pair $(\zeta, \eta) \in L^2(0,T; H^1(\Omega) \times H^2_{\boldsymbol{n}}(\Omega))$ in (3.34) for $(\phi_\theta, \psi_\theta, \mu_\theta, z_\theta)$ expressed as

$$\begin{aligned} 0 \leq \int_Q \big(F_{1,\phi}(\phi_\theta, \psi_\theta) - \mu_\theta\big)(\zeta - \phi_\theta) + \nabla(\varepsilon\phi_\theta - \sigma\psi_\theta) \cdot \nabla(\zeta - \phi_\theta) \, dx \, dt \\ + \int_Q \Delta\psi_\theta \Delta(\eta - \psi_\theta) - \sigma \nabla\phi_\theta \cdot \nabla(\eta - \psi_\theta) + \big(F_{1,\psi}(\phi_\theta, \psi_\theta) - z_\theta\big)(\eta - \psi_\theta) \, dx \, dt \\ + \int_Q \big(2\lambda\omega^2 \Delta\psi_\theta + \lambda\omega^4(\psi_\theta - \tfrac{1}{2})\big)(\eta - \psi_\theta) + F_{\log}(\zeta, \eta) - F_{\log}(\phi_\theta, \psi_\theta) \, dx \, dt. \end{aligned}$$

Due to the definition of F_0 in (1.6) and the continuity of $F_{\log}$ over $\mathcal{K}$ we see that

$$\Big| \int_Q F_{\log}(\zeta, \eta) - F_{\log}(\phi_\theta, \psi_\theta) \, dx \, dt \Big| \leq C\theta \to 0$$

as $\theta \to 0$. Employing the compactness assertions in (3.45) and weak lower semicontinuity of the Bochner norms, we obtain as $\theta \to 0$

$$\begin{aligned} 0 \leq \int_Q \big(F_{1,\phi}(\phi_*, \psi_*) - \mu_*\big)(\zeta - \phi_*) + \nabla(\varepsilon\phi_* - \sigma\psi_*) \cdot \nabla(\zeta - \phi_*) \, dx \, dt \\ + \int_Q \Delta\psi_* \Delta(\eta - \psi_*) - \sigma \nabla\phi_* \cdot \nabla(\eta - \psi_*) + \big(F_{1,\psi}(\phi_*, \psi_*) - z_*\big)(\eta - \psi_*) \, dx \, dt \\ + \int_Q \big(2\lambda\omega^2 \Delta\psi_* + \lambda\omega^4(\psi_* - \tfrac{1}{2})\big)(\eta - \psi_*) \, dx \, dt. \end{aligned}$$

Via a similar calculation to the proof of uniqueness in Section 3.2 we find that $(\phi_*, \psi_*, \mu_*, z_*)$ is the unique variational solution to (1.5) with the obstacle potential (1.7), whence in fact $\Delta\psi_* \in L^2(0,T; H^1(\Omega))$. Furthermore, by uniqueness of variational solutions we infer that the whole sequence $\{(\phi_\theta, \psi_\theta, \mu_\theta, z_\theta)\}_{\theta \in (0,1]}$ converges, and by the density of $L^2(0,T; H^2_{\boldsymbol{n}}(\Omega))$ in $L^2(0,T; H^1(\Omega))$ we recover (2.5) holding for arbitrary obstacle-admissible test function pair $(\zeta, \eta) \in L^2(0,T; H^1(\Omega))^2$.

3.4.2 Convergence rate

Let $(\phi_\theta, \psi_\theta, \mu_\theta, z_\theta)$ be the variational solution to (1.5) with the logarithmic potential (1.6) associated with the initial conditions (ϕ_0, ψ_0), and let $(\phi_*, \psi_*, \mu_*, z_*)$ be the variational solution to (1.5) with the obstacle potential (1.7) associated with the same initial conditions. We denote by $\widehat{\phi}_\theta := \phi_* - \phi_\theta$, $\widehat{\psi}_\theta := \psi_* - \psi_\theta$, $\widehat{\mu}_\theta := \mu_* - \mu_\theta$, and $\widehat{z}_\theta := z_* - z_\theta$ the differences between variational solutions and incidentally remark that $\widehat{\phi}_\theta$ is of zero mean value as $\langle \widehat{\phi}_\theta \rangle_\Omega = \langle \phi_* - \phi_\theta \rangle_\Omega = \langle \phi_0 \rangle_\Omega - \langle \phi_0 \rangle_\Omega = 0$.

Similar to the proof of uniqueness, we consider the variational inequality (2.5) for $(\phi_*, \psi_*, \mu_*, z_*)$ with test function pair $(\zeta, \eta) = (\phi_\theta, \psi_\theta)$ which we note is obstacle-admissible, as well as the alternate variational inequality (3.34) for $(\phi_\theta, \psi_\theta, \mu_\theta, z_\theta)$ with test function pair $(\zeta, \eta) = (\phi_*, \psi_*)$ which satisfies $F_{\log}(\phi_*, \psi_*) \in L^1(Q)$. Then, upon summing, we

obtain

$$\begin{aligned}
&\int_\Omega \big(F_{1,\phi}(\phi_*,\psi_*) - F_{1,\phi}(\phi_\theta,\psi_\theta) - \widehat{\mu}_\theta\big)\widehat{\phi}_\theta + \nabla(\varepsilon\widehat{\phi}_\theta - \sigma\widehat{\psi}_\theta)\cdot\nabla\widehat{\phi}_\theta\,dx \\
&\quad + \int_\Omega -\lambda\nabla\Delta\widehat{\psi}_\theta\cdot\nabla\widehat{\psi}_\theta + \big(F_{1,\psi}(\phi_*,\psi_*) - F_{1,\psi}(\phi_\theta,\psi_\theta) - \widehat{z}_\theta\big)\widehat{\psi}_\theta - \sigma\nabla\widehat{\phi}_\theta\cdot\nabla\widehat{\psi}_\theta \\
&\quad + \int_\Omega (2\lambda\omega^2\Delta\widehat{\psi}_\theta + \lambda\omega^4\widehat{\psi}_\theta)\widehat{\psi}_\theta\,dx \\
&\le \int_\Omega F_{\log}(\phi_*,\psi_*) - F_{\log}(\phi_\theta,\psi_\theta)\,dx \le C\theta,
\end{aligned}$$

where for the right-hand side we have used the definition (1.6) and the continuity of $F_{\log}$ over $\mathcal{K}$. Analogously, from the difference between (2.3a) and (2.3b) for $(\phi_*,\psi_*,\mu_*,z_*)$ and $(\phi_\theta,\psi_\theta,\mu_\theta,z_\theta)$, and choosing $u=\mathcal{N}(\widehat{\phi}_\theta)$ and $v=\widehat{\psi}_\theta$, we obtain

$$0 = \frac{1}{2}\frac{d}{dt}\|\nabla\mathcal{N}(\widehat{\phi}_\theta)\|^2 + \int_\Omega \widehat{\mu}_\theta\widehat{\psi}_\theta\,dx, \quad 0 = \frac{1}{2}\frac{d}{dt}\|\widehat{\psi}_\theta\|^2 + \int_\Omega \widehat{z}_\theta\widehat{\phi}_\theta\,dx.$$

Then, upon adding these inequalities we deduce similar to Section 3.2,

$$\begin{aligned}
&\frac{1}{2}\frac{d}{dt}\Big(\|\nabla\mathcal{N}(\widehat{\phi}_\theta)\|^2 + \|\widehat{\psi}_\theta\|^2\Big) + \frac{1}{4}\|\nabla\widehat{\phi}_\theta\|^2 + \frac{\lambda}{2}\|\Delta\widehat{\psi}_\theta\|^2 \\
&\quad \le C\Big(\|\nabla\mathcal{N}(\widehat{\phi}_\theta)\|^2 + \|\widehat{\psi}_\theta\|^2\Big) + C\theta
\end{aligned}$$

with constants independent of θ. Application of the Gronwall inequality and the elliptic regularity estimate (3.9) leads to (2.9).

4 Numerical discretization

In this section we introduce a finite element approximation of the system (1.5) with the obstacle potential (1.7) based on a suitable variational formulation that is then discretized with piecewise linear finite elements. We establish an unconditional stability result, introduce an iterative solution method for implementation and then present several numerical simulations, which exhibit a wide range of complex pattern formations.

4.1 Weak formulation

For notational convenience, we let $(\cdot,\cdot)$ denote the L^2–inner product on Ω, and define

$$K := \{\,(\eta_1,\eta_2)\in[H^1(\Omega)]^2 : (\eta_1(x),\eta_2(x))\in\mathcal{K} \text{ a.e. in } \Omega\,\}.$$

Furthermore, we introduce an auxiliary variable $q=-\Delta\psi$ and consider the following variational formulation for (1.5) with the obstacle potential (1.7). Find $(\phi,\psi)\in L^2(0,T;K)\cap(H^1(0,T;(H^1(\Omega))^*))^2$, $z\in L^2(0,T;L^2(\Omega))$ and $(\mu,q)\in(L^2(0,T;H^1(\Omega)))^2$ such that for almost all $t\in(0,T)$

$$0 = \langle\partial_t\phi,u\rangle + (\nabla\mu,\nabla u), \tag{4.1a}$$

$$0 = \langle\partial_t\psi,v\rangle + (z,v), \tag{4.1b}$$

$$\begin{aligned}
0 \le\ & (\nabla\phi - \sigma\nabla\psi, \nabla(\eta-\phi)) + (F_{1,\phi}(\phi,\psi) - \mu, \eta-\phi) \\
&+ (\lambda\omega^4(\psi-\tfrac{1}{2}) - z + F_{1,\psi}(\phi,\psi), \zeta-\psi) \\
&+ (\lambda\nabla q - 2\lambda\omega^2\nabla\psi - \sigma\nabla\phi, \nabla(\zeta-\psi)),
\end{aligned} \tag{4.1c}$$

$$0 = (\nabla\psi,\nabla\theta) - (q,\theta), \tag{4.1d}$$

for all $(\eta, \zeta) \in K$ and $(u, v, \theta) \in H^1(\Omega) \times L^2(\Omega) \times H^1(\Omega)$. This weak formulation can be derived from Definition 2.2 with the help of the new variable $q = -\Delta\psi$. For the numerical approximation we prefer the formulation (4.1) because this weak formulation can be solved with piecewise linear continuous functions at the discrete level.

4.2 Finite element approximation

We assume that Ω is a polyhedral domain and let $\mathcal{T}_h$ be a regular triangulation of Ω into disjoint open simplices. Associated with $\mathcal{T}_h$ is the piecewise linear finite element space

$$S^h = \left\{ \zeta \in C^0(\overline{\Omega}) : \zeta_{|_o} \in P_1(o) \, \forall o \in \mathcal{T}_h \right\},$$

where we denote by $P_1(o)$ the set of all affine linear functions on o, cf. [7]. In addition, we define

$$K^h = K \cap S^h,$$

and let $(\cdot, \cdot)^h$ be the usual mass lumped L^2–inner product on Ω associated with $\mathcal{T}_h$. Finally, τ denotes a chosen uniform time step size.

For what follows we assume that F_1 can be decomposed into $F_1 = F_1^+ + F_1^-$, with F_1^+ being convex and F_1^- being concave. For example, in the case (1.4) we set

$$F_1^+(\phi, \psi) = \frac{C_F}{2}(\phi^2 + \psi^2), \tag{4.2a}$$

$$F_1^-(\phi, \psi) = -\frac{\alpha}{2}\phi^2 - \frac{g}{3}(\psi - \tfrac{1}{2})^3 - \frac{\gamma}{2}(\psi - \tfrac{1}{2})^2 + \frac{\delta}{2}\phi^2(\psi - \tfrac{1}{2}) - \frac{C_F}{2}(\phi^2 + \psi^2), \tag{4.2b}$$

where $C_F \geq 0$ is a constant chosen sufficiently large. In fact, choosing

$$C_F = \max\left(0, \frac{3}{2}|\delta| - \alpha, |\delta| + |g| - \gamma\right) \tag{4.3}$$

ensures that the Hessian

$$H = \begin{pmatrix} -\alpha - C_F + \delta(\psi - \frac{1}{2}) & \delta\phi \\ \delta\phi & -\gamma - 2g(\psi - \frac{1}{2}) - C_F \end{pmatrix} = \begin{pmatrix} H_{11} & H_{12} \\ H_{12} & H_{22} \end{pmatrix}$$

of F_1^- satisfies $H_{11} \leq -|\delta|$, $H_{12} \leq -|\delta|$, $H_{11}H_{22} \geq \delta^2$, and thus $\operatorname{tr} H \leq 0$ and $\det H \geq 0$ in $\mathcal{K}$. It follows that F_1^- with the choice (4.3) is indeed concave in $\mathcal{K}$.

Then our finite element approximation of (4.1) is given as follows. Let $(\phi_h^0, \psi_h^0) \in K^h$. Then, for $n \geq 0$ and given $(\phi_h^n, \psi_h^n) \in K^h$, find $(\phi_h^{n+1}, \psi_h^{n+1}) \in K^h$ and $(\mu_h^{n+1}, z_h^{n+1}, q_h^{n+1}) \in [S^h]^3$ such that

$$0 = \tfrac{1}{\tau}(\phi_h^{n+1} - \phi_h^n, u_h)^h + (\nabla\mu_h^{n+1}, \nabla u_h), \tag{4.4a}$$

$$0 = \tfrac{1}{\tau}(\psi_h^{n+1} - \psi_h^n, v_h)^h + (z_h^{n+1}, v_h)^h, \tag{4.4b}$$

$$\begin{aligned} 0 \leq {} & (\varepsilon\nabla\phi_h^{n+1} - \tfrac{\sigma}{2}\nabla(\psi_h^{n+1} + \psi_h^n), \nabla(\eta_h - \phi_h^{n+1})) \\ & + (F_{1,\phi}^+(\phi_h^{n+1}, \psi_h^{n+1}) + F_{1,\phi}^-(\phi_h^n, \psi_h^n) - \mu_h^{n+1}, \eta_h - \phi_h^{n+1})^h \\ & + (\lambda\omega^4(\psi_h^{n+1} - \tfrac{1}{2}) - z_h^{n+1} + F_{1,\psi}^+(\phi_h^{n+1}, \psi_h^{n+1}) + F_{1,\psi}^-(\phi_h^n, \psi_h^n), \zeta_h - \psi_h^{n+1})^h \\ & + (\lambda\nabla q_h^{n+1} - 2\lambda\omega^2\nabla\psi_h^{n+1} - \tfrac{\sigma}{2}\nabla(\phi_h^{n+1} + \phi_h^n), \nabla(\zeta_h - \psi_h^{n+1})), \end{aligned} \tag{4.4c}$$

$$0 = (\nabla\psi_h^{n+1}, \nabla\theta_h) - (q_h^{n+1}, \theta_h)^h, \tag{4.4d}$$

for all $(\eta_h, \zeta_h) \in K^h$ and $(u_h, v_h, \theta_h) \in [S^h]^3$.

The convex-concave splitting of F_1 allows for an unconditional stability estimate for the discrete energy

$$E^n = \frac{\varepsilon}{2}\|\nabla\phi_h^n\|^2 + (F_1(\phi_h^n,\psi_h^n),1)^h - \sigma(\phi_h^n,q_h^n)^h + \frac{\lambda}{2}\|\omega^2(\psi_h^n - \tfrac{1}{2}) - q_h^n\|_h^2, \tag{4.5}$$

where $\|u_h\|_h = [(u,u)^h]^{\frac{1}{2}}$, and where $q_h^0 \in S^h$ is defined by (4.4d) with $n+1$ replaced by 0. Note that since q_h^n approximates $q = -\Delta\psi$, the energy (4.5) is a discrete analogue of (1.3).

Theorem 4.1. *Let $(\phi_h^{n+1},\psi_h^{n+1},\mu_h^{n+1},z_h^{n+1},q_h^{n+1})$ be a solution to (4.4). Then it holds that*

$$E^{n+1} + \tau\|\nabla\mu_h^{n+1}\|^2 + \tau\|z_h^{n+1}\|_h^2 \le E^n. \tag{4.6}$$

Moreover, there exists a constant $E_{\min}\in\mathbb{R}$ such that

$$E^n \ge E_{\min} + \frac{\lambda}{8}\|q_h^n\|_h^2 + \frac{\varepsilon}{2}\|\nabla\phi_h^n\|^2 \quad \text{for all } n\ge 0.$$

Proof. Choosing $u_h = \tau\mu_h^{n+1}$ in (4.4a), $v_h = \tau z_h^{n+1}$ in (4.4b) and $(\zeta_h,\eta_h) = (\phi_h^n,\psi_h^n)$ in (4.4c), we obtain upon summing

$$\begin{aligned}
0 \ge\ & (\varepsilon\nabla\phi_h^{n+1}, \nabla(\phi_h^{n+1}-\phi_h^n)) + (F_{1,\phi}^+(\phi_h^{n+1},\psi_h^{n+1}) + F_{1,\phi}^-(\phi_h^n,\psi_h^n), \phi_h^{n+1}-\phi_h^n)^h \\
&+ \tau\|\nabla\mu_h^{n+1}\|^2 - \tfrac{\sigma}{2}(\nabla(\psi_h^{n+1}+\psi_h^n), \nabla(\phi_h^{n+1}-\phi_h^n)) \\
&+ (\lambda\omega^4(\psi_h^{n+1}-\tfrac{1}{2}) + F_{1,\psi}^+(\phi_h^{n+1},\psi_h^{n+1}) + F_{1,\psi}^-(\phi_h^n,\psi_h^n), \psi_h^{n+1}-\psi_h^n)^h \\
&+ \tau\|z_h^{n+1}\|_h^2 + (\lambda\nabla q_h^{n+1} - 2\lambda\omega^2\nabla\psi_h^{n+1} - \tfrac{\sigma}{2}\nabla(\phi_h^{n+1}+\phi_h^n), \nabla(\psi_h^{n+1}-\psi_h^n)).
\end{aligned} \tag{4.7}$$

Furthermore, we see that

$$\begin{aligned}
&\tfrac{\sigma}{2}(\nabla(\psi_h^{n+1}+\psi_h^n), \nabla(\phi_h^{n+1}-\phi_h^n)) + \tfrac{\sigma}{2}(\nabla(\phi_h^{n+1}+\phi_h^n), \nabla(\psi_h^{n+1}-\psi_h^n)) \\
&\quad = \sigma(\nabla\psi_h^{n+1}, \nabla\phi_h^{n+1}) - \sigma(\nabla\psi_h^n, \nabla\phi_h^n) = \sigma(\phi_h^{n+1}, q_h^{n+1})^h - \sigma(\phi_h^n, q_h^n)^h,
\end{aligned} \tag{4.8}$$

while by the convexity of F_1^+ and concavity of F_1^- we have that

$$\begin{aligned}
&(F_{1,\phi}^+(\phi_h^{n+1},\psi_h^{n+1}), \phi_h^{n+1}-\phi_h^n)^h + (F_{1,\psi}^+(\phi_h^{n+1},\psi_h^{n+1}), \psi_h^{n+1}-\psi_h^n)^h \\
&\qquad + (F_{1,\phi}^-(\phi_h^n,\psi_h^n), \phi_h^{n+1}-\phi_h^n)^h + (F_{1,\psi}^-(\phi_h^n,\psi_h^n), \psi_h^{n+1}-\psi_h^n)^h \\
&\quad \ge (F_1^+(\phi_h^{n+1},\psi_h^{n+1}),1)^h - (F_1^+(\phi_h^n,\psi_h^n),1)^h \\
&\qquad + (F_1^-(\phi_h^{n+1},\psi_h^{n+1}),1)^h - (F_1^-(\phi_h^n,\psi_h^n),1)^h \\
&\quad = (F_1(\phi_h^{n+1},\psi_h^{n+1}) - F_1(\phi_h^n,\psi_h^n),1)^h.
\end{aligned} \tag{4.9}$$

Combining (4.7), (4.8) and (4.9) yields

$$\begin{aligned}
0 \ge\ & \frac{\varepsilon}{2}\|\nabla\phi_h^{n+1}\|^2 - \frac{\varepsilon}{2}\|\nabla\phi_h^n\|^2 + \frac{\varepsilon}{2}\|\nabla(\phi_h^{n+1}-\phi_h^n)\|^2 \\
&+ (F_1(\phi_h^{n+1},\psi_h^{n+1}) - F_1(\phi_h^n,\psi_h^n),1)^h + \tau\|\nabla\mu_h^{n+1}\|^2 + \tau\|z_h^{n+1}\|_h^2 \\
&- \sigma(\phi_h^{n+1},q_h^{n+1})^h + \sigma(\phi_h^n,q_h^n)^h + (\lambda\omega^4(\psi_h^{n+1}-\tfrac{1}{2}), \psi_h^{n+1}-\psi_h^n)^h \\
&+ (\lambda\nabla q_h^{n+1} - 2\lambda\omega^2\nabla\psi_h^{n+1}, \nabla(\psi_h^{n+1}-\psi_h^n)).
\end{aligned} \tag{4.10}$$

Moreover, taking the difference between (4.4d) at instance $n+1$ and n, and choosing $\theta = -\lambda q_h^{n+1}$ in the subsequent difference yields

$$(\nabla(\psi_h^{n+1}-\psi_h^n), \lambda\nabla q_h^{n+1}) = \lambda(q_h^{n+1}-q_h^n, q_h^{n+1})^h = \frac{\lambda}{2}\left(\|q_h^{n+1}\|_h^2 - \|q_h^n\|_h^2 + \|q_h^{n+1}-q_h^n\|_h^2\right).$$

Hence, together with (4.10), we obtain

$$
\begin{aligned}
0 \geq\ & \frac{\varepsilon}{2}\|\nabla\phi_h^{n+1}\|^2 - \frac{\varepsilon}{2}\|\nabla\phi_h^n\|^2 + \frac{\varepsilon}{2}\|\nabla(\phi_h^{n+1}-\phi_h^n)\|^2 \\
& + (F_1(\phi_h^{n+1},\psi_h^{n+1}) - F_1(\phi_h^n,\psi_h^n),1)^h \\
& + \tau\|\nabla\mu_h^{n+1}\|^2 + \tau\|z_h^{n+1}\|_h^2 - \sigma(\phi_h^{n+1},q_h^{n+1})^h + \sigma(\phi_h^n,q_h^n)^h \\
& + \frac{\lambda}{2}\Big(\|q_h^{n+1}\|_h^2 - 2\omega^2\|\nabla\psi_h^{n+1}\|^2 + \omega^4\|\psi_h^{n+1}-\tfrac{1}{2}\|_h^2\Big) \\
& - \frac{\lambda}{2}\Big(\|q_h^{n}\|_h^2 - 2\omega^2\|\nabla\psi_h^{n}\|^2 + \omega^4\|\psi_h^{n}-\tfrac{1}{2}\|_h^2\Big) \\
& + \frac{\lambda}{2}\Big(\|q_h^{n+1}-q_h^n\|_h^2 - 2\omega^2\|\nabla(\psi_h^{n+1}-\psi_h^n)\|^2 + \omega^4\|\psi_h^{n+1}-\psi_h^n\|_h^2\Big).
\end{aligned}
\tag{4.11}
$$

Using the relation $\|\nabla\psi_h^k\|^2 = (q_h^k, \psi_h^k - \frac{1}{2})^h$ for $k = n$ and $k = n+1$, recall (4.4d), we see that

$$
\begin{aligned}
\|q_h^k\|_h^2 - 2\omega^2\|\nabla\psi_h^k\|^2 + \omega^4\|\psi_h^k-\tfrac{1}{2}\|_h^2 &= (|q_h^k|^2 - 2\omega^2 q_h^k(\psi_h^k-\tfrac{1}{2}) + \omega^4|\psi_h^k-\tfrac{1}{2}|^2,1)^h \\
&= \|\omega^2(\psi_h^k-\tfrac{1}{2}) - q_h^k\|_h^2
\end{aligned}
$$

for $k \in \{n, n+1\}$, and similarly

$$
\begin{aligned}
&\|q_h^{n+1}-q_h^n\|_h^2 - 2\omega^2\|\nabla(\psi_h^{n+1}-\psi_h^n)\|^2 + \omega^4\|\psi_h^{n+1}-\psi_h^n\|_h^2 \\
&\quad = \|q_h^{n+1}-q_h^n\|_h^2 - 2\omega^2(q_h^{n+1}-q_h^n,\psi_h^{n+1}-\psi_h^n)^h + \omega^4\|\psi_h^{n+1}-\psi_h^n\|_h^2 \\
&\quad = \|\omega^2(\psi_h^{n+1}-\psi_h^n) - (q_h^{n+1}-q_h^n)\|_h^2.
\end{aligned}
$$

This allows us to express (4.11) as

$$
\begin{aligned}
0 \geq\ & E^{n+1} - E^n + \frac{\varepsilon}{2}\|\nabla(\phi_h^{n+1}-\phi_h^n)\|^2 + \tau\|\nabla\mu_h^{n+1}\|^2 + \tau\|z_h^{n+1}\|_h^2 \\
& + \frac{\lambda}{2}\|\omega^2(\psi_h^{n+1}-\psi_h^n) - (q_h^{n+1}-q_h^n)\|_h^2,
\end{aligned}
$$

which proves the desired result (4.6). The lower bound follows from the fact that $(\phi_h^n, \psi_h^n) \in K^h$, since then

$$
\begin{aligned}
E^n &\geq |\Omega| \min_{\mathcal{K}} F_1 - \frac{2\sigma^2}{\lambda}|\Omega| - \frac{\lambda}{8}\|q_h^n\|_h^2 + \frac{\lambda}{2}\|\omega^2(\psi_h^n-\tfrac{1}{2}) - q_h^n\|_h^2 + \frac{\varepsilon}{2}\|\nabla\phi_h^n\|^2 \\
&\geq |\Omega| \min_{\mathcal{K}} F_1 - \frac{2\sigma^2}{\lambda}|\Omega| - \frac{\lambda}{8}\|q_h^n\|_h^2 + \frac{\lambda}{2}\left(\omega^2\|\psi_h^n-\tfrac{1}{2}\|_h - \|q_h^n\|_h\right)^2 + \frac{\varepsilon}{2}\|\nabla\phi_h^n\|^2 \\
&\geq |\Omega| \min_{\mathcal{K}} F_1 - \frac{2\sigma^2}{\lambda}|\Omega| - \frac{\lambda}{8}\|q_h^n\|_h^2 + \frac{\lambda}{2}\left(\tfrac{1}{2}\|q_h^n\|_h^2 - 2\omega^4\|\psi_h^n-\tfrac{1}{2}\|_h^2\right) + \frac{\varepsilon}{2}\|\nabla\phi_h^n\|^2 \\
&\geq |\Omega| \min_{\mathcal{K}} F_1 - \frac{2\sigma^2}{\lambda}|\Omega| - \frac{\lambda\omega^4}{4}|\Omega| + \frac{\lambda}{8}\|q_h^n\|_h^2 + \frac{\varepsilon}{2}\|\nabla\phi_h^n\|^2.
\end{aligned}
$$

This completes the proof. □

4.3 Iterative solution method

Following [3] we now discuss a possible algorithm to solve the resulting system of algebraic equations for $(\phi_h^{n+1}, \psi_h^{n+1}, \mu_h^{n+1}, z_h^{n+1}, q_h^{n+1})$ arising at each time level from the finite element approximation (4.4). To this end, let $\mathcal{J}$ denotes the number of nodes of $\mathcal{T}^h$. Then,

on introducing the obvious notations, the system (4.4) can be written in matrix-vector form as follows. Find $(\Phi^{n+1},\Psi^{n+1})\in\mathcal{K}^{\mathcal{J}}$ and $W^{n+1},Z^{n+1},Q^{n+1}\in\mathcal{R}^{\mathcal{J}}$ such that

$$
\begin{aligned}
&M\Phi^{n+1}+\tau AW^{n+1}=M\Phi^{n}, && \text{(4.12a)}\\
&M\Psi^{n+1}+\tau MZ^{n+1}=M\Psi^{n}, && \text{(4.12b)}\\
&(\eta_h-\Phi^{n+1})^{\top}(\varepsilon A\Phi^{n+1}-\tfrac{\sigma}{2}A\Psi^{n+1}+MF^{+}_{1,\phi}(\Phi^{n+1},\Psi^{n+1})-MW^{n+1}) && \text{(4.12c)}\\
&\quad+(\zeta_h-\Psi^{n+1})^{\top}(\lambda\omega^4M\Psi^{n+1}-\tfrac{\sigma}{2}A\Phi^{n+1}-MZ^{n+1}+MF^{+}_{1,\psi}(\Phi^{n+1},\Psi^{n+1})\\
&\qquad\qquad+\lambda AQ^{n+1}-2\lambda\omega^2A\Psi^{n+1})\\
&\geq(\eta_h-\Psi^{n+1})^{\top}R^{n}+(\zeta_h-\Psi^{n+1})^{\top}S^{n}\quad\forall\,(\eta_h,\zeta_h)\in\mathcal{K}^{\mathcal{J}},\\
&A\Psi^{n+1}-MQ^{n+1}=0, && \text{(4.12d)}
\end{aligned}
$$

where M and A denote the lumped mass matrix and stiffness matrix, respectively, $R^n=\frac{\sigma}{2}A\Psi^n-MF^{-}_{1,\phi}(\Phi^n,\Psi^n)$ and $S^n=\frac{1}{2}\lambda\omega^4M\underline{1}-MF^{-}_{1,\psi}(\Phi^n,\Psi^n)+\frac{\sigma}{2}A\Phi^n$.

Let $A=A_D-A_L-A_L^{\top}$ and recall that M is a diagonal matrix. Then we can formulate a "Gauss–Seidel type" iterative scheme as follows. Given $(\Phi^{n+1,0},\Psi^{n+1,0})\in\mathcal{K}^{\mathcal{J}}$ and $W^{n+1,0},Z^{n+1,0},Q^{n+1,0}\in\mathcal{R}^{\mathcal{J}}$, for $k\geq 0$ find $(\Phi^{n+1,k+1},\Psi^{n+1,k+1})\in\mathcal{K}^{\mathcal{J}}$ and $W^{n+1,k+1},Z^{n+1,k+1},Q^{n+1,k+1}\in\mathcal{R}^{\mathcal{J}}$ such that

$$
\begin{aligned}
&M\Phi^{n+1,k+1}+\tau(A_D-A_L)W^{n+1,k+1}=M\Phi^{n}+\tau A_L^{\top}W^{n+1,k}, && \text{(4.13a)}\\
&M\Psi^{n+1,k+1}+\tau MZ^{n+1,k+1}=M\Psi^{n}, && \text{(4.13b)}\\
&(\eta_h-\Phi^{n+1,k+1})^{\top}(\varepsilon(A_D-A_L)\Phi^{n+1,k+1}-\tfrac{\sigma}{2}(A_D-A_L)\Psi^{n+1,k+1} && \text{(4.13c)}\\
&\qquad\qquad+MF^{+}_{1,\phi}(\Phi^{n+1,k+1},\Psi^{n+1,k+1})-MW^{n+1,k+1})\\
&\quad+(\zeta_h-\Psi^{n+1,k+1})^{\top}(\lambda\omega^4M\Psi^{n+1,k+1}-\tfrac{\sigma}{2}(A_D-A_L)\Phi^{n+1,k+1}-MZ^{n+1,k+1}\\
&\qquad\qquad+MF^{+}_{1,\psi}(\Phi^{n+1,k+1},\Psi^{n+1,k+1})\\
&\quad+\lambda(A_D-A_L)Q^{n+1,k+1}-2\lambda\omega^2(A_D-A_L)\Psi^{n+1,k+1})\\
&\geq(\eta_h-\Phi^{n+1,k+1})^{\top}(R^{n}+\varepsilon A_L^{\top}\Phi^{n+1,k}-\tfrac{\sigma}{2}A_L^{\top}\Psi^{n+1,k})\\
&\qquad+(\zeta_h-\Psi^{n+1,k+1})^{\top}(S^{n}-\frac{\sigma}{2}A_L^{\top}\Phi^{n+1,k}+\lambda A_L^{\top}Q^{n+1,k}-2\lambda\omega^2A_L^{\top}\Psi^{n+1,k})\\
&\qquad\qquad\qquad\qquad\qquad\qquad\forall\,(\eta_h,\zeta_h)\in\mathcal{K}^{\mathcal{J}},\\
&(A_D-A_L)\Psi^{n+1,k+1}-MQ^{n+1,k+1}=A_L^{\top}\Psi^{n+1,k}. && \text{(4.13d)}
\end{aligned}
$$

From now on we fix our discussion to the choice (4.2). Then (4.13) can be explicitly solved for $j=1,\ldots,\mathcal{J}$. To this end let

$$
\begin{aligned}
r_1&=M\Phi^{n}+\tau(A_LW^{n+1,k+1}+A_L^{\top}W^{n+1,k}),\\
r_2&=R^{n}+\varepsilon A_L\Phi^{n+1,k+1}+\varepsilon A_L^{\top}\Phi^{n+1,k}-\tfrac{\sigma}{2}A_L\Psi^{n+1,k+1}-\tfrac{\sigma}{2}A_L^{\top}\Psi^{n+1,k}),\\
r_3&=M\Psi^{n},\\
r_4&=S^{n}-\tfrac{\sigma}{2}A_L\Phi^{n+1,k+1}-\tfrac{\sigma}{2}A_L^{\top}\Phi^{n+1,k}+\lambda(A_LQ^{n+1,k+1}+A_L^{T}Q^{n+1,k})\\
&\quad-2\lambda\omega^2(A_L\Psi^{n+1,k+1}+A_L^{\top}\Psi^{n+1,k}),\\
r_5&=A_L\Psi^{n+1,k+1}+A_L^{\top}\Psi^{n+1,k}.
\end{aligned}
$$

Then $(\Phi_j^{n+1,k+1},\Psi_j^{n+1,k+1})$ is the solution of the following problem: Find $(\Phi_j,\Psi_j)\in\mathcal{K}$ such that, for every $(\eta_h,\zeta_h)\in\mathcal{K}$,

$$
(\eta_h-\Phi_j)^{\top}(\alpha_{11}\Phi_j-\alpha_{12}\Psi_j-\beta_1)+(\zeta_h-\Psi_j)^{\top}(\alpha_{22}\Psi_j-\alpha_{12}\Phi_j-\beta_2)\geq 0, \qquad \text{(4.14)}
$$

where $\alpha_{12} = \frac{\sigma}{2} A_{jj}$. The values of $\alpha_{11}, \beta_1, \alpha_{22}, \beta_2$ can be identified from the above, on writing, for $j = 1, ..., \mathcal{J}$,

$$\begin{aligned} W_j^{n+1,k+1} &= ([r_1]_j - M_{jj}\Phi_j^{n+1,k+1})/(\tau A_{jj}), \\ Z_j^{n+1,k+1} &= ([r_3]_j - M_{jj}\Psi_j^{n+1,k+1})/(\tau M_{jj}), \\ Q_j^{n+1,k+1} &= -([r_5]_j - A_{jj}\Psi_j^{n+1,k+1})/M_{jj}, \end{aligned} \tag{4.15}$$

and then substituting these into the variational inequality in (4.13). In fact, overall we obtain

$$\begin{aligned} \alpha_{11} &= \varepsilon A_{jj} + C_F M_{jj} + M_{jj}^2/(\tau A_{jj}), \\ \beta_1 &= [r_2]_j + M_{jj}[r_1]_j/(\tau A_{jj}), \\ \alpha_{22} &= (\lambda^{\frac{1}{2}}\omega^2 M_{jj}^{\frac{1}{2}} - \lambda^{\frac{1}{2}} A_{jj} M_{jj}^{-\frac{1}{2}})^2 + C_F M_{jj} + M_{jj}/\tau, \\ \beta_2 &= [r_4]_j + [r_3]_j/\tau + \lambda A_{jj}[r_5]_j/M_{jj}. \end{aligned}$$

We can rewrite (4.14) as

$$\begin{pmatrix} \eta_h - \Phi_j \\ \zeta_h - \Psi_j \end{pmatrix}^T \mathfrak{A} \left[\begin{pmatrix} \Phi_j \\ \Psi_j \end{pmatrix} - \mathfrak{A}^{-1} \begin{pmatrix} \beta_1 \\ \beta_2 \end{pmatrix} \right] \geq 0 \quad \forall\ (\eta_h, \zeta_h) \in \mathcal{K}, \tag{4.16}$$

where $\mathfrak{A} = \left(\begin{smallmatrix} \alpha_{11} & -\alpha_{12} \\ -\alpha_{12} & \alpha_{22} \end{smallmatrix}\right)$. The matrix is symmetric positive definite if $\alpha_{12}^2 < \alpha_{11}\alpha_{22}$, which is guaranteed as long as the time step size τ is chosen sufficiently small. In that case, the unique solution to (4.16) is

$$(\Phi_j, \Psi_j) = \mathrm{P}_{\mathcal{K}}^{\mathfrak{A}} \left(\mathfrak{A}^{-1} \begin{pmatrix} \beta_1 \\ \beta_2 \end{pmatrix} \right),$$

where $\mathrm{P}_{\mathcal{K}}^{\mathfrak{A}}(x_1, x_2)$ is the orthogonal projection of the point $\underline{x} = (x_1, x_2)^\top \in \mathbb{R}^2$ onto $\mathcal{K}$ with respect to the inner product $\langle \underline{p}, \underline{q} \rangle_{\mathfrak{A}} := \underline{p}^T \mathfrak{A}\, \underline{q}$. The projection $\underline{y} = \mathrm{P}_{\mathcal{K}}^{\mathfrak{A}}(\underline{x})$ can be computed as follows.

1. If $\underline{x} \in \mathcal{K}$, then $\underline{y} = \underline{x}$, else
2. If $x_2 \leq 0$ then $\underline{y} := (\max\{-1, \min\{x_1 - \frac{\sigma}{2\alpha_{11}} x_2, 1\}\}, 0)^\top$, else
3. If $x_1 \geq 0$ then $\underline{v} := (1, -1)^\top$, else $\underline{v} := -(1, 1)^\top$.
4. $\gamma := \dfrac{\langle \underline{x} - (0,1)^\top, \underline{v} \rangle_{\mathfrak{A}}}{\|\underline{v}\|_{\mathfrak{A}}^2}$.
5. $\underline{y} := (0,1)^\top + \min\{\max\{\gamma, 0\}, 1\}\, \underline{v}$.

Having found $(\Phi_j^{n+1,k+1}, \Psi_j^{n+1,k+1}) = (\Phi_j, \Psi_j)$ from (4.14), we can then find $W_j^{n+1,k+1}$, $Z_j^{n+1,k+1}$ and $Q_j^{n+1,k+1}$ via (4.15). Repeating this procedure for $j = 1, \ldots, \mathcal{J}$ we obtain the solution to (4.13). In practice the iteration (4.13) is performed until a suitable stopping criterion is met.

4.4 Numerical simulations

We implemented the scheme (4.4) with the help of the finite element toolbox ALBERTA, see [27]. To increase computational efficiency, we employ adaptive meshes, which have a

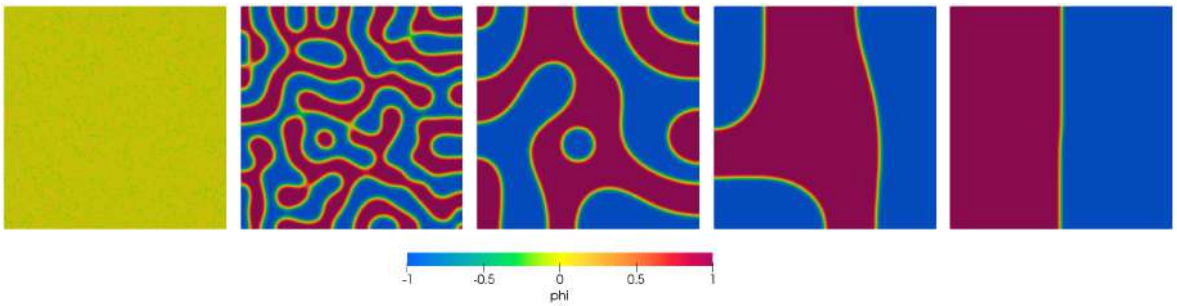

Figure 2: Spinodal decomposition for CH. We display ϕ_h^n at times $t = 0$, 10^{-4}, 0.001, 0.01, 1.

finer mesh size h_f within the regions $|\phi_h^n| < 1$ and a coarser mesh size h_c in the regions $|\phi_h^n| = 1$, see [2, 3, 4] for a more detailed description.

In all our numerical simulations we make use of the splitting (4.2) for F_1 as defined in (1.4), together with the choice (4.3) for the value of C_F.

Throughout the numerical experiments we set $\Omega = (-\frac{1}{2}, \frac{1}{2})^d$ and use $\varepsilon = \frac{1}{16\pi}$ and $\lambda = 10^{-5}$. For the computations for Cahn–Hilliard (CH) and Cahn–Hilliard–Swift–Hohenberg (CHSH) we let $\alpha = 100$, unless stated otherwise. For the computations for Swift–Hohenberg (SH) and CHSH, unless otherwise stated, we always set $\omega = 100$ and $\delta = \sigma = 0$. Of course, for CH we set $\lambda = g = \gamma = \delta = \sigma = 0$, while for SH we use $\alpha = \delta = \sigma = 0$. Moreover, for the initial data for CH and CHSH we always choose a random ϕ_0 with zero mean value and values inside $[-0.01, 0.01]$, while for SH we simply set $\phi_0 = 0$. Similarly, for SH we choose a random ψ_0 with mean 0.5 and values inside $[0.49, 0.51]$, while for CHSH we set $\psi_0 = \frac{1}{2}(1 - |\phi_0|)$, and for CH we use $\psi_0 = 0$.

For demonstrative purposes, we begin with a simulation for CH in two dimensions. Then, the usual spinodal decomposition can be observed in Figure 2. The color map shown in Figure 2 will be used throughout for the visualizations of ϕ_h^n. Next we consider some simulations for SH, in order to obtain some insights into the role of the different parameters in the free energy of the system. Here we ran our finite element approximation for a very long time, until the numerical solutions ψ_h^n have settled on a stable profile, or changed only very little. These profiles, for different parameters, are visualized in Figure 3. The color map shown in Figure 3 will be used throughout for the visualizations of ψ_h^n. In the first row of Figure 3 we can see that increasing the value of ω leads to a higher frequency of the observed oscillations. In the second row we see that increasing γ, with $\omega = 100$ fixed, leads to more intricate patterns. Finally, the third row demonstrates that increasing $|g|$, while keeping $\omega = 100$ and $\gamma = 10$ fixed, leads to the phase $\psi = 1$ being preferred, so that small islands of the phase $\psi = 0$ are created. If we now combine the parameters from Figure 2 and the last image in the second row of Figure 3 for the full CHSH model, we see a dramatically different evolution. We refer to Figure 4 for the numerical results, which can be compared to Figure 7f in [23]. As a comparison we show the time evolution for SH on its own in Figure 5. Comparing the evolving patterns in Figure 4, with the pure CH evolution in Figure 2 and the pure SH evolution in Figure 5, we note that only by combining the two gives rise to the kind of complex patterns that motivates our current study.

If we repeat the CHSH simulation from Figure 4 for a smaller value of γ, we obtain the results in Figure 6. We observe that they show some resemblance to the patterns in [23].

Our next simulations investigate the effect of the parameter g on the CHSH evolutions.

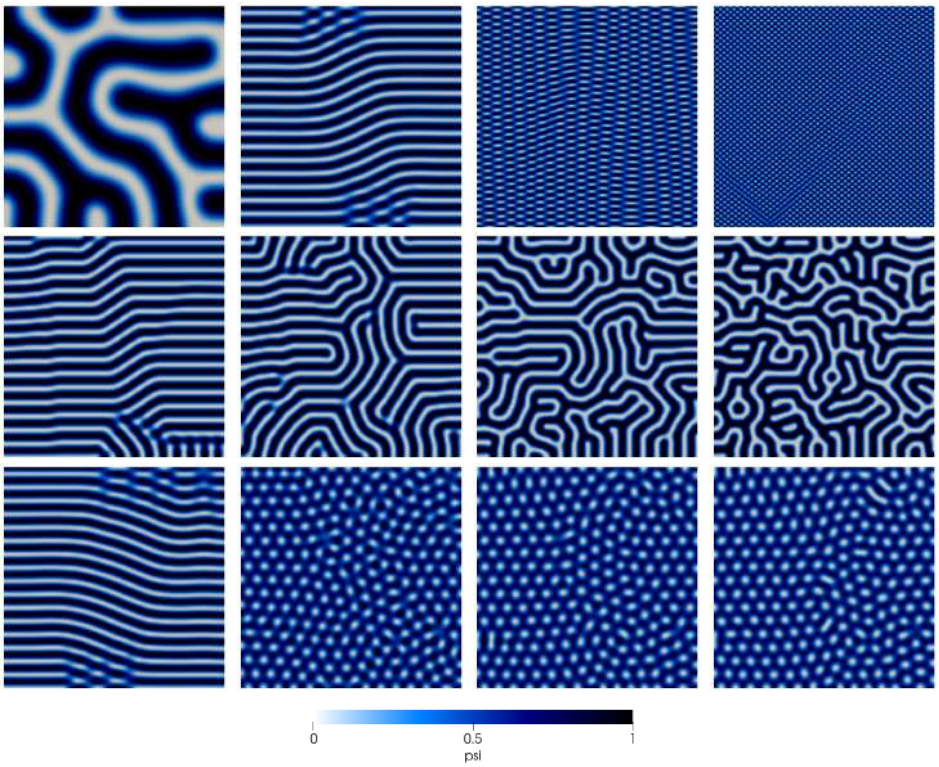

Figure 3: Obtained steady states for SH. First row: $g = 0$, $\gamma = 10$ and $\omega = 30, 100, 200, 300$. Second row: $\omega = 100$, $g = 0$ and $\gamma = 100, 200, 500, 1000$. Third row: $\omega = 100$, $\gamma = 10$ and $g = -100, -150, -500, -1000$.

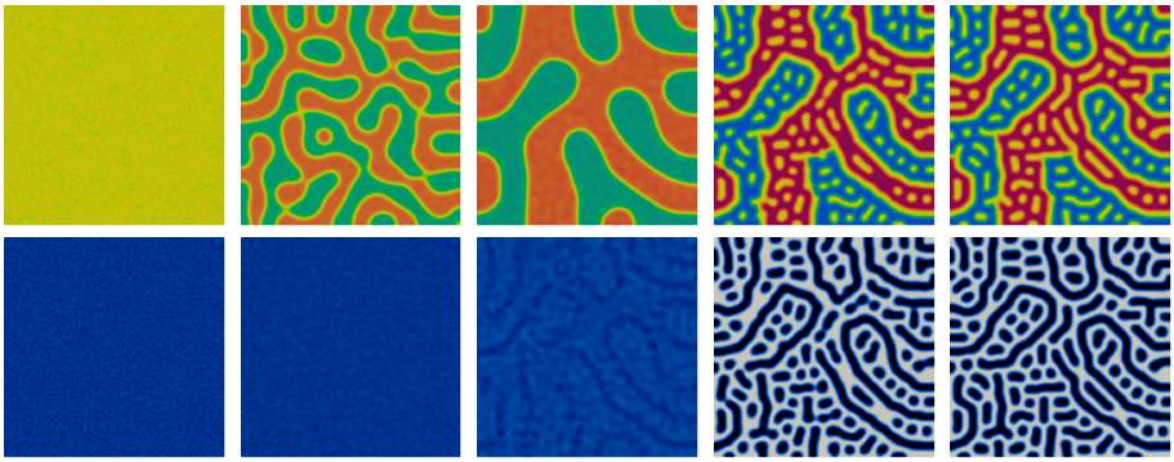

Figure 4: Computation for CHSH with $g = 0$, $\gamma = 1000$. We display ϕ_h^n at times $t = 0$, 10^{-4}, 0.001, 0.01, 0.1. Below we show ψ_h^n at the same times.

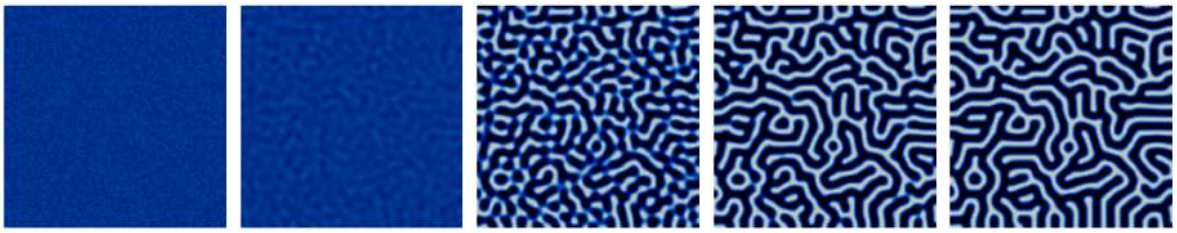

Figure 5: Computation for SH with $g = 0$, $\gamma = 1000$. (Compare with Figure 4.) We display ψ_h^n at times $t = 0$, 0.001, 0.005, 0.01, 0.1.

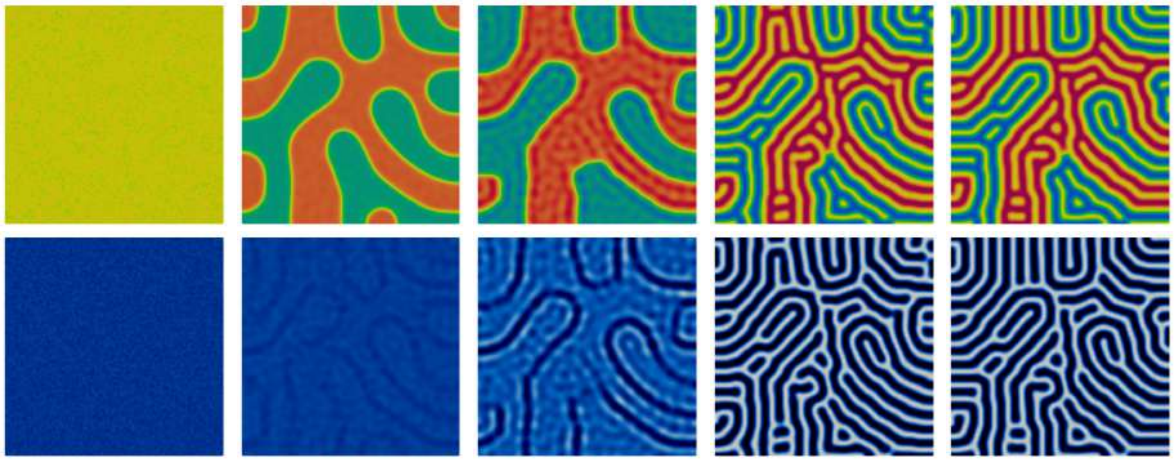

Figure 6: Computation for CHSH with $g = 0$, $\gamma = 500$. We display ϕ_h^n at times $t = 0$, 0.001, 0.005, 0.05, 0.5. Below we show ψ_h^n at the same times.

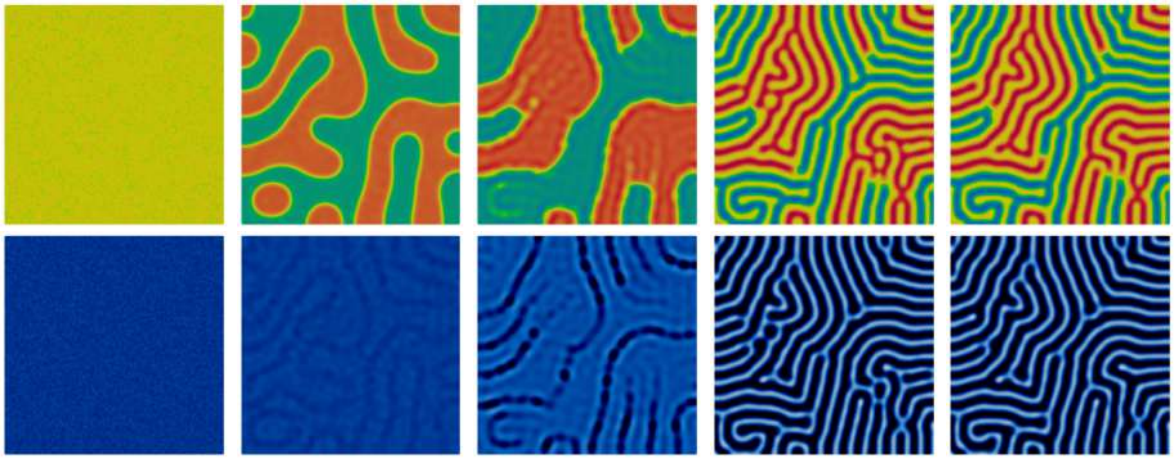

Figure 7: The same as Figure 6, but with $g = 2000$. We display ϕ_h^n at times $t = 0$, 0.001, 0.005, 0.05, 0.5. Below we show ψ_h^n at the same times.

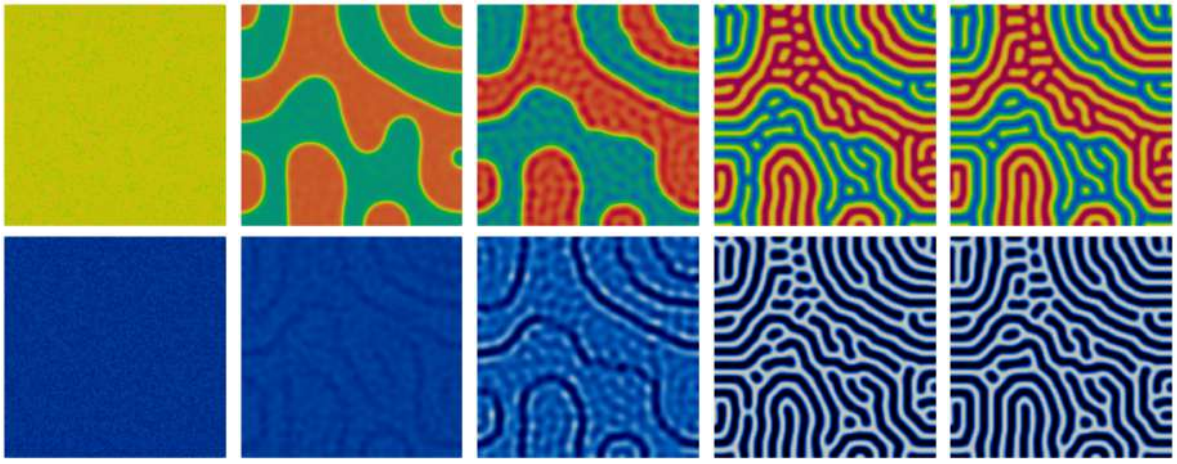

Figure 8: The same as Figure 6, but with $g = -300$. We display ϕ_h^n at times $t = 0$, 0.001, 0.005, 0.05, 0.5. Below we show ψ_h^n at the same times.

An experiment with $g = 2000$ can be seen in Figure 7. Here the phase $\psi = 1$ is preferred by the evolution, which in turn has an effect on the pattern that develops for ϕ. Numerical simulations with $g \in \{-300, -1000, -2000\}$ can be seen in Figures 8, 9 and 10, respectively. In Figure 10 we observe the formation of islands in ϕ and ψ, cf. Figure 7d in [23].

Varying the value of δ leads to the evolution in Figure 11 for $\delta = 200$, and the evolution in Figure 12 for $\delta = -100$. It can be seen that in the two pure phases of ϕ, the value of ψ is very small when $\delta > 0$ while ψ is close to 1 when $\delta < 0$. This is the expected behavior attributed to the term $\frac{\delta}{2}\phi^2(\psi - \frac{1}{2})$ in the total free energy.

Finally, a computation for $\sigma = 0.05$ can be seen in Figure 13. The presence of the σ term in the energy leads to the absence of oscillations in the phase characterized by $\phi = 1$ and $\psi = 0$. If we use the larger value $\alpha = 200$, then this effects becomes even more pronounced, see Figure 14 and compare to Figure 7b in [23].

We conclude this section with some numerical simulations in three dimensions shown in Figures 15, 16 and 17. All the parameters are chosen as in the corresponding two dimensional experiments in Figures 2, 4 and 5.

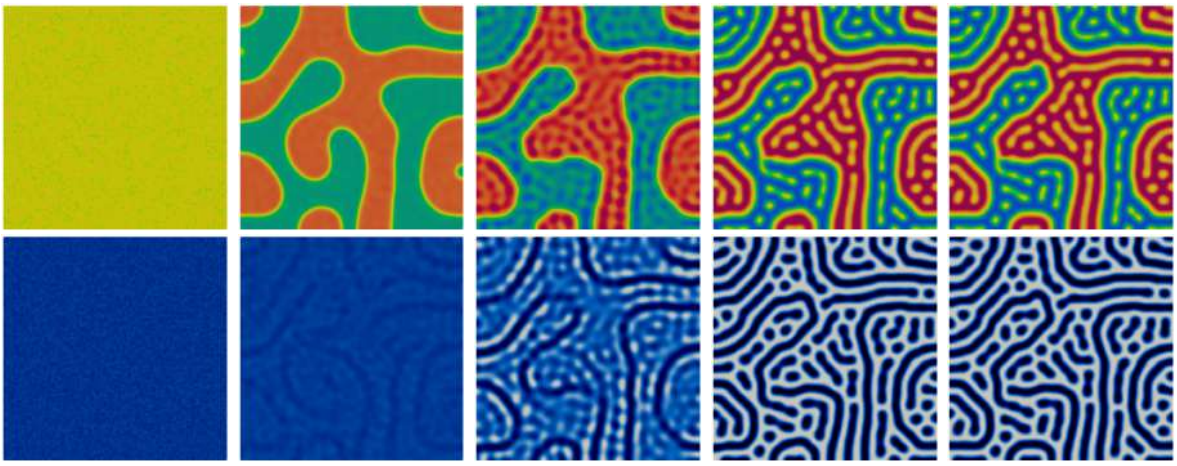

Figure 9: The same as Figure 6, but with $g = -1000$. We display ϕ_h^n at times $t = 0$, 0.001, 0.005, 0.05, 0.5. Below we show ψ_h^n at the same times.

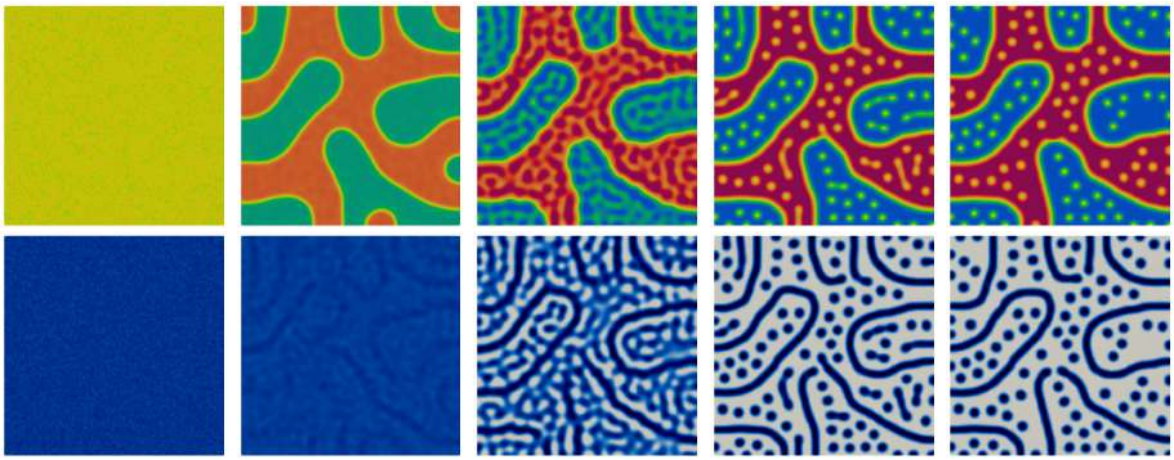

Figure 10: The same as Figure 6, but with $g = -2000$. We display ϕ_h^n at times $t = 0$, 0.001, 0.005, 0.05, 0.5. Below we show ψ_h^n at the same times.

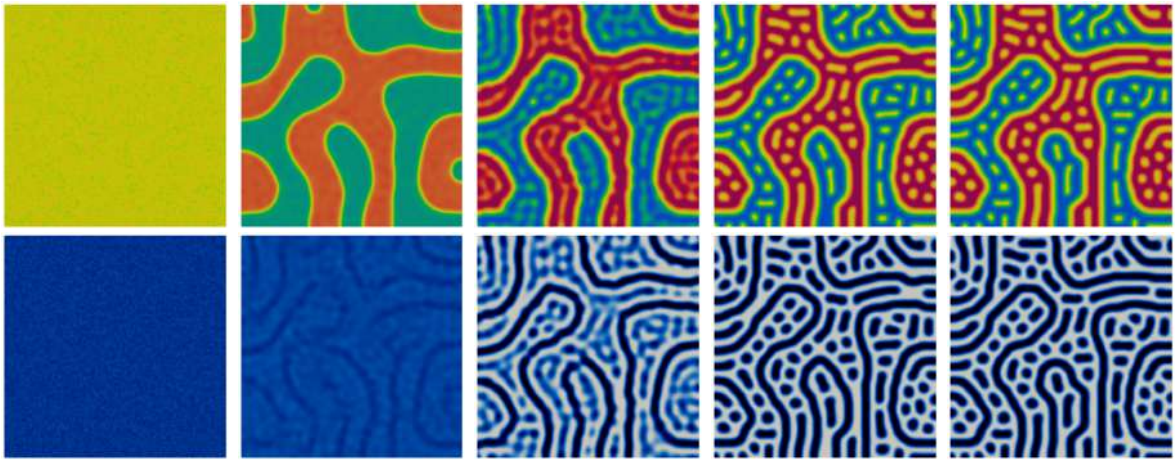

Figure 11: The same as Figure 6, but with $\delta = 200$. We display ϕ_h^n at times $t = 0$, 0.001, 0.005, 0.05, 0.5. Below we show ψ_h^n at the same times.

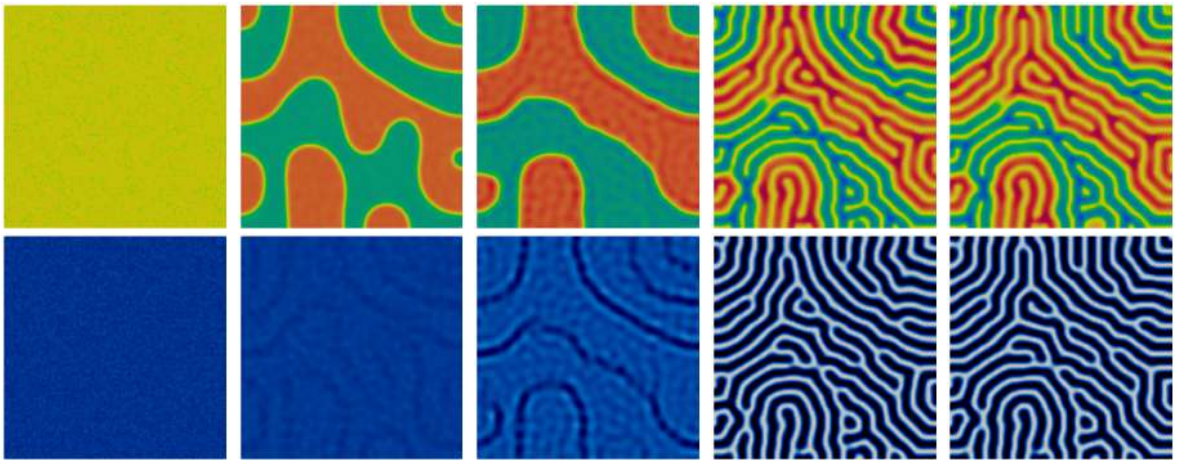

Figure 12: The same as Figure 6, but with $\delta = -100$. We display ϕ_h^n at times $t = 0$, 0.001, 0.005, 0.05, 0.5. Below we show ψ_h^n at the same times.

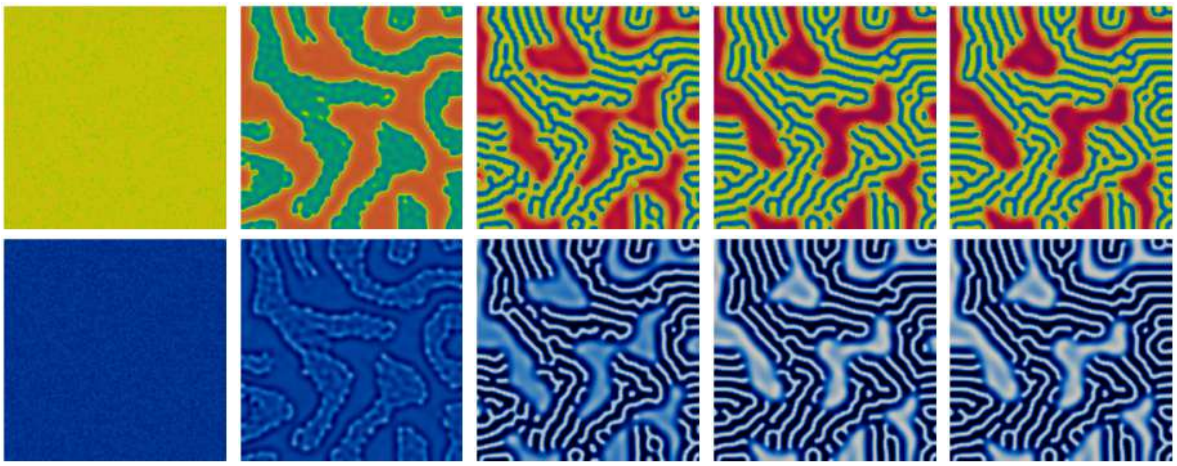

Figure 13: The same as Figure 6, but with $\sigma = 0.05$. We display ϕ_h^n at times $t = 0$, 0.001, 0.005, 0.05, 0.5. Below we show ψ_h^n at the same times.

Figure 14: The same as Figure 6, but with $\sigma = 0.05$ and $\alpha = 200$. We display ϕ_h^n at times $t = 0$, 0.001, 0.005, 0.05, 0.5. Below we show ψ_h^n at the same times.

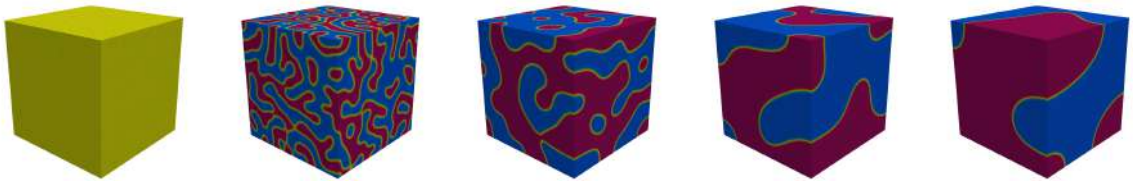

Figure 15: Spinodal decomposition for CH. We display ϕ_h^n at times $t = 0$, 10^{-4}, 0.001, 0.01, 0.05.

Figure 16: Computation for SH with $g = 0$, $\gamma = 1000$. We display ψ_h^n at times $t = 0$, 0.001, 0.005, 0.01, 0.1.

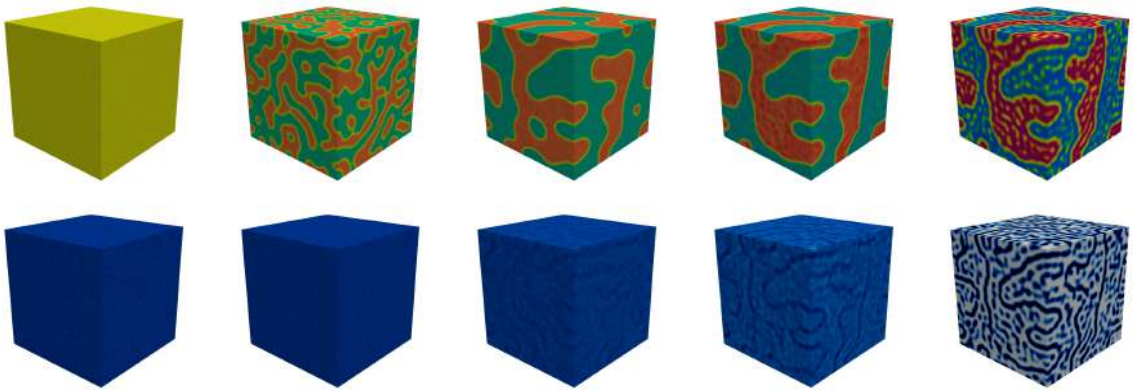

Figure 17: Computation for CHSH with $g = 0$, $\gamma = 1000$. We display ϕ_h^n at times $t = 0$, 10^{-4}, 0.001, 0.002, 0.005. Below we show ψ_h^n at the same times.

Acknowledgements

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