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MINIMIZERS FOR THE CAHN–HILLIARD ENERGY FUNCTIONAL UNDER STRONG ANCHORING CONDITIONS*

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Abstract. We study analytically and numerically the minimizers for the Cahn–Hilliard energy functional with a symmetric quartic double-well potential and under a strong anchoring condition (i.e., the Dirichlet condition) on the boundary of an underlying bounded domain. We show a bifurcation phenomenon determined by the boundary value and a parameter that describes the thickness of a transition layer separating two phases of an underlying system of binary mixtures. For the case that the boundary value is exactly the average of the two pure phases, if the bifurcation parameter is larger than or equal to a critical value, then the minimizer is unique and is exactly the homogeneous state. Otherwise, there are exactly two symmetric minimizers. The critical bifurcation value is inversely proportional to the first eigenvalue of the negative Laplace operator with the zero Dirichlet boundary condition. For a boundary value that is larger (or smaller) than that of the average of the two pure phases, the symmetry is broken and there is only one minimizer. We also obtain the bounds and morphological properties of the minimizers under additional assumptions on the domain. Our analysis utilizes the notion of the Nehari manifold and connects it to the eigenvalue problem for the negative Laplacian with the homogeneous boundary condition. We numerically minimize the functional E by solving the gradient-flow equation of E, i.e., the Allen–Cahn equation, with the designated boundary conditions, and with random initial values. We present our numerical simulations and discuss them in the context of our analytical results.

Key words. Cahn–Hilliard functional, minimizations, strong anchoring condition, bifurcation

AMS subject classifications. 35B36, 35B30, 35Q92, 49J40

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1. Introduction.

We consider the Cahn–Hilliard functional for the free energy of a binary mixture [8]

$$E[u] = \int_\Omega \left[\frac{\kappa}{2}|\nabla u|^2 + W(u)\right] dx, \qquad u \in H^1(\Omega). \tag{1.1}$$

Here, Ω is a bounded domain in $\mathbb{R}^d$ ($d = 2$ or 3) with a C^2 boundary, $\kappa > 0$ is a constant, and W is a double-well potential with two equal depth minima at $u = u^-$ and $u = u^+$, respectively, where u^- and u^+ are given distinct real numbers. We call u^- and u^+ the two pure phases. To be concrete, we consider the quartic double-well potential

$$W(u) = \gamma(u - u^-)^2(u - u^+)^2 \qquad (u \in \mathbb{R}), \tag{1.2}$$

where $\gamma > 0$ is a constant. Such form of a double-well potential is also generally used in application. Common examples include (1) $W(u) = 18u^2(u-1)^2$ with $u^- = 0$ and

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$u^+ = 1$, where the prefactor 18 is chosen so that

$$\int_0^1 \sqrt{2W(u)}\, du = 1;$$

and (2) $W(u) = (1/4)(u^2 - 1)^2$ with $u^- = -1$ and $u^+ = 1$.

If the energy $E[u]$ is small and the system described by the function u is not in a single, pure phase, then it decomposes the system region Ω into mainly two regions or phases $\{u = u^-\}$ and $\{u = u^+\}$, respectively. The parameter $\kappa > 0$, if it is small, then characterizes the width of the transition layer where u changes from $u \approx u^-$ to $u \approx u^+$. To be more precise, the thickness of the transition layer is $O(\sqrt{\kappa})$ as $0 < \kappa \ll 1$. Indeed, it is known that as $\kappa \to 0$ the functional $E =: E_\kappa$ converges in some sense to the area functional (with a possible multiplicity constant); cf. [36, 39]. Recently, Dai, Li, and Lu [16] proved that, as $\kappa \to 0$, the first variation of the Cahn–Hilliard functional converges to the mean curvature which is the first variation of the area functional.

The Cahn–Hilliard functional, and the related Cahn–Hilliard equation and Allen–Cahn equation that govern the dynamics of relaxing the Cahn–Hilliard energy with respect to the $H^{-1}(\Omega)$ and $L^2(\Omega)$ inner product, respectively, have been useful modeling tools to understand many physical properties of an underlying system of binary mixtures or other two-phase material. Such properties include the phase separation, coarsening dynamics, and pattern formation. An important issue arising from such modeling of the system confined spatially in a region Ω is the treatment of the interaction of the mixture with the boundary $\partial\Omega$. Mathematically, this corresponds to boundary conditions on u. A common choice of such a boundary condition is the Neumann condition in which $\partial_n u = \nabla u \cdot n$ is prescribed on the boundary $\partial\Omega$, where n is the exterior unit normal at the boundary $\partial\Omega$ (cf., e.g., [3, 1, 2, 7, 19, 26, 32, 38, 40]). Enforcing the homogeneous (i.e., zero) Neumann condition is equivalent to requiring ∇u to be perpendicular to the normal vector n of $\partial\Omega$. Since ∇u is perpendicular to the level surfaces of u, we see that a necessary condition resulting from the zero Neumann condition is that, near the boundary $\partial\Omega$, the level surfaces of u are perpendicular to $\partial\Omega$. Thus the geometric shape of $\partial\Omega$ affects u. Periodic boundary conditions are also commonly used in the related studies, particularly computational studies (cf., e.g., [9, 11, 14, 15, 23, 28, 30, 31, 12, 41]).

In this work, we consider the Dirichlet boundary condition in which the value of u at each point of the boundary $\partial\Omega$ is prescribed (or the trace of u on the boundary $\partial\Omega$ is prescribed). Mathematically this means we have a prescribed function g defined on $\partial\Omega$, and u needs to match g on the boundary. The Dirichlet boundary condition $u = g$ on $\partial\Omega$ requires a pointwise match, which is the strongest possible match. Thus we call it the strong anchoring condition. There are other ways to measure how well u matches g on the boundary. For instance, we may require the $L^2(\Omega)$-norm $\|u - g\|_{L^2(\partial\Omega)}$ to be sufficiently small, say smaller than a prescribed tolerance. We call such matches weak anchoring conditions. Strong anchoring conditions are critical in physical modeling. For instance, such conditions can describe the ambient medium which is at rest relative to front motion inside the confined region Ω [18]. Such boundary conditions also come into play in systems where the patterns are modulated through templates on the boundary (cf. [33] and references therein).

We notice that only a few studies have been concerned with the Dirichlet boundary conditions, particularly in terms of the analysis of the minimizers of the functional or solution to the corresponding equation. For instance, Du and Nicolaides [18] proposed

a finite element scheme for the 1D Cahn–Hilliard equation using Dirichlet boundary conditions with the total energy decreasing in time. Bronsard and Hilhorst [5] studied the limiting behavior of the solution to the Cahn–Hilliard equation with the Dirichlet boundary condition using energy-type methods. Bates and Han [4] studied the existence, uniqueness, and continuous dependence on initial data of the solution for a nonlocal Cahn–Hilliard equation with Dirichlet boundary conditions on a bounded domain. Li et al. [34] presented a conservative numerical method for the Cahn–Hilliard equation with Dirichlet boundary conditions in complex domains. Garcke and Lam [25] established the well-posedness of the system equipped with Dirichlet boundary conditions for regular potentials with polynomial growth of order less than six and also the existence and uniqueness of weak solutions for some singular potentials.

Our main results of analysis consist of two parts.

(1) If the boundary value is the average of the two pure phases, then there is a bifurcation of the minimizer for the Cahn–Hilliard energy functional. Such bifurcation depends on the value of κ/γ. If this value is larger than or equal to a critical value that is inversely proportional to the first eigenvalue of the negative Laplace operator with the homogeneous Dirichlet boundary condition, then the minimizer is unique and is exactly the homogeneous state. Otherwise, there are exactly two symmetric minimizers.

(2) For a boundary value that is in between the average of the two pure phases and one of them, the symmetry is broken, and there is only one minimizer which is in the same range.

Our analysis utilizes the notion of the Nehari manifold and connects it to the eigenvalue problem for the negative Laplacian with the homogeneous boundary condition. To gain insight into our analysis, we carry out numerical simulations. We minimize the Cahn–Hilliard functional E by solving the gradient-flow equation, i.e., the Allen–Cahn equation, with the strong anchoring boundary conditions. We use uniformly distributed random initial values and seek positive solutions.

The rest of the paper is organized as follows: In section 2, we state our main theorems. In section 3, we introduce the notion of the Nehari manifold and prove some of its properties that will be used in proving our main theorems. In sections 4 and 5, we prove our main theorems. In section 6, we present numerical simulations to showcase the theoretical results. Finally, in section 7, we draw conclusions and point out directions for further explorations.

2. Main theorems. Let $g \in H^{1/2}(\partial\Omega)$. Using the direct method in the calculus of variations, one can prove that the Cahn–Hilliard energy functional E defined in (1.1) has a minimizer in the admissible set

$$\mathcal{A}_g := \left\{ u \in H^1(\Omega) : \, u = g \text{ on } \partial\Omega \right\}; \tag{2.1}$$

see, for instance, [20, 21]. Due to the nonconvexity of $W(u)$, the minimizer is generally not unique. Every minimizer $u \in \mathcal{A}_g$ satisfies the time-independent Allen–Cahn equation

$$-\kappa\Delta u + W'(u) = 0 \qquad \text{in } \Omega \tag{2.2}$$

in the sense that

$$\langle \delta E[u], v \rangle = \int_\Omega \left[\kappa \nabla u \cdot \nabla v + W'(u) v \right] dx = 0 \qquad \forall v \in H_0^1(\Omega). \tag{2.3}$$

Note that the first equality above defines the first variation $\delta E[u] : H_0^1(\Omega) \to \mathbb{R}$ of the energy functional E at u as a bounded linear functional of $H_0^1(\Omega)$, i.e., $\delta E[u] \in H^{-1}(\Omega)$ (the dual space of $H_0^1(\Omega)$).

In this paper, we study the morphology of minimizers for E when the boundary data g satisfy one of the following three conditions on $\partial\Omega$:

(i) $g(x) \equiv \frac{u^+ + u^-}{2}$ for all $x \in \partial\Omega$;
(ii) $\frac{u^+ + u^-}{2} < g(x) < u^+$ for all $x \in \partial\Omega$;
(iii) $u^- < g(x) < \frac{u^+ + u^-}{2}$ for all $x \in \partial\Omega$.

One example of such a boundary function g is given by

$$g(x) = g_\alpha(x) := \alpha(x)u^+ + (1 - \alpha(x))u^- \qquad \text{on } \partial\Omega,$$

where $0 < \alpha(x) < 1$ is a function on $\partial\Omega$.

The study of case (i) is motivated in part by discussions in [17] on the existence of positive solution for nonlinear elliptic problems. In this case, since the boundary condition

$$u = \frac{u^+ + u^-}{2} \quad \text{on } \partial\Omega \tag{2.4}$$

keeps the symmetry of the functional E, there may exist more than one minimizer for E, but only when the parameter κ is small enough. Indeed, the parameter κ is a bifurcation parameter, with a critical value $4\gamma/\lambda_1$, where λ_1 is the first eigenvalue for the negative Laplace operator in Ω with the homogeneous Dirichlet boundary condition

$$-\Delta u = \lambda u \qquad \text{in } \Omega, \tag{2.5}$$

$$u = 0 \qquad \text{on } \partial\Omega. \tag{2.6}$$

For cases (ii) and (iii), it turns out there is a unique minimizer for E. In other words, the choice of boundary conditions breaks the symmetry of the energy functional E.

We summarize these results in the following two theorems.

THEOREM 2.1 (the case $g = (u^+ + u^-)/2$ on $\partial\Omega$). *Assume $g = (u_+ + u_-)/2$ on $\partial\Omega$.*

(i) *If $\kappa \geq 4\gamma/\lambda_1$, then the constant function $u = (u^+ + u^-)/2$ is the only minimizer for E in $\mathcal{A}_g$, and*

$$\min\{E[u] : u \in \mathcal{A}_g\} = \frac{\gamma(u^+ - u^-)^2}{4}|\Omega|.$$

(ii) *If $\kappa < 4\gamma/\lambda_1$, then there are exactly two minimizers, u_{pos} and u_{neg}, for E in $\mathcal{A}_g$, and*

$$\min\{E[u] : u \in \mathcal{A}_g\} < \frac{\gamma(u^+ - u^-)^2}{4}|\Omega|.$$

Moreover, these two minimizers u_{pos} and u_{neg} satisfy

$$u_{\text{pos}} + u_{\text{neg}} = u^- + u^+ \qquad \text{in } \Omega$$

and

$$u^- < u_{\text{neg}} < \frac{u^- + u^+}{2} < u_{\text{pos}} < u^+ \qquad \text{in } \Omega.$$

Remark. Suppose $g = (u_+ + u_-)/2$ on $\partial\Omega$. Suppose also that Ω is axial symmetric with respect to a hyperplane, say,

$$L := \{x = (x_1, x') \in \mathbb{R}^d : x_1 = 0 \text{ and } x' = (x_2, \dots, x_d)\},$$

in the sense that $(x_1, x') \in \Omega$ if and only if $(-x_1, x') \in \Omega$. Then it follows from a classical result of Gidas, Ni, and Nirenberg [27] (see also [29]) that the solution $u_{g,\mathrm{pos}}$ is an even function with respect to L, that is,

$$u_{g,\mathrm{pos}}(-x_1, x') = u_{g,\mathrm{pos}}(x_1, x') \qquad \forall (x_1, x') \in \Omega.$$

Furthermore,

$$\frac{\partial u_{g,\mathrm{pos}}}{\partial x_1}(x_1, x') < 0 \qquad \text{if } x_1 > 0.$$

If Ω is a ball, say, $\Omega = B(0, R)$, then the solution $u_{g,\mathrm{pos}}$ is radially symmetric, and

$$\frac{\partial u_{g,\mathrm{pos}}}{\partial r} < 0 \qquad \text{if } 0 < r < R.$$

Similar results hold for the solution $u_{g,\mathrm{neg}}$.

THEOREM 2.2 (the case $(u^+ + u^-)/2 < g < u^+$ on $\partial\Omega$ or $u^- < g < (u^+ + u^-)/2$ on $\partial\Omega$). *Let $g \in C(\partial\Omega)$.*

(i) *If $(u^+ + u^-)/2 < g < u^+$ on $\partial\Omega$, then there exists a unique minimizer $u_{g,\mathrm{pos}}$ for E in $\mathcal{A}_g$. Moreover,*

$$\min_{\partial\Omega} g < u_{g,\mathrm{pos}} < u^+ \qquad \text{in } \Omega.$$

(ii) *If $u^- < g < (u^+ + u^-)/2$ on $\partial\Omega$, then there exists a unique minimizer $u_{g,\mathrm{neg}}$ for E in $\mathcal{A}_g$. Moreover,*

$$u^- < u_{g,\mathrm{neg}} < \max_{\partial\Omega} g \qquad \text{in } \Omega.$$

To simplify the notation, we will rescale all the parameters in the Cahn–Hilliard functional and the boundary data g. We set

$$\tilde{u} := \frac{2u - (u^+ + u^-)}{u^+ - u^-}, \tag{2.7}$$

$$\tilde{g} := \frac{2g - (u^+ + u^-)}{u^+ - u^-}. \tag{2.8}$$

Then $u \in \mathcal{A}_{(u^+ + u^-)/2}$ if and only if $\tilde{u} \in H_0^1(\Omega)$, and more generally $u \in \mathcal{A}_g$ if and only if $\tilde{u} \in \mathcal{A}_{\tilde{g}}$. Moreover,

$$E[u] = \gamma(u^+ - u^-)^2 \int_\Omega \left[\frac{\tilde{\kappa}}{2}|\nabla\tilde{u}|^2 + \frac{1}{4}(\tilde{u}^2 - 1)^2\right] dx, \tag{2.9}$$

where $\tilde{\kappa} = \kappa/(4\gamma)$. We shall then consider the Cahn–Hilliard functional in the specific form of the integral above.

3. The Nehari manifold. We consider the functional

$$E[u] = \int_\Omega \left[\frac{\kappa}{2}|\nabla u|^2 + \frac{1}{4}(u^2-1)^2\right] dx, \qquad u \in H^1(\Omega). \tag{3.1}$$

We define the associated Nehari manifold [6]

$$S = \left\{u \in H_0^1(\Omega) : \langle \delta E[u], u\rangle = 0\right\}.$$

Thus, by (2.3), $u \in S$ if and only if $u \in H_0^1(\Omega)$ and

$$\int_\Omega \left[\kappa|\nabla u|^2 + W'(u)u\right] dx = 0. \tag{3.2}$$

It is clear that $0 \in S$ and every critical point of E lies in S.

LEMMA 3.1. *The set S is bounded in $H_0^1(\Omega)$.*

Proof. Let $u \in S$. We have by the definition of S that

$$\begin{aligned} 0 &= \int_\Omega \left(\kappa|\nabla u|^2 + u^4 - u^2\right) dx \\ &= \int_\Omega \left[\kappa|\nabla u|^2 + \frac{3u^4}{4} + \left(\frac{u^2}{2} - 1\right)^2 - 1\right] dx \\ &\geq \int_\Omega \left(\kappa|\nabla u|^2 + \frac{3u^4}{4} - 1\right) dx. \end{aligned} \tag{3.3}$$

Thus

$$\int_\Omega \left(\kappa|\nabla u|^2 + \frac{3u^4}{4}\right) dx \leq |\Omega|.$$

Hence

$$\|\nabla u\|_{L^2(\Omega)} \leq \sqrt{\frac{|\Omega|}{\kappa}}$$

and

$$\|u\|_{L^2(\Omega)} \leq |\Omega|^{1/4}\|u\|_{L^4(\Omega)} \leq \left(\frac{4}{3}|\Omega|^2\right)^{1/4}.$$

This completes the proof. ∎

Let $E|_S$ be the restriction of the energy functional E on the Nehari manifold S. We shall classify the local minimizers for $E|_S$ and show that some local minimizers of $E|_S$ are actually critical points of E. For each $u \in H^1(\Omega)$, we denote

$$F_u = \{su : s \in \mathbb{R}\} = \operatorname{Span}\{u\}$$

and call it the fiber associated to u. We define the fibering map (see, e.g., [6])

$$\Phi_u(s) := E[su] \qquad \forall s \in \mathbb{R}.$$

Clearly, if u is a local minimizer of E, then Φ_u has a local minimum at $s = 1$.

The first and second derivatives of the fibering map Φ_u are related to the first and second variations of E at u, respectively. Let $u \in H^1(\Omega)$. The first variation $\delta E[u]$ is defined in (2.3). The second variation $\delta^2 E[u] : H_0^1(\Omega) \times H_0^1(\Omega) \to \mathbb{R}$ of the functional E at u is defined by

$$\delta^2 E[u](v,w) = \int_\Omega \left[\kappa \nabla v \cdot \nabla w + W''(u)vw\right] dx \qquad \forall v, w \in H_0^1(\Omega). \tag{3.4}$$

LEMMA 3.2. *If $u \in H_0^1(\Omega)$, then*

$$\Phi_u'(s) = \langle \delta E[su], u \rangle = \int_\Omega \left[s\kappa |\nabla u|^2 + W'(su)u \right] dx, \tag{3.5}$$

$$\Phi_u''(s) = \delta^2 E[su](u,u) = \int_\Omega \left[\kappa |\nabla u|^2 \ + W''(su)u^2 \right] dx. \tag{3.6}$$

Proof. By the definition of Φ_u and (2.3), we have

$$\begin{aligned} \Phi_u'(s) &= \lim_{h\to 0} \frac{\Phi_u(s+h) - \Phi_u(s)}{h} \\ &= \lim_{h\to 0} \frac{E[(s+h)u] - E[su]}{h} \\ &= \langle \delta E[su], u \rangle \\ &= \int_\Omega \left[s\kappa |\nabla u|^2 + W(su)u \right] dx, \end{aligned}$$

leading to (3.5). Taking another derivative, we obtain that

$$\Phi_u''(s) = \int_\Omega \left[\kappa |\nabla u|^2 \ + W''(su)u^2 \right] dx = \delta^2 E[su](u,u),$$

leading to (3.6). ∎

COROLLARY 3.3. *If $u \in H_0^1(\Omega) \setminus \{0\}$ and $s \in \mathbb{R} \setminus \{0\}$, then $su \in S$ if and only if $\Phi_u'(s) = 0$.*

Proof. We have by (3.5) that

$$\Phi_u'(s) = \langle \delta E[su], u \rangle = \frac{1}{s} \langle \delta E[su], su \rangle ,$$

implying the assertion. ∎

Thus, $0 \neq u \in S$ if and only if $s = 1$ is a stationary point of $\Phi_u(s)$, i.e., u is a critical point of E restricted on the fiber F_u. It is therefore natural to split the manifold S into three parts, S^+, S^-, and S^0, corresponding to when u is a local minimum, local maximum, and point of inflection of E along the fiber F_u. Hence, we define

$$\begin{aligned} S^+ &= \left\{ u \in S : \delta^2 E[u](u,u) > 0 \right\}, \\ S^- &= \left\{ u \in S : \delta^2 E[u](u,u) < 0 \right\}, \\ S^0 &= \left\{ u \in S : \delta^2 E[u](u,u) = 0 \right\}. \end{aligned}$$

LEMMA 3.4. *Let $u_0 \in S - S^0$ be a local minimizer for $E|_S$. Then $\delta E[u_0] = 0$.*

Proof. If u_0 is a local minimizer for $E|_S$, then u_0 is a solution to the following optimization problem:

$$\begin{aligned} &\text{Minimize } E[u] \text{ among all } u \in H_0^1(\Omega) \\ &\text{subject to } \Gamma[u] := \int_\Omega \left[\kappa |\nabla u|^2 + W'(u)u \right] dx = 0. \end{aligned}$$

Then there exists a Lagrange multiplier $\mu \in \mathbb{R}$ such that $\delta E[u_0] = \mu \delta \Gamma[u_0]$ in the sense that

$$\langle \delta E[u_0], v\rangle = \mu \langle \delta \Gamma[u_0], v\rangle \qquad \forall v \in H_0^1(\Omega). \tag{3.7}$$

Since $u_0 \in S \subset H_0^1(\Omega)$, we have

$$0 = \langle \delta E[u_0], u_0\rangle = \mu \langle \delta \Gamma[u_0], u_0\rangle . \tag{3.8}$$

On the other hand,

$$\begin{aligned}
\langle \delta \Gamma[u_0], u_0\rangle &= \int_\Omega \left[2\kappa|\nabla u_0|^2 + W''(u_0)u_0^2 + W'(u_0)u_0\right] dx \\
&= \int_\Omega \left[\kappa|\nabla u_0|^2 + W''(u_0)u_0^2\right] dx \qquad \text{by (3.2)} \\
&= \delta^2 E[u_0](u_0, u_0) \\
&\neq 0 \qquad \text{since } u_0 \notin S^0.
\end{aligned}$$

This and (3.8) imply that $\mu = 0$, and hence by (3.7)

$$\langle \delta E[u_0], v\rangle = 0 \qquad \forall v \in H_0^1(\Omega).$$

That is, $\delta E[u_0] = 0$. ∎

Corollary 3.5. *We have*

$$\begin{aligned}
S &= \left\{ u \in H_0^1(\Omega) : \int_\Omega \left(\kappa|\nabla u|^2 + u^4 - u^2\right) dx = 0 \right\}, \\
S^+ &= \left\{ u \in S : \int_\Omega \left(\kappa|\nabla u|^2 + 3u^4 - u^2\right) dx > 0 \right\} \\
&= \left\{ u \in S : \int_\Omega u^4\, dx > 0 \right\} \\
&= \{u \in S : u \neq 0\}, \\
S^- &= \left\{ u \in S : \int_\Omega u^4\, dx < 0 \right\} = \emptyset, \\
S^0 &= \left\{ u \in S : \int_\Omega u^4\, dx = 0 \right\} = \{0\}.
\end{aligned}$$

Proof. By (1.2), $W'(u) = -u + u^3$. Thus the expression of S follows from its definition; cf. (3.2). Now, $u \in S$ if and only if $u \in H_0^1(\Omega)$ and

$$\int_\Omega \kappa|\nabla u|^2 dx = \int_\Omega \left(u^2 - u^4\right) dx.$$

Since $W''(u) = 3u^2 - 1$, we thus obtain the expression of S^+, S^-, and S^0 by their definitions and the formula of the second variation (3.4). ∎

Lemma 3.6. *Let* $u \in H_0^1(\Omega) \setminus \{0\}$.

(i) *If*

$$\int_\Omega \left(\kappa|\nabla u|^2 - u^2\right) dx \geq 0, \tag{3.9}$$

then Φ_u has no positive critical points or positive turning points, Φ_u is monotonically increasing in $s > 0$, and

$$\lim_{s\to\infty} \Phi_u(s) = \infty.$$

(ii) *If*

$$\int_\Omega \left(\kappa|\nabla u|^2 - u^2\right)\, dx < 0, \tag{3.10}$$

then Φ_u has exactly one positive critical point

$$s_u = \left[-\frac{\int_\Omega \left(\kappa|\nabla u|^2 - u^2\right) dx}{\int_\Omega u^4\, dx}\right]^{1/2}, \tag{3.11}$$

$\Phi_u''(s_u) > 0$, and $s_u u \in S^+$.

Proof. Since $W(u) = (u^2-1)^2/4$, we have by (3.5) and (3.6) that

$$\Phi_u'(s) = \int_\Omega \left[s\left(\kappa|\nabla u|^2 - u^2\right) + s^3u^4\right] dx,$$
$$\Phi_u''(s) = \int_\Omega \left(\kappa|\nabla u|^2 - u^2 + 3s^2u^4\right) dx.$$

Therefore, $\Phi_u'(s) = 0$ if and only if $s = 0$ or

$$s^2 = -\frac{\int_\Omega \left(\kappa|\nabla u|^2 - u^2\right) dx}{\int_\Omega u^4\, dx}.$$

If (3.9) holds true, then

$$\Phi_u'(s) \geq s^3 \int_\Omega u^4\, dx > 0 \qquad \forall s > 0$$

and

$$\Phi_u''(s) \geq 3s^2 \int_\Omega u^4\, dx > 0 \qquad \forall s > 0.$$

These imply the assertion of part (i). If (3.10) holds true, then s_u defined in (3.11) is the unique solution to $\Phi_u'(s) = 0$ for $s \in (0,\infty)$. Moreover,

$$\Phi_u''(s_u) = -2\int_\Omega \left(\kappa|\nabla u|^2 - u^2\right) dx > 0.$$

By Corollary 3.3, $s_u u \in S$. By Corollary 3.5, $s_u u \in S^+$. Part (ii) is proved. ∎

4. Proof of Theorem 2.1. By the change of variables (2.7), (2.8), and (2.9), we will consider the rescaled functional E defined in (3.1). Note that the parameter κ in the energy E defined in (2.9) is $\kappa/(4\gamma)$ with κ and γ in the original functional E defined in (1.1).

Case 1: $\kappa \geq 1/\lambda_1$. We need to prove that $u = 0$ is the unique minimizer of the functional E defined in (3.1) over $H_0^1(\Omega)$ and that the minimum energy is $|\Omega|/4$.

We recall that $\lambda_1 > 0$ is the smallest eigenvalue of the eigenvalue problem (2.5) and (2.6). By Rayleigh's principle, we have

$$\lambda_1 = \min\left\{ \frac{\int_\Omega |\nabla u|^2\,dx}{\int_\Omega u^2\,dx} : \ u \in H_0^1(\Omega), u \neq 0 \right\}. \tag{4.1}$$

Hence

$$\int_\Omega |\nabla u|^2\,dx \geq \lambda_1 \int_\Omega u^2\,dx \qquad \forall u \in H_0^1(\Omega).$$

If $\kappa \geq 1/\lambda_1$, we have for any $u \in H_0^1(\Omega)$ that

$$\begin{aligned} E[u] &= \int_\Omega \left(\frac{1}{2}(\kappa|\nabla u|^2 - u^2) + \frac{u^4+1}{4} \right) dx \\ &\geq \int_\Omega \left(\frac{1}{2}(\kappa\lambda_1 - 1)u^2 + \frac{u^4}{4} + \frac{1}{4} \right) dx \\ &\geq \frac{1}{4}|\Omega|. \end{aligned}$$

The equality holds if and only if $u = 0$. Therefore, $u = 0$ is the unique minimizer of E defined in (3.1) and the minimum value is $|\Omega|/4$. Part (i) of Theorem 2.1 is proved.

Case 2: $0 < \kappa < 1/\lambda_1$. We need to prove that there are exactly two minimizers, $u_{\rm pos}$ and $u_{\rm neg}$, of the energy functional (3.1) in $H_0^1(\Omega)$, the minimum energy value is less than $|\Omega|/4$, and

$$u_{\rm pos} + u_{\rm neg} = 0 \qquad \text{in } \Omega, \tag{4.2}$$

$$-1 < u_{\rm neg} < 0 < u_{\rm pos} < 1 \qquad \text{in } \Omega. \tag{4.3}$$

We prove all these in three steps. But first we note that there exists $u^* \in H_0^1(\Omega)$ that minimizes the energy functional E defined in (3.1) over $H_0^1(\Omega)$; cf. Theorem 3.3 in [13].

Step 1. *An estimate of the minimum energy.* Let ψ_1 be an eigenfunction corresponding to λ_1. Then we have

$$\int_\Omega |\nabla \psi_1|^2\,dx = \lambda_1 \int_\Omega \psi_1^2\,dx.$$

Hence

$$\int_\Omega \left(\kappa|\nabla\psi_1|^2 - \psi_1^2 \right) dx = (\kappa\lambda_1 - 1) \int_\Omega \psi_1^2\,dx < 0.$$

We define s_{ψ_1} by (3.11) with ψ_1 replacing u. Then, by Lemma 3.6, $s_{\psi_1}\psi_1 \in S^+ \subset S$. Hence, by the expression of elements in S in Corollary 3.5, we have

$$\int_\Omega \left[\kappa|\nabla(s_{\psi_1}\psi_1)|^2 + (s_{\psi_1}\psi_1)^4 - (s_{\psi_1}\psi_1)^2 \right] dx = 0.$$

Thus

$$\begin{aligned} E[s_{\psi_1}\psi_1] &= \int_\Omega \left[\frac{\kappa}{2}|\nabla(s_{\psi_1}\psi_1)|^2 + \frac{1}{4}((s_{\psi_1}\psi_1)^4 - 2(s_{\psi_1}\psi_1)^2 + 1)\right] dx \\ &= \frac{1}{4}\int_\Omega \left[1 - (s_{\psi_1}\psi_1)^4\right]\, dx \\ &= \frac{|\Omega|}{4} - \frac{\left[\int_\Omega (\kappa|\nabla\psi_1|^2 - \psi_1^2)\, dx\right]^2}{\int_\Omega \psi_1^4\, dx} \\ &= \frac{|\Omega|}{4} - (\kappa\lambda_1 - 1)^2 \frac{\left(\int_\Omega \psi_1^2\, dx\right)^2}{\int_\Omega \psi_1^4\, dx} \\ &< \frac{|\Omega|}{4}. \end{aligned}$$

Therefore,

$$E[u^*] = \min\left\{E[u] : u \in H_0^1(\Omega)\right\} \le E[s_{\psi_1}\psi_1] < \frac{|\Omega|}{4}. \tag{4.4}$$

Step 2. *Properties of minimizers* $u_{\rm pos}$ *and* $u_{\rm neg}$. We define $u_{\rm pos} = |u^*| \in H_0^1(\Omega)$ and $u_{\rm neg} = -|u^*| \in H_0^1(\Omega)$. Since $|\nabla u^*| = |\nabla u_{\rm pos}| = |\nabla u_{\rm neg}|$ a.e., and $W(u) = (u^2-1)^2/4$ is an even function, we have $E[u_{\rm pos}] = E[u_{\rm neg}] = E[u^*]$. That is, both $u_{\rm pos}$ and $u_{\rm neg}$ are minimizers for E over $H_0^1(\Omega)$. Clearly,

$$u_{\rm pos} \ge 0, \quad u_{\rm neg} \le 0, \quad \text{and} \quad u_{\rm pos} + u_{\rm neg} = 0 \qquad \text{in } \Omega.$$

We now obtain the bounds for these minimizers. We will only analyze the bounds for $u_{\rm pos}$, since the bound for $u_{\rm neg}$ can be obtained by the relation $u_{\rm neg} = -u_{\rm pos}$.

Consider nonnegative solutions for the Euler–Lagrange equation for E in $H_0^1(\Omega)$:

$$-\kappa\Delta u + u^3 - u = 0 \quad \text{in } \Omega, \tag{4.5}$$

$$u = 0 \quad \text{on } \partial\Omega, \tag{4.6}$$

$$u \ge 0 \quad \text{in } \Omega. \tag{4.7}$$

This system has a trivial solution $u \equiv 0$. Since $u_{\rm pos}$ is a minimizer for E in $H_0^1(\Omega)$, $u_{\rm pos}$ is a nontrivial weak solution for (4.5)–(4.7). By the Sobolev embedding theorem with the space dimension $d = 2$ or 3, we have $f := u_{\rm pos} - u_{\rm pos}^3 \in L^2(\Omega)$. Then by the regularity theory for $-\kappa\Delta u_{\rm pos} = f$, we see that $u \in H^2(\Omega)$. By the Sobolev embedding theorem again we have $u \in C^{0,\beta}(\bar\Omega)$ for $\beta = 1/2$ if $d = 3$ for any $\beta \in (0,1)$ if $d = 2$. For the interior regularity, we can use a bootstrap argument to show that $u \in H^m_{\rm loc}(\Omega)$ for any positive integer m, and hence $u \in C^\infty(\Omega)$. Thus $u \in C^\infty(\Omega) \cap C^{0,\beta}(\overline{\Omega})$.

Claim 1. $u_{\rm pos}$ *is a positive solution to* (4.5)–(4.7). *That is,* $u_{\rm pos} > 0$ *in* Ω.

Proof of Claim 1. If not, then there exists $x_0 \in \Omega$ such that $u_{\rm pos}(x_0) = 0$. Let $v = -u_{\rm pos}$. Then $v \le 0$ in Ω and v attains a nonnegative maximum at x_0. But since $u_{\rm pos}$ satisfies (4.5), we have

$$\kappa\Delta v - cv = -v \ge 0, \qquad \text{with } c = v^2 \ge 0.$$

By the maximum principle [21, 29], we conclude that $v =$ constant. Since $v = 0$ on $\partial\Omega$, we must have $v \equiv 0$ in Ω, i.e., $u_{\rm pos} \equiv 0$ in Ω. This contradicts the fact that the 0 function is not a minimizer as its energy is $|\Omega|/4$, which is strictly greater than the minimum energy by (4.4). Claim 1 is proved. ∎

Claim 1 also eliminates the existence of minimizers that have both positive and negative parts. Indeed, if v is a minimizer that has both positive and negative parts, then there exists $x_0 \in \Omega$ such that $v(x_0) = 0$, and hence $|v(x_0)| = 0$. But since $|v|$ is a nonnegative minimizer, by Claim 1, $|v|$ must be strictly positive in Ω. This is a contradiction.

CLAIM 2. $u_{\text{pos}} < 1$ *in* $\overline{\Omega}$.

Proof of Claim 2. Since $u_{\text{pos}} = 0$ on $\partial\Omega$, u_{pos} must attain its maximum at some interior point $x_0 \in \Omega$. Then $u_{\text{pos}}(x_0) > 0$ and $\Delta u_{\text{pos}}(x_0) \le 0$. Consequently by (4.5) we get

$$u_{\text{pos}}(x_0)^3 = \kappa\Delta u_{\text{pos}}(x_0) + u_{\text{pos}}(x_0) \le u_{\text{pos}}(x_0).$$

Hence $u_{\text{pos}}(x_0)^2 \le 1$ and $u_{\text{pos}}(x_0) \le 1$. Consequently $u_{\text{pos}}(x) \le 1$ for all $x \in \Omega$.

To show that $u_{\text{pos}} < 1$ for all Ω, we need only to show that $u_{\text{pos}}(x_0) < 1$. If not, then $u_{\text{pos}}(x_0) = 1$. Define $v = u_{\text{pos}} - 1$. Then $-1 \le v \le 0$ in Ω and $v(x_0) = 0$ is the nonnegative maximum of v in Ω. By (4.5), we have

$$\kappa\Delta v - (v+1)(v+2)v = 0.$$

Since $(v+1)(v+2) \ge 0$, by the maximum principle we conclude that $v =$ constant. Since $v(x_0) = 0$, we get $v \equiv 0$ and $u_{\text{pos}} \equiv 1$, contradicting the fact that $u_{\text{pos}} = 0$ on $\partial\Omega$. Claim 2 is proved. ∎

Step 3. *Uniqueness of a positive minimizer.* We will prove the uniqueness of positive minimizer by contradiction. Recall that all minimizers of E are in S. By the expression of element in S in Corollary 3.5, we have for any $u \in S$

$$E[u] = \frac{1}{4}\int_\Omega (1 - u^4)\,dx. \tag{4.8}$$

Suppose there are two positive minimizers $u_1, u_2 \in H_0^1(\Omega)$ for $E[u]$, and $u_1 \not\equiv u_2$ in the sense that

$$|\{x \in \Omega : u_1(x) \ne u_2(x)\}| > 0.$$

Then

$$E[u_1] = E[u_2] = \inf\{E[u] : u \in H_0^1(\Omega)\}.$$

Define

$$\Omega_1 := \{x \in \Omega : u_1(x) \ge u_2(x)\},$$
$$\Omega_2 := \{x \in \Omega : u_1(x) < u_2(x)\}.$$

Correspondingly, we define for all $u \in H_0^1(\Omega)$

$$E_i[u] := \int_{\Omega_i}\left[\frac{\kappa}{2}|\nabla u|^2 + \frac{1}{4}(u^2-1)^2\right]dx, \qquad i = 1, 2. \tag{4.9}$$

Then $E[u] = E_1[u] + E_2[u]$. If Ω_1 or Ω_2 is of measure zero, say $|\Omega_2| = 0$, then

$$u_1 \ge u_2 \quad \text{a.e. in } \Omega \qquad \text{and} \qquad |\{x \in \Omega : u_1(x) > u_2(x)\}| > 0.$$

So, by (4.8) and $u_1 \ge u_2 > 0$ in Ω, we have

$$E[u_1] = \frac{1}{4}\int_\Omega (1 - u_1^4)\,dx < \frac{1}{4}\int_\Omega (1 - u_2^4)\,dx = E[u_2], \tag{4.10}$$

a contradiction. Thus we must have $|\Omega_1| > 0$ and $|\Omega_2| > 0$.

We now analyze the identity

$$E_1[u_1] + E_2[u_1] = E_1[u_2] + E_2[u_2] = \inf E$$

by considering three cases.

(a) If $E_1[u_1] = E_1[u_2]$, then $E_2[u_1] = E_2[u_2]$. Define

$$w := \max\{u_1, u_2\} = \begin{cases} u_1 & \text{in } \Omega_1, \\ u_2 & \text{in } \Omega_2. \end{cases} \tag{4.11}$$

Then it is easy to show [21, 22] that $w \in H_0^1(\Omega)$ and

$$\nabla w = \begin{cases} \nabla u_1 & \text{a.e. in } \Omega_1, \\ \nabla u_2 & \text{a.e. in } \Omega_2. \end{cases} \tag{4.12}$$

So

$$E[w] = E_1[u_1] + E_2[u_2] = E_1[u_2] + E_2[u_2] = E[u_2] = \inf E.$$

Thus w is a minimizer for E and $w \in S$. But $w \geq u > 0$ a.e. in Ω and $|\{x \in \Omega : w(x) > u_1(x)\}| > 0$. Hence,

$$E[w] = \frac{1}{4}\int_\Omega (1 - w^4)\, dx < \frac{1}{4}\int_\Omega (1 - u_1^4)\, dx = E[u_1] = \inf E,$$

a contradiction.

(b) If $E_1[u_1] < E_1[u_2]$, then $E_2[u_1] > E_2[u_2]$. Again we consider w defined by (4.11). Then

$$E[w] = E_1[u_1] + E_2[u_2] < E_1[u_2] + E_2[u_2] = E[u_2] = \inf E,$$

a contradiction.

(c) If $E_1[u_1] > E_1[u_2]$, then $E_2[u_1] < E_2[u_2]$. Consider

$$w_2 := \min\{u_1, u_2\} = \begin{cases} u_2 & \text{in } \Omega_1, \\ u_1 & \text{in } \Omega_2. \end{cases} \tag{4.13}$$

Then $w_2 \in H_0^1(\Omega)$ and

$$E[w_2] = E_1[u_2] + E_2[u_1] < E_1[u_1] + E_2[u_1] = E[u_1] = \inf E,$$

a contradiction.

The proof of Theorem 2.1 is complete.

5. Proof of Theorem 2.2. By (2.7), (2.8), and (2.9), the two cases in Theorem 2.2 are simplified as follows: (i) $0 < g < 1$, and (ii) $-1 < g < 0$. Let u_g^* be a minimizer for E in $\mathcal{A}_g$.

Case $0 < g < 1$. Since $E[|u|] = E[u]$ for any $u \in H^1(\Omega)$, we define $u_{g,\text{pos}} = |u_g^*| \geq 0$; then $u_{g,\text{pos}} \in \mathcal{A}_g$ and $E[u_{g,\text{pos}}] = E[u_g^*]$. Thus $u_{g,\text{pos}}$ is a minimizer for E in $\mathcal{A}_g$. The proofs for the bound and the uniqueness of u_{pos} in the previous section have nothing to do with the boundary condition of u_{pos}. So using the same proofs, we establish that $u_{g,\text{pos}}$ is the unique minimizer for E in $\mathcal{A}_g$ and $0 < u_{g,\text{pos}} < 1$.

Since $u_{g,\mathrm{pos}}$ is a solution to the Euler–Lagrange equation

$$-\kappa\Delta u + u^3 - u = 0 \quad \text{in } \Omega, \tag{5.1}$$

$$u = g \quad \text{on } \partial\Omega, \tag{5.2}$$

by (5.1) and $0 < u_{g,\mathrm{pos}} < 1$, we have

$$\kappa\Delta u_{g,\mathrm{pos}} = u_{g,\mathrm{pos}}^3 - u_{g,\mathrm{pos}} < 0 \quad \text{in } \Omega. \tag{5.3}$$

Thus $u_{g,\mathrm{pos}}$ cannot attain its minimum over $\overline{\Omega}$ at an interior point of Ω. Consequently,

$$\min_{\partial\Omega} g < u_{g,\mathrm{pos}} < 1 \quad \text{in } \Omega.$$

Case $-1 < g < 0$. We define $u_{g,\mathrm{neg}} = -|u_g^*| \le 0$. The rest of the proof is similar to that of (i).

The proof of Theorem 2.2 is complete. ∎

6. Numerical simulations. In this section, we present some numerical simulations to showcase the properties of the energy minimizers that we have described in Theorem 2.1. To find the minimum of E, we solve the equation of the L^2-gradient flow of E, that is, the Allen–Cahn equation

$$\frac{\partial u}{\partial t} = \kappa\Delta u - W'(u), \tag{6.1}$$

with the homogeneous Dirichlet boundary condition $u = 0$ on $\partial\Omega$. Our goal is to eventually reach an equilibrium state, or its numerical approximation, of (6.1) and hope that the equilibrium state is a minimizer of E. In principle, it is possible for the gradient flow to get stuck at local minimizers of E. When we consider only positive solutions of (6.1), we expect, however, that our numerical solutions may approximate global minimizers.

We choose a square domain $\Omega = (0, L) \times (0, L)$ with $L = \sqrt{2}\pi$ so that $\lambda_1 = 1$. We use the forward Euler finite difference scheme for the time discretization and the standard 5-point central differencing scheme for the discretization of the Laplacian operator:

$$\frac{u_{i,j}^{n+1} - u_{i,j}^n}{\Delta t} = \kappa\frac{u_{i+1,j}^n + u_{i,j+1}^n - 4u_{i,j}^n + u_{i-1,j}^n + u_{i,j-1}^n}{h^2} - W'(u_{i,j}^n). \tag{6.2}$$

The parameters are $h = L/128$ and $\Delta t = 1 \times 10^{-4}$. The time step is small enough for our numerical simulations to be stable; see, e.g., [37] for stability conditions for parabolic equations. Since our interest is to find minimizers u of E which solve (2.2), we define the error term err^n by

$$err_{i,j}^n := \kappa\frac{u_{i+1,j}^n + u_{i,j+1}^n - 4u_{i,j}^n + u_{i-1,j}^n + u_{i,j-1}^n}{h^2} - W'(u_{i,j}^n). \tag{6.3}$$

We assign random initial values for u^0 and run the simulations from $t = 0$ to at least $t = 50$ and $\|err^n\|_\infty < 1 \times 10^{-7}$, whichever comes later. When both criteria are met, we consider the solution u^n as an equilibrium state of (6.1) and treat u^n as a minimizer of E. We use two types of random initial values. The first consists of random initial values uniformly distributed in $[-0.5, 0.5]$. The second consists of positive random initial values uniformly distributed in $[0, 1]$. Since in our setting $\lambda_1 = 1$, the critical

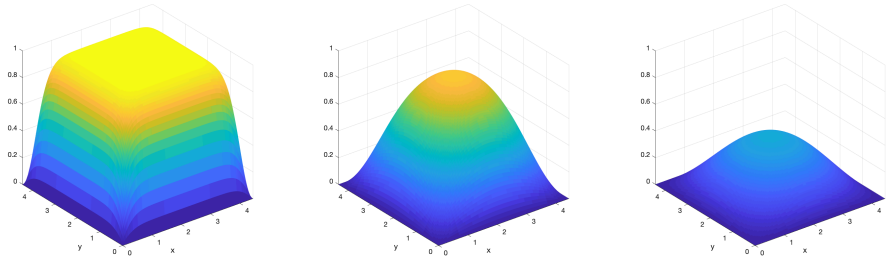

FIG. 6.1. *Surface plots of the positive minimizer of the functional E for different values of κ. Left: $\kappa = 0.05$; middle: $\kappa = 0.50$; right: $\kappa = 0.90$.*

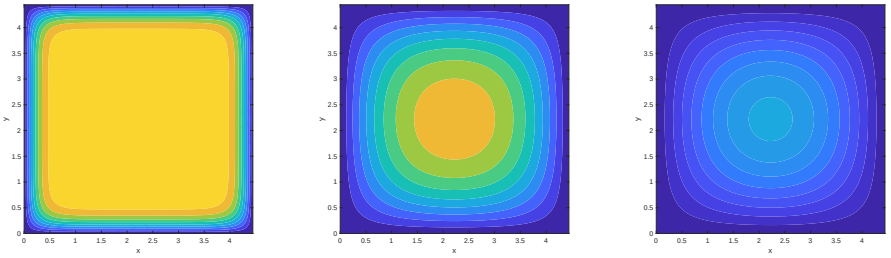

FIG. 6.2. *Contour plots of the positive minimizer of the functional E for different values of κ. Left: $\kappa = 0.05$; middle: $\kappa = 0.50$; right: $\kappa = 0.90$.*

value for κ is 1. To clarify the dependence of energy on κ, we denote the energy by E^κ, and the positive and negative minimizers by u^κ_{pos} and u^κ_{neg}.

In Figures 6.1 and 6.2, we plot the surface and contour of the positive minimizer of the functional E, respectively, for different values of the parameter κ. In Figure 6.3 (left), we plot the minimum energy $\min E$ vs. the parameter κ. In Figure 6.3 (right), we plot the profiles of the positive minimizer u^κ_{pos} along the diagonal $y = x$ of the domain.

Here are our observations from our numerical simulations:

(i) For $\kappa > 1$, for both types of initial values, the numerical solution converges to the constant solution $u = 0$. The energy $E^\kappa[u^n]$ approaches $E[0] = |\Omega|/4$.

(ii) For $0 < \kappa < 1$, if initial values are between $[-0.5, 0.5]$, then the solutions u^n can converge to either a positive solution u^κ_{pos} or a negative solution u^κ_{neg}. In addition, $u^\kappa_{\text{neg}} = -u^\kappa_{\text{pos}}$.

(iii) For $0 < \kappa < 1$, u^κ_{pos} is symmetric with respect to $x = L/2$, $y = L/2$, $y = x$, and $y = L - x$ and attains its maximum at the center of the domain; see Figures 6.1 and 6.2. In addition, the contours are concentric. This is the symmetry property stated in the remark after Theorem 2.1.

(iv) The minimum energy is a strictly increasing function of $\kappa \in (0, 1)$ and is a constant for $\kappa > 1$; see Figure 6.3 (left). This can be easily proved by observing for $0 < \kappa_1 < \kappa_2 < 1$, $E^{\kappa_1}[u^{\kappa_1}_{\text{pos}}] \le E^{\kappa_1}[u^{\kappa_2}_{\text{pos}}] < E^{\kappa_2}[u^{\kappa_2}_{\text{pos}}]$, since $u^{\kappa_2}_{\text{pos}}$ is not a constant.

(v) The positive minimizers u^κ_{pos} also exhibit a monotonicity for $0 < \kappa < 1$; see Figures 6.1 and 6.3 (right). The study of this phenomenon is beyond the scope of this paper.

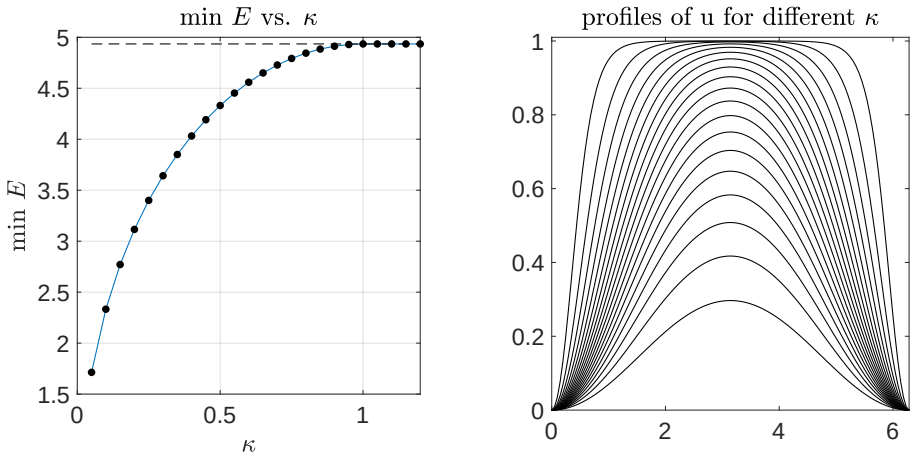

FIG. 6.3. *Left:* $\min E$ *vs.* κ. *The dashed line corresponds to the value* $|\Omega|/4$. *For* $\kappa \geq 1$, $\min E$ *remains a constant that is equal to* $|\Omega|/4$. *For* $0 < \kappa < 1$, $\min E < |\Omega|/4$. *The value* $\min E$ *decreases as* κ *decreases. Right: the profiles of the positive minimizer* u^{κ}_{pos} *along the diagonal* $y = x$ *of the domain. From bottom to top:* $\kappa = 0.95,\ 0.90,\ 0.85,\ \ldots, 0.05$.

For $\kappa = 1$ we observe that the solution u^n converges very slowly to the equilibrium solution $u = 0$. A heuristic spectral analysis indicates that it is an intrinsic feature of the Allen–Cahn equation (6.1) with $W(u) = \frac{1}{4}(u^2 - 1)^2$. Namely, the Allen–Cahn equation (6.1) resolves the lowest frequency very slowly when $\kappa = 1/\lambda_1$. Let λ_i and $\{\phi_i\}$ be the eigenvalues and the normalized eigenfunctions for the negative Laplace operator with homogeneous Dirichlet boundary condition, i.e.,

$$-\Delta\phi_i = \lambda_i\phi_i \quad \text{in } \Omega, \qquad \phi_i = 0 \quad \text{on } \partial\Omega, \qquad \text{and} \qquad \int_\Omega \phi_i^2(x)\,dx = 1.$$

Then we can decompose the solution $u(x,t)$ for (6.1) as $u(x,t) = \sum_{i=1}^{\infty} \alpha_i(t)\phi_i(x)$. Since $W'(u) = u^3 - u$, we also write $u^3 = \sum_{i=1}^{\infty} \beta_i(t)\phi_i(x)$. Plugging these expressions into (6.1), we have

$$\sum_{i=1}^{\infty} \alpha_i'(t)\phi_i(x) = \sum_{i=1}^{\infty} \left((1 - \kappa\lambda_i)\alpha_i(t) - \beta_i(t)\right)\phi_i(x).$$

For each mode we have an ODE

$$\alpha_i'(t) = (1 - \kappa\lambda_i)\alpha_i(t) - \beta_i(t),$$

whose solution satisfies

$$\alpha_i(t) = e^{-(\kappa\lambda_i - 1)(t - t_0)}\alpha_i(t_0) - \int_{t_0}^{t} e^{-(\kappa\lambda_i - 1)(t-s)}\beta_i(s)\,ds \quad \forall t > t_0 > 0$$

for any fixed $t_0 > 0$. For the lowest frequency mode $i = 1$, if $\kappa = 1$, since $\lambda_1 = 1$ we have

$$\alpha_1(t) = \alpha_1(t_0) - \int_{t_0}^{t} \beta_1(s)\,ds. \tag{6.4}$$

By our theoretical result in Theorem 2.1, we know that u approaches 0. Suppose at time $t \geq t_0$ that u is of magnitude $O(\varepsilon)$ for some $0 < \varepsilon < 1$ and $\alpha_1(t_0) \neq 0$. Then

$$\alpha_1(t_0) = \int_\Omega u(t_0, x)\phi_1(x)\, dx \sim O(\varepsilon),$$
$$\beta_1(t) = \int_\Omega u(t, x)^3\phi_1(x)\, dx \sim O(\varepsilon^3).$$

By (6.4), heuristically it takes at least a period of time $O(\varepsilon^{-2})$ to drive $\alpha_1(t)$ into the magnitude of $O(\varepsilon^2)$. Afterward $\beta_1 \sim O(\varepsilon^6)$ and it takes a period of time $O(\varepsilon^{-4})$ to drive α_1 from $O(\varepsilon^2)$ into the magnitude of $O(\varepsilon^3)$. If $\kappa \neq 1$, then for $i = 1$ we do not encounter this slowdown issue for $\alpha_1(t)$ because of the exponential term $e^{-(\kappa\lambda_1 - 1)t}\alpha_1(t_0)$.

For all other modes $i \geq 2$, we do not have such a slow resolution issue. If $\kappa \neq 1/\lambda_i$ for all $i \geq 2$, then the exponential term $e^{-(\kappa\lambda_i - 1)t}\alpha_i(t_0)$ will dominate. If $\kappa = 1/\lambda_i$ for some $i \geq 2$, then since $\lambda_i > \lambda_1$, we have $\kappa < 1/\lambda_1$. By Theorem 2.1 we know $u^\kappa_{\text{pos}} > 0$ in Ω. So if u is close to u^κ_{pos}, then $\beta_i = \int_\Omega u^3\phi_i\, dx$ is of magnitude $O(1)$, and $\alpha_i(t)$ can be resolved in reasonable time by (6.4) (with the subscript 1 replaced by i).

7. Discussions. In this paper, we study the minimizers of the Cahn–Hilliard energy functional under some strong anchoring conditions that are related to the two pure phases that define the double well in the functional. We have found a bifurcation phenomenon for the minimizers when the boundary value is exactly the average of the two pure phases. In such a case, depending on the bifurcation parameter, there can be a unique minimizer or there can be two distinct minimizers. If the boundary value is in between one pure phase and the average of the two pure phases, then the minimizer is unique and is also within the same range. Therefore, our analysis indeed shows a significant effect of the strong anchoring conditions to the minimizers of the Cahn–Hilliard functional. Our numerical simulations indeed confirm our analysis.

Our work is a first step toward detailed analysis of the minimizers of Cahn–Hilliard energy functional under strong anchoring conditions. There are, however, many more interesting problems along the lines of our analysis. First, it is natural to extend our work to more general Dirichlet boundary data that are related to the two phases u_- and u_+. For instance, it will be interesting to understand the morphology of minimizers when the boundary value is a convex combination of the two phases u_- and u_+ with volume fractions $\lambda \in (0, 1)$ and $1 - \lambda$, respectively. Second, we have not considered the mass conservation in our current study. In fact, in our setting, the total mass in the domain Ω (i.e., the integral of u on Ω) is not constrained to be a constant. We have showed the bifurcation phenomenon based on the sign of the boundary value and the value of the parameter κ. If the total mass in Ω is constrained to be a constant, then we expect that such a constraint will play some essential roles in the morphology and properties of the minimizers. Third, the existence of multiple and structured energy minimizers due to a special strong anchoring condition motivates strongly a new study of the kinetics pathways through which the system goes from one of the minimizers to the other. Important in application, such kinetics is often understood through the study of the dynamics of an underlying system, i.e., the time-dependent equations, such as the Cahn–Hilliard or Allen–Cahn equations. However, variational methods, particularly energy minimization methods, can often provide the information of minimizers and saddle points, and further the transition paths and energy barriers [42, 10]. Last but not least, if there is phase separation on the boundary in addition to the phase transition in the bulk domain, and if these two

processes interact and mutually influence each other, a dynamic boundary condition is needed. See [24, 35] and references therein for details. This is another direction for our future studies.

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