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Minimizers for the de Gennes–Cahn–Hilliard energy under strong anchoring conditions

Shibin Dai | **Abba Ramadan**

Department of Mathematics, University of Alabama, Tuscaloosa, Alabama, USA

Correspondence
Shibin Dai, Department of Mathematics, University of Alabama, Tuscaloosa, AL, 35487, USA.
Email: sdai4@ua.edu

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Abstract

In this article, we use the Nehari manifold and the eigenvalue problem for the negative Laplacian with Dirichlet boundary condition to analytically study the minimizers for the de Gennes–Cahn–Hilliard energy with quartic double-well potential and Dirichlet boundary condition on the bounded domain. Our analysis reveals a bifurcation phenomenon determined by the boundary value and a bifurcation parameter that describes the thickness of the transition layer that segregates the binary mixture's two phases. Specifically, when the boundary value aligns precisely with the average of the pure phases, and the bifurcation parameter surpasses or equals a critical threshold, the minimizer assumes a unique form, representing the homogeneous state. Conversely, when the bifurcation parameter falls below this critical value, two symmetric minimizers emerge. Should the boundary value be larger or smaller from the average of the pure phases, symmetry breaks, resulting in a unique minimizer. Furthermore, we derive bounds of these minimizers, incorporating boundary conditions and features of the de Gennes–Cahn–Hilliard energy.

KEYWORDS

bifurcation, De Gennes-Cahn-Hilliard functional, minimizations, strong anchoring condition

1 | INTRODUCTION

The Cahn–Hilliard functional

$$E_{\mathrm{CH}}[u] = \int_{\Omega} \left(\frac{\kappa}{2} |\nabla u|^2 + W(u) \right) dx \tag{1.1}$$

is extensively employed as a phenomenological diffuse-interface model to characterize the free energy of a system undergoing phase separation [6, 7]. Here Ω is a bounded domain in $\mathbb{R}^n$, u is the relative concentration of the two phases and $W(u)$ is a double-well potential with two equal minima at $u^- < u^+$ corresponding to the two pure phases, and $\kappa > 0$ is a parameter such that $\sqrt{\kappa}$ is proportional to the thickness of the transition region between the two phases.

The Cahn–Hilliard functional and the related Cahn–Hilliard equation and Allen-Hilliard equation have been used as models to understand many physical properties of two-phase materials. These properties include but are not limited to phase separation, coarsening dynamics and pattern formation. These studies are done on a domain Ω, thus the interaction of the mixture and the boundary $\partial\Omega$ is equally important. The Neumann boundary condition $\partial_n u = 0$ is commonly used, where n is the exterior unit normal at the boundary [2, 5, 18, 22, 26, 31–33, 36]. Other forms of boundary conditions such as the periodic boundary conditions are also popularly used, especially in computational studies [8–10, 12, 13, 20, 23–25, 37]. Recently Dai et al. [14] investigated the characterization of the minimizer of the Cahn–Hilliard functional for the free energy (1.1) with quartic double-well potential under the strong anchoring condition, that is, the Dirichlet condition. The authors required that u to be strongly anchored on the boundary, by matching a prescribed function g on $\partial\Omega$ pointwisely, which is the strongest possible match. This type of strong anchoring conditions is very important in physical modeling [17, 27]. The anchoring could be weakened by requiring the match to be within a small tolerance when measured in some norm say L^2.

It is worth mentioning that the study of the Cahn–Hilliard functional under Dirichlet boundary condition has been scarce. Notwithstanding, Du and Nicolaides [17] proposed it for a finite element scheme for the 1D Cahn–Hilliard equation. Bronsard and Hilhorst [4] also studied the limiting behavior of the solution to the Cahn–Hilliard equation with the Dirichlet boundary condition using the energy method. Other avenues where the Dirichlet boundary condition was considered can be found in [3, 21, 29].

This article was motivated by the recent work of Dai et al. [14] where in particular they showed that if the Dirichlet boundary value is the average of the two pure phases then there is a bifurcation of the minimizer for the Cahn–Hilliard energy functional. In fact, such bifurcation depends on the value κ and this range for κ is related to the first eigenvalue of the negative Laplacian with Dirichlet boundary condition. Moreover, they also showed that for the boundary value that is between the average of the two pure phases, the symmetry is broken and there is only one minimizer in the same range. Their analysis was conducted via the Nihari manifold and linked the problem to the negative Laplacian with homogenous boundary data.

Some numerical simulations for applications in materials science utilize a model that deviates slightly from the original Cahn–Hilliard equation [30, 35]. In particular, these simulations incorporate an additional degeneracy, and the equation is represented by the following non-variational system of equations, named the doubly degenerate Cahn–Hilliard (DDCH) equation:

$$u_t = \nabla \cdot (M_0(u) \nabla \mu), \tag{1.2}$$

$$G_0(u)\mu = -\kappa \Delta u + W'(u). \tag{1.3}$$

Here the diffusion mobility $M(u)$ is nonnegative and generally depends on u, and can be degenerate. The additional degeneracy comes from the diffusion restriction function $G_0(u)$ [35]. Numerical simulations and asymptotic analysis indicate that the DDCH equation has the potential to be a more precise approximation of surface diffusion [1]. Nevertheless, there was a drawback to this model—it lacks variationality. In simpler terms, Equations (1.2) and (1.3) lack a recognized free energy. Having an expression for the energy facilitates the numerical analysis and analytical validation of the model's properties. For instance, the absence of energy makes it impossible to construct variational derivatives. As a solution to these limitations, a variational diffuse interface model, called the de Gennes–Cahn–Hilliard (dGCH) model, was developed in [35] and studied in [15]. Similar to the expression of the free energy in (1.1), the free energy is defined as

$$E_{\mathrm{dGCH}}[u] = \int_\Omega \frac{1}{g_0(u)}\left(\frac{\kappa}{2}|\nabla u|^2 + W(u)\right)dx, \quad u \in H^1(\Omega). \tag{1.4}$$

Here

$$W(u) = \gamma(u-u^+)^2(u-u^-)^2 \tag{1.5}$$

is a double well potential with two equal minima at $u^- < u^+$ corresponding to the two pure phases, and γ is a normalizing constant which satisfies $\int_{u^-}^{u^+}\sqrt{2W(s)}ds = 1$. g_0 is a function of the form $g_0(u) = |(u-u^+)(u-u^-)|^p$, $p > 0$. We are only going to analyze the numerically convenient case $p = 1$, that is,

$$g_0(u) = |(u-u^+)(u-u^-)|. \tag{1.6}$$

The factor $\frac{1}{g_0}$ is called the energy restriction function or the de Gennes coefficient [16, 28]. Due to the singularity of $g_0(u)$ at $u = u^\pm$, it is tempting to conjecture that we need only to consider $u \in H^1(\Omega)$ with values confined between u^- and u^+. However, realizing that $W(u)/g_0(u) = \gamma|(u-u^+)(u-u^-)|$ and that

$$\nabla u = 0 \quad \text{a.e. in the set } \{x \in \Omega : u(x) = u^\pm\},$$

it is natural to interpret the integrand of (1.4) as

$$\begin{cases} \frac{1}{g_0(u)}\left(\frac{\kappa}{2}|\nabla u|^2 + W(u)\right) & \text{if } u \neq u^\pm \\ 0 & \text{if } u = u^\pm. \end{cases}$$

In this sense, all $u \in H^1(\Omega)$ aer allowable for E_{dGCH}, although some of them may make $E_{\mathrm{dGCH}}[u] = \infty$. More discussions regarding the chemical potential and the dGCH system with a degenerate mobility can be found in the references above. It is also worth mentioning that Dai, Renzi and Wise recently established the Gamma convergence of (1.4) [15].

2 | MAIN RESULT

In this article, we are interested in characterizing minimizers for the dGCH energy E_{dGCH}. The starting point is to use a transformation to obtain a form that is easier to handle the challenges imposed by the factor $\frac{1}{g_0}$. For convenience and without loss of generality we can rescale the energy and boundary data such that $u^- = -1$, $u^+ = 1$, and

$$W(u) = \frac{1}{4}(u^2-1)^2, \qquad g_0(u) = |u^2 - 1|. \tag{2.1}$$

Introduce the transformation

$$h(t) := \int_0^t \frac{ds}{\sqrt{g_0(s)}}. \tag{2.2}$$

Since $g_0(s)$ is zero at $s = \pm 1$, this transformation is a singular integral. Now let $w(x) = h(u(x))$ for all $x \in \Omega$. Then we can construct a new set of energy functional using a change of variables and the Sobolev chain rule

$$\tilde{E}[w] = \int_\Omega \left(\frac{\kappa}{2} |\nabla w|^2 + \frac{W(h^{-1}(w))}{g_0(h^{-1}(w))} \right) dx.$$

For our choices of g_0 and W in (2.1), we have the following explicit expressions for $h(t)$ and h^{-1} [34]

$$h(t) := \begin{cases} -\ln(\sqrt{t^2-1} - t) - \frac{\pi}{2}, & \text{if } t < -1 \\ \sin^{-1}(t), & \text{if } t \in [-1,1] \\ \ln(t + \sqrt{t^2-1}) + \frac{\pi}{2}, & \text{if } t > 1 \end{cases} \tag{2.3}$$

and

$$h^{-1}(t) := \begin{cases} -\frac{1}{2}\left(e^{-\left(t+\frac{\pi}{2}\right)} + e^{\left(t+\frac{\pi}{2}\right)} \right), & \text{if } t < -1 \\ \sin(t), & \text{if } t \in [-1,1] \\ \frac{1}{2}\left(e^{-\left(t+\frac{\pi}{2}\right)} + e^{\left(t+\frac{\pi}{2}\right)} \right), & \text{if } t > 1. \end{cases} \tag{2.4}$$

If we restrict on the region $u \in [-1,1]$ and hence $w \in [-\frac{\pi}{2}, \frac{\pi}{2}]$, we then have that

$$\frac{W(h^{-1}(w))}{g_0(h^{-1}w)} = \frac{\cos^2(w)}{4}.$$

This motivated us to study the following energy

$$E[w] = \int_\Omega \left(\frac{\kappa}{2} |\nabla w|^2 + \frac{\cos^2(w)}{4} \right) dx, \quad w \in H^1(\Omega), \tag{2.5}$$

with the hope that under appropriate boundary conditions, minimizers for $E(w)$ indeed lie in $[-\pi/2, \pi/2]$. See Lemma 3.1 for details.

Now we consider a given boundary value $m(x) \in H^{\frac{1}{2}}(\partial\Omega)$. Using direct method in the calculus of variations, one can prove that the energy functional (2.5) has a minimizer in the admissible set

$$\mathcal{A}_m := \{ w \in H^1(\Omega) : w = m(x) \text{ on } \partial\Omega \}. \tag{2.6}$$

Due to the lack of convexity of $W(u)$, uniqueness of such minimizers is not guaranteed. Every minimizer $w \in \mathcal{A}_m$ satisfies the Euler-Lagrange equation

$$-\kappa \Delta w - \frac{\sin(2w)}{4} = 0 \quad \text{in} \quad \Omega. \tag{2.7}$$

Note that the above equation is defined in the weak sense, more specifically in the sense that

$$\langle \delta E[w], v \rangle = \int_\Omega \left(\kappa \nabla w \cdot \nabla v - \frac{v \sin(2w)}{4} \right) dx \quad \text{for all } v \in H_0^1(\Omega). \tag{2.8}$$

In this article, we analyze the minimizers of (2.5) under the following three situations of boundary data.

1. $m(x) \equiv 0$, for all $x \in \partial\Omega$,
2. $0 < m(x) < \pi/2$, for all $x \in \partial\Omega$,
3. $-\pi/2 < m(x) < 0$, for all $x \in \partial\Omega$.

Analysis of these minimizers with different boundary data boils down to the parameter κ, which is a bifurcation parameter, and the minimum eigenvalue λ_1 of the negative Laplacian with Dirichlet boundary data, that is, the minimum value λ that solves the eigenvalue problem

$$\begin{aligned} -\Delta w &= \lambda w \text{ in } \Omega, \\ w &= 0 \text{ on } \partial\Omega. \end{aligned} \tag{2.9}$$

We can now summarize our results as follows.

Theorem 2.1. *Assume $m(x) = 0$ for all $x \in \partial\Omega$.*

(i) If $\kappa \geq \frac{1}{2\lambda_1}$, then $w = 0$ is the only minimizer for E in $\mathcal{A}_m$ and

$$\min\{E[w] : w \in \mathcal{A}_m\} = \frac{|\Omega|}{4},$$

(ii) If $0 < \kappa < \frac{1}{2\lambda_1}$, then there exist two and only two minimizers w_+, w_- for E in $\mathcal{A}_m$ and

$$\min\{E[w] : w \in \mathcal{A}_m\} < \frac{|\Omega|}{4}.$$

Moreover, $w_+ + w_- = 0$ and $-\frac{\pi}{2} < w_- < 0 < w_+ < \frac{\pi}{2}$ in Ω.

Theorem 2.2. *Let $m(x) \in C(\partial\Omega)$.*

(i) If $0 < m(x) < \frac{\pi}{2}$ for all $x \in \partial\Omega$, then there exists a unique minimizer for E in $\mathcal{A}_m$. Moreover

$$\min_{\partial\Omega} m < w_{+,m} < \frac{\pi}{2}.$$

(ii) If $-\frac{\pi}{2} < m(x) < 0$ for all $x \in \partial\Omega$, then there exists a unique minimizer for E in $\mathcal{A}_m$. Moreover

$$-\frac{\pi}{2} < w_{-,m} < \max_{\partial\Omega} m.$$

Theorems 2.1 and 2.2 will easily translate back into the following results about E_{dGCH}.

Theorem 2.3. *Let W be defined by (1.5), g be defined by (1.6), and $h \in C(\partial\Omega)$. Consider minimizers for the energy E_{dGCH} in the the admissible set*

$$\mathcal{A}_h = \{u \in H^1(\Omega) : u = h \text{ on } \partial\Omega\}.$$

For $h = \frac{u^+ + u^-}{2}$,

(i) If $\kappa \geq \frac{\gamma}{8\lambda_1}$, then $u = \frac{u^+ + u^-}{2}$ is the only minimizer for E_{dGCH} in $\mathcal{A}_h$ and

$$\min\{E_{\text{dGCH}}[u] : u \in \mathcal{A}_h\} = \frac{\gamma(u^+ - u^-)^2}{4}|\Omega|,$$

(ii) If $0 < \kappa < \frac{\gamma}{8\lambda_1}$, then there exist two and only two minimizers u_+, u_- for E_{dGCH} in $\mathcal{A}_h$ and

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

Moreover, $u_+ + u_- = 0$ and $u^- < u_- < 0 < u_+ < u^+$ in Ω.

Furthermore,

(i) If $\frac{u^-+u^+}{2} < h(x) < u^+$ *for all* $x \in \partial\Omega$, *then there exists a unique minimizer for* E_{dGCH} *in* $\mathcal{A}_h$. *Moreover*

$$\min_{\partial\Omega} h < u_{+,h} < u^+.$$

(ii) If $u^- < h(x) < \frac{u^-+u^+}{2}$ *for all* $x \in \partial\Omega$, *then there exists a unique minimizer for* E_{dGCH} *in* $\mathcal{A}_h$. *Moreover*

$$u^- < u_{-,h} < \max_{\partial\Omega} h.$$

Remark 2.4. Note that the translation of Theorem 2.1 and 2.2 into Theorem 2.3 is possible thanks to the transformation (2.2).

Remark 2.5. We want to emphasize that similar to [14], in this article we concentrate on the quartic double well potential (1.5). There are technical challenges if we apply the same framework to other potentials such as the logarithmic potential

$$W_{\log}(u) = \begin{cases} \frac{\theta}{2}((1+u)\ln(1+u) + (1-u)\ln(1-u)) + \frac{1}{2}(1-u^2) & \text{if } |u| < 1, \\ +\infty & \text{otherwise.} \end{cases}$$

We also want to clarify that the results in this study are about global minimizers of the dGCH energy (1.4) under Dirichlet boundary conditions. it is an interesting question whether we could relate these results with properties of solutions for the H^{-1} and L^2 gradient flows, that is, the dGCH equations or de Gennes–Allen–Cahn equations. It is also interesting to study properties of other critical points of this energy, local minimizers in particular. We will save these topics for future explorations.

The rest of the article is devoted to proving Theorems 2.1 and 2.2. First in Section 3 we prove that, if the boundary value $m(x)$ satisfies $-\pi/2 \le m(x) \le \pi/2$ for all $x \in \partial\Omega$, then the minimizers for E are bounded between $-\pi/2$ and $\pi/2$. In Section 4, we discuss the results about the Nehari manifold, which are essential for the proof of Theorem 2.1. In Sections 5, we prove Theorems 2.1 and 2.2.

3 | BOUNDEDNESS OF MINIMIZERS WHEN $-\pi/2 \le m(x) \le \pi/2$ ON $\partial\Omega$

The following lemma justifies our motivation to transform the minimization of E_{dGCH} into the minimization of E.

Lemma 3.1. *Suppose* $-\pi/2 \le m(x) \le \pi/2$ *on* $\partial\Omega$ *and* $w \in \mathcal{A}_m$ *is a minimizer for* E *in the admissible set* $\mathcal{A}_m$. *Then we have* $-\pi/2 \le w(x) \le \pi/2$ *for all* $x \in \Omega$.

Proof. Let $A := \{x \in \Omega : |w(x)| > \pi/2\}$. Suppose $|A| > 0$. Define

$$\tilde{w}(x) = \begin{cases} \pi/2 & \text{if } w(x) > \pi/2, \\ w(x) & \text{if } -\pi/2 \le w(x) \le \pi/2, \\ -\pi/2 & \text{if } w(x) < -\pi/2. \end{cases} \tag{3.1}$$

Then $\tilde{w} \in \mathcal{A}_m$. Since $\nabla\tilde{w} = 0, \cos(\tilde{w}) = 0$ in A and $E[w] \le E[\tilde{w}]$, we have

$$0 \le \int_A \left(\frac{\kappa}{2}|\nabla w|^2 + \frac{\cos^2(w)}{4} \right) dx = E[w] - E[\tilde{w}] \le 0.$$

Then we must have $\nabla w = 0$ and $\cos(w) = 0$ in A. That is, for $x \in A$, $w(x)$ can only take discrete values $k\pi + \pi/2$ for $k \in \mathbf{Z}$. This is impossible since $w \in H^1(\Omega)$ and $w(x) \in [-\pi/2, \pi.2]$ for $x \in \Omega \setminus A$. Consequently $|A| = 0$ and hence $-\pi/2 \leq w(x) \leq \pi/2$ for all $x \in \Omega$. ■

4 | THE NEHARI MANIFOLD (FOR $m(x) \equiv 0$)

Considering the energy functional (2.5) we define the associated Nehari manifold

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

where $\langle \delta E[w], v \rangle$ is the first variations defined in (2.8). Then by Equation (2.8), $w \in S$ if and only if $w \in H_0^1(\Omega)$ and

$$\int_\Omega \left(\kappa |\nabla w|^2 - \frac{w \sin(2w)}{4} \right) dx = 0. \tag{4.1}$$

Note that every critical point of the energy functional (2.5) lies in S and also $0 \in S$. Next we will show that S is bounded in $H_0^1(\Omega)$.

Lemma 4.1. *The set S is bounded in $H_0^1(\Omega)$.*

Proof. Let $w \in S$. By (4.1), Hölder's inequality, and Poincaré's inequality, we have

$$\begin{aligned} \kappa \|\nabla w\|^2_{L^2(\Omega)} &= \kappa \int_\Omega |\nabla w|^2 \, dx = \int_\Omega \frac{w \sin(2w)}{4} dx \\ &\leq \frac{1}{4} \int_\Omega |w| \, dx \leq \frac{1}{4} |\Omega|^{1/2} \|w\|_{L^2(\Omega)} \leq C \|\nabla w\|_{L^2(\Omega)}. \end{aligned}$$

Here C depends only on Ω. So $\|\nabla w\|_{L^2(\Omega} \leq C/\kappa < \infty$. This completes the proof. ■

Our goal is to classify the minimizers of E. To that end, let $E|_S$ be the restriction of the energy functional E on S. We will show that critical points of $E|_S$ are indeed critical points of E. To do so, for each $w \in H^1(\Omega)$ define the associated fiber

$$F_w = \{ws : s \in \mathbb{R}\} = \text{span}\{w\}.$$

We can also define the fiber map

$$T_w(s) := E[sw], \forall s \in \mathbb{R}.$$

Note that if w is a local minimizer of E then T_w has a local minimizer at $s = 1$. Just like the first variations, the second variation $\delta^2 E[w] : H_0^1(\Omega) \times H_0^1(\Omega) \to \mathbb{R}$ plays an important role in the classification of the set S. This is defined as

$$\delta^2 E[w](u, v) = \int_\Omega \left(\kappa \nabla u \cdot \nabla v - \frac{uv \cos(2w)}{2} \right) dx, \ \forall u, v \in H_0^1(\Omega). \tag{4.2}$$

The first and second variations and the fiber map $T_w(s)$ are related as follows.

Lemma 4.2. *If $w \in H_0^1(\Omega)$ then*

$$T_w'(s) = \langle \delta E[sw], w \rangle = \int_\Omega \left(\kappa |s \nabla w|^2 - \frac{w \sin(2sw)}{4} \right) dx \tag{4.3}$$

and

$$T''_w(s) = \delta^2 E[sw](w,w) = \int_\Omega \left(\kappa |s\nabla w|^2 - \frac{w^2 \cos(2sw)}{2} \right) dx. \tag{4.4}$$

Proof. The proof follows from the limit definition of variations. ■

The above lemma allows us to get the following characterization.

Corollary 4.3. *If $w \in H_0^1(\Omega) \setminus \{0\}$ and $s \in \mathbb{R} \setminus \{0\}$ then $sw \in S \Leftrightarrow T'_w(s) = 0$.*

Proof. By (4.3) we have that

$$T'_w(s) = \langle \delta E[sw], w \rangle = \frac{1}{s} \langle \delta E[sw], sw \rangle.$$

Thus we have the equivalency. ■

Observe that $0 \neq w \in S \Leftrightarrow w$ is a critical point of $E|_{F_w}$. This motivates the splitting of the set S into local minimum, local maximum or inflection points of E along the fiber. Thus define the following sets

$$S^+ = \{w \in S : \delta^2 E[w](w,w) > 0\},$$

$$S^- = \{w \in S : \delta^2 E[w](w,w) < 0\},$$

$$S^0 = \{w \in S : \delta^2 E[w](w,w) = 0\}.$$

Lemma 4.4. *Let $w_0 \in S - S^0$ be a local minimizer of $E|_S$ then $\delta E[w_0] = 0$.*

Proof. The proof is analogous to Lemma 3.4 of [14]. ■

Since we concentrate on the global minimizers for E, by Lemma 3.1, we only need to classify the functions $w \in S \cap X$, where

$$X := \{w \in H_0^1(\Omega) : |w(x)| \leq \pi/2 \text{ a.e. in } \Omega\}.$$

Corollary 4.5. *We have the following characterization of S, S^0, S^+, S^- and their intersections with X.*

$$S = \left\{ w \in H_0^1(\Omega) : \int_\Omega \left(\kappa |\nabla w|^2 - \frac{w \sin(2w)}{4} \right) dx = 0 \right\}, \tag{4.5}$$

$$S^+ = \left\{ w \in S : \int_\Omega \left(\kappa |\nabla w|^2 - \frac{w^2 \cos(2w)}{2} \right) dx > 0 \right\}, \tag{4.6}$$

$$= \left\{ w \in S : \int_\Omega \left(\frac{w \sin(2w)}{4} - \frac{w^2 \cos(2w)}{2} \right) dx > 0 \right\}, \tag{4.7}$$

$$S^- = \left\{ w \in S : \int_\Omega \left(\frac{w \sin(2w)}{4} - \frac{w^2 \cos(2w)}{2} \right) dx < 0 \right\}, \tag{4.8}$$

$$S^0 = \left\{ w \in S : \int_\Omega \left(\frac{w \sin(2w)}{4} - \frac{w^2 \cos(2w)}{2} \right) dx = 0 \right\}. \tag{4.9}$$

In addition,

$$S^+ \cap X = \{w \in S \cap X : w \neq 0\}, \tag{4.10}$$

$$S^- \cap X = \emptyset, \tag{4.11}$$

$$S^0 \cap X = \{0\}. \tag{4.12}$$

Proof. Equation (4.5)–(4.9) follow from the definitions of the set S of and the second variation (4.2). For the rest, we only need to prove (4.10).

1. Define $\phi(t) := \frac{\sin t}{t} - \cos t$ for $t \neq 0$ and $\phi(0) = 0$. For $-\pi \leq t \leq \pi$ and $t \neq 0$, by Taylor expansion,

$$\begin{aligned}
\phi(t) = \frac{\sin t}{t} - \cos t &= \frac{1}{t}\left(t - \frac{t^3}{3!} + \frac{t^5}{5!} - \frac{t^7}{7!} + \frac{t^9}{9!} - \cdots\right) - \left(1 - \frac{t^2}{2!} + \frac{t^4}{4!} - \frac{t^6}{6!} + \frac{t^8}{8!} - \cdots\right) \\
&= \left(\frac{1}{2!} - \frac{1}{3!}\right)t^2 - \left(\frac{1}{4!} - \frac{1}{5!}\right)t^4 + \left(\frac{1}{6!} - \frac{1}{7!}\right)t^6 - \left(\frac{1}{8!} - \frac{1}{9!}\right)t^8 + \cdots \\
&= \frac{2t^2}{3!} - \frac{4t^4}{5!} + \frac{6t^6}{7!} - \frac{8t^8}{9!} + \cdots \\
&= t^2\left(\frac{2}{3!} - \frac{4t^2}{5!}\right) + t^6\left(\frac{6}{7!} - \frac{8t^2}{9!}\right) + \cdots \\
&\geq t^2\left(\frac{2}{3!} - \frac{4\pi^2}{5!}\right) + t^6\left(\frac{6}{7!} - \frac{8\pi^2}{9!}\right) + \cdots
\end{aligned} \tag{4.13}$$

It is easy to check every term in the right-hand side of (4.13) is positive for $t \neq 0$. So

$$\phi(t) = \frac{\sin t}{t} - \cos t > 0 \qquad \text{for all } -\pi \leq t \leq \pi,\ t \neq 0. \tag{4.14}$$

Note that we may allow $|t|$ to be in a range bigger than π, but it is not our priority to find the optimal bound on $|t|$.

2. For any $w \in S \cap X$ with $w \neq 0$, let $B := \{x \in \Omega : w(x) \neq 0\}$. Then $|B| > 0$ and for $x \in B$, we have $\phi(2w) > 0$ by (4.14). Therefore

$$\int_\Omega \left(\frac{w\sin(2w)}{4} - \frac{w^2\cos(2w)}{2}\right)dx = \int_\Omega \frac{w^2}{2}\left(\frac{\sin(2w)}{2w} - \cos(2w)\right)dx = \int_\Omega \frac{w^2}{2}\phi(2w)\, dx > 0.$$

By (4.7), we see that $w \in S^+$.

■

Lemma 4.6. *Let* $w \in H_0^1(\Omega) \setminus \{0\}$.

1. If

$$\int_\Omega \kappa|\nabla w|^2\, dx \geq \frac{1}{2}\int_\Omega w^2 dx, \tag{4.15}$$

then T_w *has no positive critical points or positive turning points,* $T_w'(s) > 0$, $T_w''(s) > 0$ *for all* $s > 0$ *and*

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

2. If

$$\int_\Omega \kappa|\nabla w|^2\, dx > \frac{1}{2}\int_\Omega w^2\, dx, \tag{4.16}$$

then $s = 0$ *is the unique critical point for* T_w.

3. If

$$\int_\Omega \kappa|\nabla w|^2\, dx < \frac{1}{2}\int_\Omega w^2\, dx \tag{4.17}$$

then there exists some $s_w > 0$ such that $T'_w(s_w) = 0$, that is T_w has a critical point s_w. Moreover, if $|s_w w| \leq \pi/2$ for all $x \in \Omega$ then $T''_w(s_w) > 0$, which implies that $s_w w \in S^+$.

Proof. From the definition of $T_w(s)$ and (2.5) we have

$$T_w(s) = \int_\Omega \left(\frac{s^2\kappa}{2}|\nabla w|^2 + \frac{\cos^2(ws)}{4} \right) dx.$$

1. Suppose (4.15) holds and $s > 0$. Since $w(x) \not\equiv 0$, there exists $\delta > 0$ such that the set

$$\Omega_\delta := \{x \in \Omega : |w(x)| \geq \delta\}$$

has positive measure. By the following elementary inequality

$$t^2 - t\sin t \geq t_0^2 - t_0\sin(t_0) > 0 \text{ for all } |t| \geq |t_0| > 0,$$

for all $x \in \Omega$ we have

$$\frac{sw^2}{2} - \frac{w\sin(2ws)}{4} = \frac{1}{8s}((2sw)^2 - (2sw)\sin(2sw)) \geq 0$$

and for all $x \in \Omega_\delta$ we can go one step further to obtain

$$\begin{aligned}\frac{sw^2}{2} - \frac{w\sin(2ws)}{4} &= \frac{1}{8s}((2sw)^2 - (2sw)\sin(2sw)) \\ &\geq \frac{1}{8s}((2s\delta)^2 - (2s\delta)\sin(2s\delta)) = \frac{\delta}{4}(2s\delta - \sin(2s\delta)) > 0.\end{aligned}$$

So by (4.15)

$$\begin{aligned}T'_w(s) &= \int_\Omega \left(s\kappa|\nabla w|^2 - \frac{w\sin(2ws)}{4} \right) dx \geq \int_\Omega \left(\frac{sw^2}{2} - \frac{w\sin(2ws)}{4} \right) dx \\ &\geq \int_{\Omega_\delta} \left(\frac{sw^2}{2} - \frac{w\sin(2ws)}{4} \right) dx \geq \frac{\delta}{4}(2s\delta - \sin(2s\delta))|\Omega_\delta| > 0.\end{aligned}$$

Integrating the above inequality, we have

$$T_w(s) \geq T_w(0) + \left(\frac{s^2\delta^2}{4} + \frac{\cos(2s\delta)}{8} \right)|\Omega_\delta| \to \infty \text{ as } s \to \infty.$$

The second derivative

$$T''_w(s) = \int_\Omega \left(\kappa|\nabla w|^2 - \frac{w^2\cos(2ws)}{2} \right) dx \geq \frac{1}{2}\int_\Omega w^2(1 - \cos(2ws))\, dx > 0.$$

The last inequality is because $w^2(1 - \cos(2ws) \geq 0$ and equality holds if and only if $w = k\pi/s$ for $k \in \mathbb{Z}$, which is impossible since we need $w \in H^1_0(\Omega) \setminus \{0\}$. This completes the proof of Statement (1).

2. Clearly $s = 0$ is a critical point for T_w since $T'_w(0) = 0$ by (4.3). We need to show that T_w has no other critical points if (4.16) holds. Note that $T'_w(s) = 0$ is equivalent to $s\int_\Omega \kappa|\nabla w|^2 dx = \int_\Omega \frac{w\sin(2ws)}{4} dx$. Let

$$\alpha := \int_\Omega \kappa|\nabla w|^2 dx, \quad \varphi(s) := \int_\Omega \frac{w\sin(2ws)}{4} dx.$$

Then $T_w'(s) = 0$ if and only if $\alpha s = \varphi(s)$, or equivalently, s is a fix point for $G(s) := \varphi(s)/\alpha$. Observe that for any $s \neq t$ we have

$$\begin{aligned} |G(s) - G(t)| &\leq \frac{1}{4\alpha} \int_\Omega |w|| \sin(2ws) - \sin(2wt)| dx \\ &\leq \frac{1}{2\alpha} \int_\Omega w^2 |s - t| dx \\ &\leq |s - t| \frac{1}{2\alpha} \int_\Omega w^2 dx. \end{aligned}$$

This is a contraction since $\frac{1}{2\alpha} \int_\Omega w^2 dx < 1$ by (4.16). Thus G has a unique fixed point and hence $s = 0$ is the unique critical point for T_w.

3. Now suppose (4.17) holds. Then $T_w''(0) = \int_\Omega \left(\kappa |\nabla w|^2 - \frac{w^2}{2} \right) dx < 0$. Since $T_w'(0) = 0$, by the definition of derivative there exists $s_1 > 0$ such that $T_w'(s_1) < 0$. However

$$\begin{aligned} T_w'(s) = s \int_\Omega \kappa |\nabla w|^2 \, dx - \int_\Omega \frac{w \sin(2ws)}{4} dx \geq s \int_\Omega \kappa |\nabla w|^2 \, dx - \frac{1}{4} \int_\Omega |w| \, dx \\ \to \infty \text{ as } s \to \infty. \end{aligned} \tag{4.18}$$

By the continuity of $T_w'(s)$ in s, there exists $s_w > s_1$ such that $T_w'(s_w) = 0$.

To show that $T_w''(s_w) > 0$, we need to notice $T_w'(s_w) = 0$ implies

$$\int_\Omega \kappa |\nabla w|^2 \, dx = \int_\Omega \frac{w \sin(2ws_w)}{4s_w} dx.$$

Hence

$$\begin{aligned} T_w''(s_w) &= \int \left(\kappa |\nabla w|^2 - \frac{w^2 \cos(2ws_w)}{2} \right) dx \\ &= \int_\Omega \left(\frac{w \sin(2ws_w)}{4s_w} - \frac{w^2 \cos(2ws_w)}{2} \right) dx \\ &= \int_\Omega \frac{w^2}{2} \left(\frac{\sin(2ws_w)}{2ws_w} - \cos(2ws_w) \right) dx. \end{aligned}$$

If $|s_w w| \leq \pi/2$ then by (4.14) we have $T_w''(s_w) > 0$. Hence by Corollaries 4.5 and 4.3 $s_w w \in S^+$.

■

5 | PROOF OF THEOREMS 2.1 AND 2.2

Now we are ready to begin the proof of Theorem (2.1). First note that there exists $w^* \in H_0^1(\Omega)$ that minimizes the energy functional E defined by (2.5) over $H_0^1(\Omega)$, compare Theorem 3.3 in [11]. By Lemma 3.1 we know also $|w^*| \leq \pi/2$ for all $x \in \Omega$. We recall that if $w \neq 0$ is a minimizer for E, then the corresponding fiber map $T_w(s) = E[sw],\ s \in \mathbf{R}$ has a minimum at $s = 1$ and hence $s = 1$ is a critical point of T_w. Utilizing the Dirichlet eigenvalue problem (2.9) and by Rayleigh's quotient, we have

$$\lambda_1 = \min \left\{ \frac{\int_\Omega |\nabla w|^2 dx}{\int w^2 dx} : w \in H_0^1(\Omega) \setminus \{0\} \right\}, \tag{5.1}$$

from which we can clearly get that for all $w \in H_0^1(\Omega)$ we have

$$\int_\Omega |\nabla w|^2 dx \geq \lambda_1 \int_\Omega w^2 dx. \tag{5.2}$$

Case 1. $\kappa \geq \frac{1}{2\lambda_1}$. In this case, by (5.2) we have

$$\kappa \int_\Omega |\nabla w|^2 \, dx \geq \frac{1}{2} \int_\Omega w^2 \, dx, \text{ for all } w \in H_0^1(\Omega).$$

By Case 1 of Lemma 4.6, if $w \neq 0$ then $T_w(s)$ has no positive critical point. Hence $w \neq 0$ cannot be a minimizer for E. In other words, $w = 0$ is the unique minimizer for E and $\min\{E[w] : w \in H_0^1(\Omega)\} = E[0] = \frac{|\Omega|}{4}$.

Case 2. $0 < \kappa < \frac{1}{2\lambda_1}$. In this case we first show that the minimum of E is less than $\frac{|\Omega|}{4}$. Since

$$\cos^2 w = \frac{1}{2}(1 + \cos 2w) \leq \frac{1}{2}\left(1 + 1 - \frac{(2w)^2}{2} + \frac{(2w)^4}{4!}\right),$$

we have

$$E[w] \leq \hat{E}[w] \quad \text{for all } w \in H_0^1(\Omega),$$

where

$$\hat{E}[w] := \int_\Omega \left(\frac{\kappa}{2}|\nabla w|^2 + \frac{1}{4} - \frac{w^2}{4} + \frac{w^4}{12}\right) dx. \tag{5.3}$$

For each $w \in H_0^1(\Omega) \setminus \{0\}$, let $\hat{T}_w(s)$ be the fiber map for $\hat{E}$. Since $0 < \kappa < \frac{1}{2\lambda_1}$, by similar calculations as in [14], $\hat{T}_w(s)$ has exactly one critical point at

$$\hat{s}_w = \left(\frac{\frac{1}{2}\int_\Omega w^2 dx - \kappa \int_\Omega |\nabla w|^2}{\frac{1}{3}\int_\Omega w^4 dx}\right)^{1/2}, \tag{5.4}$$

and $\hat{s}_w$ is a minimizer for $\hat{T}_w$. Thus, for ψ_1 the corresponding eigenfunction of λ_1 we have

$$E[w^*] \leq E[\hat{s}_{\psi_1}\psi_1] \leq \hat{E}[\hat{s}_{\psi_1}\psi_1] = \int_\Omega \frac{\kappa}{2}|\tilde{s}_{\psi_1}\nabla\psi_1|^2 + \frac{1}{4} - \frac{\tilde{s}_{\psi_1}^2\psi_1^2}{4} + \frac{(\tilde{s}_{\psi_1}\psi_1)^4}{12} dx. \tag{5.5}$$

Using the corresponding Nehari manifold for $\hat{E}$ we have

$$\hat{E}[\hat{s}_{\psi_1}\psi_1] = \frac{1}{4}\int_\Omega \left(1 - \frac{(\hat{s}_{\psi_1}\psi_1)^4}{3}\right) dx < \frac{|\Omega|}{4}.$$

Together with Equation (5.4) we have

$$E[w^*] < \frac{|\Omega|}{4}$$

and hence $w^* \neq 0$.

Define $w_+ = |w^*|$ and $w_- = -|w^*|$. Clearly $\cos^2(w_+) = \cos^2(w_-) = \cos^2(w^*)$ and $|\nabla w_+| = |\nabla w_-| = |\nabla w^*|$. Thus $E[w_+] = E[w_-] = E[w^*]$ and both w_+ and w_- are minimizer of E over $H_0^1(\Omega)$. Also $w_+ \geq 0$ and $w_- \leq 0$ in Ω with

$$w_+ + w_- = 0 \quad \text{in} \quad \Omega.$$

Then w_+ is a nonnegative and nonzero solution for the Euler–Lagrange equation

$$-\kappa\Delta w - \frac{\sin(2w)}{4} = 0 \quad \text{in} \quad \Omega, \tag{5.6}$$

$$w = 0 \quad \text{on} \quad \partial\Omega. \tag{5.7}$$

Standard regularity theory (see, e.g., [19]) shows that $w_+ \in C^\infty(\Omega) \cap C(\overline{\Omega})$.

Next we show that $w_+ > 0$. in Ω. We prove by contradiction. To that end assume that there exists $x_0 \in \Omega$ such that $w_+(x_0) = 0$. Then $w_+(x_0)$ is the minimum of w_+. However, since $0 \le w_+ \le \pi/2$, we have

$$-\kappa\Delta w_+ = \frac{\sin(2w_+)}{4} \ge 0. \tag{5.8}$$

By the strong maximum principle, w_+ is a constant and hence is zero in Ω. This contradicts the energy estimate above. This also implies that the minimizer w^* cannot have both negative and positive parts.

To show that $w_+ < \frac{\pi}{2}$ for all $x \in \Omega$, we assume there exists $x_1 \in \Omega$ such that $w_+(x_1) = \frac{\pi}{2}$. Define $v := w_+ - \frac{\pi}{2}$. Then $-\frac{\pi}{2} \le v \le 0$ in Ω and $v(x_1) = 0$ is the non-negative maximum of u in Ω. Going back to the Euler–Lagrange equation (5.6) we have

$$-\kappa\Delta v - \frac{\sin(2v + \pi)}{4} = 0.$$

Thus

$$-\kappa\Delta v = -\frac{\sin(2v)}{4} \le -\frac{v}{2}$$

and

$$-\kappa\Delta v + \frac{v}{2} \le 0.$$

Then by the strong maximum principle, v is a constant and hence $v \equiv 0$. This implies that $w_+ \equiv \frac{\pi}{2}$ but this contradicts the boundary value of $w_+ = 0$. Thus $w_+ < \frac{\pi}{2}$.

To prove the uniqueness of positive minimizers for E, we will use the following lemma.

Lemma 5.1. *Suppose $G[w]$ is an energy functional given by*

$$G[w] := \int_\Omega (\Phi(|\nabla w|) + F(|w|))dx, \quad w \in H_0^1(\Omega), \tag{5.9}$$

where Ω is a domain and F is a strictly decreasing function. Then G allows at most one positive minimizer.

This lemma can be proved using similar arguments as in [14]. By taking $\Phi(|\nabla u|) = \frac{\kappa}{2}|\nabla w|^2$ and $F(w) = \frac{\cos^2(w)}{4}$ with $|w| \le \pi/2$, we obtain the uniqueness of positive minimizers for E. This completes the proof of Theorem 2.1.

Theorem 2.2 follows from the identity $E[|w|] = E[w]$, the Euler–Lagrange equation (5.6) and (5.7) and the strong maximum principle.

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DATA AVAILABILITY STATEMENT

Data sharing not applicable to this article as no datasets were generated or analyzed during the current study.

ORCID

Shibin Dai https://orcid.org/0000-0002-1726-4745

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