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CRITICAL POINTS OF FUNCTIONALIZED LAGRANGIANS

Keith Promislow

Department of Mathematics, Michigan State University
East Lansing, MI, 48824, USA

Hang Zhang

Nico Holding LLC, 222 W. Adams Street
Chicago, IL, 60606, USA

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Abstract. We present a novel class of higher order energies motivated by the study of network formation in binary mixtures of functionalized polymers and solvent. For a broad class of Lagrangians, we introduce their *functionalized* form, which is a higher order energy balancing the square of the variational derivative against the original energy. We show that the functionalized energies have global minimizers over several natural spaces of admissible functions. The critical points of the functionalized Lagrangian contain those of the original Lagrangian, however we demonstrate that for a sufficient strength of the functionalization all the critical points of the original Lagrangian are saddle points of the functionalized Lagrangian, and the global minima is a new structure.

1. **Introduction.** A goal of polymer chemistry is to design materials with novel macroscopic properties by controlling the spontaneous generation of nanoscaled, phase separated networks. A primary mechanism to generate such networks is through the "functionalization" of hydrophobic polymer chains and nanoparticles by the addition of acid or alkaline tipped side-chains. In the presence of a polar solvent the end groups interact exothermically, driving the generation of polymer-solvent or nanoparticle-solvent interface. The resulting phase-separated network structures can be exploited for charge selective conduction, and have important applications to efficient energy conversion devices such as polymer electrolyte membranes for fuel cells, [14, 16], dye sensitized solar cells [10], and bulk-heterojunction solar cells, [13, 3].

In 1958 Cahn and Hilliard, [1], introduced their classical energy

$$\mathcal{E}(u) = \int_\Omega \frac{1}{2}|\nabla u|^2 + W(u)\,dx, \tag{1}$$

which describes binary mixtures of inert materials in terms of a scalar quantity u representing the volume fraction over a domain $\Omega \subset \mathbb{R}^d$, $d \geq 2$. The potential W typically has two local minima, and satisfies growth conditions as $u \to \pm\infty$. Constrained minimizers of $\mathcal{E}$ are well understood, and under an appropriate spatial

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scaling, the Γ-convergence of $\mathcal{E}$ to a scaled surface area functional has long been established [12, 18].

While mixtures of inert materials generically seek to minimize surface area, the embedded charge groups in functionalized materials interact exothermically with polar solvents, spontaneously generating polymer-solvent interface. A prime example is Nafion, a functionalized fluorocarbon polymer frequently used as a membrane separator in polymer electrolyte membrane fuel cells. From their small angle x-ray scattering (SAXS) experiments, [9], Hsu and Gierke hypothesized that the water domain within the Nafion forms small 4-5 nanometer balls interconnected by thin 1-2 nanometer cylindrical pores. They further suggested such a network could arise from a balance between the elastic energy of the interface and the hydrophilic surface interactions among the charged functional groups and the solvent. Motivated by these observations, a model has been proposed, [14, 6], for interfacial development in functionalized polymer-solvent mixtures which assigns a negative value to interfacial energy via the Cahn-Hilliard energy and balances this against the square of its own variational derivative. More generally, we introduce the quadratic functionalization, $\mathcal{F}$, of the energy $\mathcal{E}$ with respect to the balance parameter $\eta > 0$,

$$\mathcal{F}(u) = \int_\Omega \frac{1}{2}\left(\frac{\delta \mathcal{E}}{\delta u}(u)\right)^2 dx - \eta\, \mathcal{E}(u). \tag{2}$$

and in particular the Functionalized Cahn-Hilliard (FCH) energy takes the form

$$\mathcal{F}_{\rm CH}(u) = \int_\Omega \frac{1}{2}\Big(\Delta u - W'(u)\Big)^2 - \eta\left(\frac{1}{2}|\nabla u|^2 + W(u)\right) dx. \tag{3}$$

In the sequel we establish two broad theorems which show that functionalized energies of the form (2) sit inside an appealing mathematical framework. In Theorem 1 we show that a broad class of energies $\mathcal{E}$ have quadratic functionalizations which possess absolute minimizers over a variety of natural admissible function spaces. In Theorem 2 we show that the critical points of the the original energies are critical points of the functionalized energies, however if the strength of the functionalization, as measured by η, is large enough, then these inherited critical points are saddles, and the global minimizer is a novel structure. Thus the functionalized energies have a rich family of critical points. Indeed, in [6] the novel global minimizers of the one-dimensional problem, bifurcating from the classical minimizers, are used to parameterize the bi-layer network structures which dominate the energy landscape in $\mathbb{R}^n$, for $n > 1$.

The FCH energy is has appeared before in the literature. In [7], an energy was proposed for amphiphilic systems, in which two immiscible fluids are mixed with a surfactant forming a microemulsion at the interface. This energy was motivated by small-angle X-ray scattering (SAXS) data which can be related to the reciprocal of the Fourier transform of the second variation of the energy evaluated at a constant background state. Based upon the data, the authors proposed an energy with a discontinuous dependence on the mixture fraction u. In subsequent work, [17], the authors smoothed out the coefficients, obtaining a form equivalent to the FCH.

Although not addressed here, $\Gamma-$limit of the FCH energy raises intriguing issues. The case $\eta < 0$, when both terms in (3) are positive, is the perview of conjecture of De Giorgi, which posits the Γ-convergence of a scaled version (3) to a modified Willmore energy. This result has recently been established, [11, 15], as well as a related problem concerning the minimization of the FCH with $\eta = 0$ subject to a surface area constraint, [4]. However the formal results of [6] suggest that the nature of the FCH energy is fundamentally different in the case $\eta > 0$. Indeed, for a fixed, smooth hypersurface $\Gamma \subset \mathbb{R}^n$, the authors showed a convergence to a Canham-Helfrich energy, [2, 8], written in terms of the mean curvature H as

$$\mathcal{E}_{CH}(\Gamma) = \int_\Gamma a_1 + a_2(H - a_3)^2 \, dS, \tag{4}$$

with a negative interfacial coefficient $a_1 < 0$ and a positive curvature coefficient $a_2 > 0$. Most significantly, due to its higher-order nature, the FCH energy supports a variety of interfacial structures, with the resulting values of the limiting coefficients depending upon the nature of the interfacial structure chosen. Moreover, preliminary results suggest that for non-zero volume fractions of both phases, the minimizing hypersurfaces of the FCH will have unbounded length, and the limit of zero-interfacial width will more resemble a homogenization problem than a traditional $\Gamma-$convergence one.

2. **Notation.** We consider functions $A : \mathbb{R}^n \times \mathbb{R}^n \mapsto \mathbb{R}$ with values $A(\mathbf{p}, x)$ and denote the full k-contraction of the k-order derivative with respect to $\mathbf{p}$ by

$$D^k_{\mathbf{p}} A(\mathbf{p})(\vec{h}_1, \dots, \vec{h}_k) = \sum_{i_1=1}^n \cdots \sum_{i_k=1}^n \frac{\partial^k A}{\partial \mathbf{p}_{i_1} \dots \partial \mathbf{p}_{i_k}}(\mathbf{p}) \vec{h}_{1,i_1} \cdots \vec{h}_{k,i_k}, \tag{5}$$

where $\vec{h}_j \in \mathbb{R}^n$ for $j = 1, \dots, n$. The l contraction of the k tensor $D^k_{\mathbf{p}} A$ by vectors $(\vec{h}_1, \dots, \vec{h}_l)$ is a $k - l$ tensor with entries

$$\left[D^k_{\mathbf{p}} A(\mathbf{p})(\vec{h}_1, \dots \vec{h}_l) \right]_{(j_1, \dots, j_{k-l})} = D^k_{\mathbf{p}} A(\mathbf{p})(\vec{h}_1, \dots, \vec{h}_l, \vec{e}_{j_1}, \dots, \vec{e}_{j_{k-l}}), \tag{6}$$

where $\{\vec{e}_1, \dots, \vec{e}_n\}$ is the canonical basis of $\mathbb{R}^n$. In particular for $k = 2$ we employ the notation

$$D^2_p A(\mathbf{p})(\vec{h}_1, \vec{h}_2) = \vec{h}_2^t D^2_{\mathbf{p}} A(p) \vec{h}_1 = \vec{h}_2 \cdot D^2_{\mathbf{p}} A(\mathbf{p}) \vec{h}_1 = \vec{h}_1 \cdot D^2_{\mathbf{p}} A(\mathbf{p}) \vec{h}_2. \tag{7}$$

We also use the matrix inner product for $M, N \in \mathbb{R}^{n \times n}$,

$$M : N = \sum_{i,j=1}^n M_{i,j} N_{i,j}. \tag{8}$$

The set $\Omega \subset \mathbb{R}^n$ will be bounded with a $\mathcal{C}^2$ boundary. For $f \in L^1(\Omega)$ we denote the mass of f by

$$< f >= \int_\Omega f dx, \tag{9}$$

while the L^2 pairing of $f, g \in L^2(\Omega)$ is denoted

$$\langle f, g \rangle = \int_\Omega f(x) g(x) \, dx. \tag{10}$$

3. **Functionalization.** Fix a bounded domain $\Omega \subset \mathbb{R}^n$ and consider a Langrangian $L(\mathbf{p}, z, x) : \mathbb{R}^n \times \mathbb{R} \times \overline{\Omega} \to \mathbb{R}$, which is smooth in its arguments. The associated energy $\mathcal{E}$ maps an admissible set $\mathcal{A}$ into $\mathbb{R}$ according to

$$\mathcal{E}(u) = \int_\Omega L(Du, u, x) dx. \tag{11}$$

If L satisfies the natural growth conditions and appropriate boundary conditons on $W^{1,q}$, then the Frechet derivative of $\mathcal{E}$ lies in the dual of $W^{1,q}$,

$$\frac{\delta \mathcal{E}}{\delta u} = -\nabla \cdot D_{\mathbf{p}} L(Du, u, x) + L_z(Du, u, x), \tag{12}$$

and acts on an appropriate classes of test functions v by

$$\left\langle \frac{\delta \mathcal{E}}{\delta u}, v \right\rangle = \int_\Omega \left[D_{\mathbf{p}} L(Du, u, x) Dv + L_z(Du, u, x) v \right] dx. \tag{13}$$

If L is coercive and convex then the energy $\mathcal{E}$ has a global minimizer over a broad class of admissible sets, and the set of critical points of $\mathcal{E}$,

$$\mathcal{C}_{\mathcal{E}} = \left\{ u \in \mathcal{A} \;\middle|\; \frac{\delta \mathcal{E}}{\delta u}(u) = 0 \right\}, \tag{14}$$

is non-empty. The primary goal of the direct methods of the calculus of variations is to establish the existence of critical points of classes of Lagrangians, that is, to construct minima and saddle points of the energy $\mathcal{E}$.

Occasionally it is possible in a physical setting to “flip the sign” of the dominant feature of an energy landscape, for example modifying a constituent material so that its interfacial energy changes from a positive to a negative contribution to the total energy balance. A fundamental question is whether the resulting energy can be regularized in a systematic fashion so as to construct new classes of critical points. A natural, and in some settings, physically meaningful approach is to regularize with the square of the variational derivative. Drawing upon the example of functionalization of polymers, we call the resultant energy the functionalization of the original energy.

Definition 1. If the energy $\mathcal{E}$ is differentiable for $u \in \mathcal{A}$ with its variational derivative lying in $L^2(\Omega)$, then for any $\eta \in L^\infty(\Omega)$ we define the *quadratic functionalization* of $\mathcal{E}$ relative to the local balance η to be

$$\mathcal{F}(u) = \int_\Omega \left[\frac{1}{2} \left(\frac{\delta \mathcal{E}}{\delta u} \right)^2 - \eta L(u) \right] dx. \tag{15}$$

The functionalized energy is typically higher order and requires more regularity be imposed upon the admissible function space. If for example $\mathcal{A} \subset W^{2,q}(\Omega)$ for $q > \max\{n, 2\}$, then $\mathcal{A} \subset W^{1,\infty}(\Omega)$ and the Frechet derivative, $\frac{\delta \mathcal{E}}{\delta u}$, given by (12), lies in $L^q(\Omega) \subset L^2(\Omega)$. The functionalized energy, $\mathcal{F}$, maps $\mathcal{A}$ into $\mathbb{R}$, and its critical points balance the original energy against its own variational derivative. To focus our efforts, we restrict our attention to Lagrangians of the separated form

$$L(\mathbf{p}, z, x) = A(\mathbf{p}) + B(z, x), \tag{16}$$

where A has bounded second deriviative and is uniformly convex, while B satisfies growth conditions and is sufficiently convex at ∞. More specifically we consider a bounded set $\Omega \subset \mathbb{R}^n$ with a $\mathcal{C}^2$ boundary and we assume there exist $\mu, \alpha > 0$, $p_1 \in \left(1, \frac{n}{n-2}\right]$, $p_2 \in \left(0, \frac{2}{n-4}\right]$, $z_0 > 0$, and $\beta > 1$ sufficiently large, such that

$$\begin{aligned} |D^2_{\mathbf{p}} A(\mathbf{p})| &\leq \mu, && (17)\\ \xi^t D^2_{\mathbf{p}} A(\mathbf{p})\xi &\geq \alpha|\xi|^2, \qquad \forall \xi \in \mathbb{R}^n, && (18)\\ |B_z| &\leq \mu(1+|z|^{p_1}), && (19)\\ |B_{zz}| &\leq \beta(1+|z|^{p_2}), && (20)\\ B_{zz}(z,x) &\geq \beta, \qquad \forall |z| \geq z_0, x \in \Omega, && (21) \end{aligned}$$

hold for all $\mathbf{p} \in \mathbb{R}^n$.

With these restrictions the functionalized energy is well defined on the following natural spaces of admissible functions,

$$\begin{aligned} \mathcal{A}_0 &= H^2(\Omega) \cap H^1_0(\Omega), && (22)\\ \mathcal{A}_N &= \left\{ u \in H^2(\Omega) \middle| D_{\mathbf{p}} A(Du) \cdot \vec{n} = 0 \right\}, && (23) \end{aligned}$$

and $\mathcal{A}_{0,N} = \mathcal{A}_0 \cap \mathcal{A}_N$, where $\vec{n}$ is the normal on $\partial\Omega$. The tangent planes of the function spaces are given by $\mathcal{A}'_0 = \mathcal{A}_0$ and

$$\begin{aligned} \mathcal{A}'_N(u) &= \left\{ v \in H^2(\Omega) \middle| D_u v = 0 \right\}, && (24)\\ \mathcal{A}'_{0,N} &= H^2(\Omega) \cap H^1_0(\Omega) \cap \{Dv \cdot \mathbf{n} = 0\}, && (25) \end{aligned}$$

where for all $u, v \in H^2$ we define

$$D_u v = D^2_{\mathbf{p}} A(Du)(Dv, \vec{n}). \qquad (26)$$

From the coercivity condition (18) it follows that the normal component of the D_u derivative is bounded away from zero, and in conjunction with homogenious Dirichlet conditions, the D_u derivative reduces to a homogenious Neumann condtion in (25). Denoting the spaces of admissible functions generically by $\mathcal{A}$ and its tangent space by $\mathcal{A}'(u)$, the critical points, $\mathcal{C}_{\mathcal{E}}$, satisfy the weak formulation

$$\int_\Omega D_{\mathbf{p}} A(Du) Dv + B_z(u,x) v \mathrm{dx} = 0, \qquad (27)$$

for all $v \in \mathcal{A}'$. However, since $u \in \mathcal{A} \subset H^2$, the elements of $\mathcal{C}_{\mathcal{E}}$ are strong solutions of

$$\frac{\delta \mathcal{E}}{\delta u}(u) = 0, \qquad (28)$$

where the first variation of $\mathcal{E}$ takes the form

$$\frac{\delta \mathcal{E}}{\delta u} = -\nabla \cdot D_{\mathbf{p}} A(Du) + B_z(u,x) = -D^2_{\mathbf{p}} A(Du) : D^2 u + B_z(u,x). \qquad (29)$$

From the assumptions (17), (19), and standard Sobolev embeddings, the first variation lies in $L^2(\Omega)$. The quadratic part, $Q_{\mathcal{E}}$, of $\mathcal{E}$ takes the form

$$Q_{\mathcal{E}}(v,v) = \int_\Omega Dv^t D^2_{\mathbf{p}} A(Du) Dv + B_{zz}(u,x)\, \mathrm{dx}, \qquad (30)$$

for $v \in \mathcal{A}'$, which induces a self-adjoint operator, the second variation of $\mathcal{E}$,

$$\mathcal{L}_{\mathcal{E}} v \equiv \frac{\delta^2 \mathcal{E}}{\delta u^2} v = -\nabla \cdot \left(D^2_{\mathbf{p}} A(Du) Dv \right) + B_{zz}(u,x) v. \qquad (31)$$

Since the functionalized energy is not obviously bounded from below, nor coercive, it is natural to ask under what circumstances it has a global minimizer over $\mathcal{A}$.

4. **Minimization of the Functionalized Lagrangian.** The essential step in constructing minimizers of $\mathcal{F}$ is to establish its coercivity, and this relies on the H^2 regularity of the variational problem for $\mathcal{E}$ over $\mathcal{A}$, which under conditions (17) and (18) follows from classical results, [5, 19], which we restate below.

Proposition 1. *If $\Omega \subset \mathbb{R}^n$ is bounded with C^2 boundary, and A satisfies (17-18) then there exists $c > 0$ such that any weak solution $u \in \mathcal{A}$ of*

$$\nabla \cdot D_{\mathbf{p}} A(Du) = f, \tag{32}$$

satisfies the estimate

$$\|u - \langle u \rangle\|_{H^2} \leq c\|f\|_{L^2}. \tag{33}$$

Our first result is the existence of global minimizers of the functionalized Lagrangian

Theorem 1. *Let $\Omega \subset \mathbb{R}^n$ be bounded with a C^2 boundary with local balance function $\eta \in W^{1,\infty}(\Omega)$ given. Then there exists $\beta_0 > 1$ such that for any Lagrangian L of the form (16) with A and B satisfying (17-21) for some $\beta \geq \beta_0$, then the functionalized energy $\mathcal{F}$ given by (15) has a global minimizer over each of the admissible sets $\mathcal{A} = \mathcal{A}_0, \mathcal{A}_N$, or $\mathcal{A}_{0,N}$.*

Remark: We may extend Theorem 1 to include existence of a minimizer under the free boundary conditions, $\mathcal{A}_f = H^2(\Omega)$, if we modify the functionalized energy to include a boundary term

$$\mathcal{F}(u) = \int_\Omega \left[\frac{1}{2}\left(\frac{\delta \mathcal{E}}{\delta u}\right)^2 - \eta L\right] \mathrm{dx} + \int_{\partial\Omega} \eta u D_{\mathbf{p}} A(Du) \cdot \vec{n}\, \mathrm{dS}. \tag{34}$$

The boundary term vanishes for the admissible sets considered in Theorem 1.

4.1. **Lower Bounds and H^2 coercivity.** The first step in the proof is to show that the functionalized energy is bounded below.

Lemma 1. *There exists a constant $C = C(|\Omega|, B, \|\eta\|_{W^{1,\infty}}) > 0$ such that for all $u \in \mathcal{A}$, the functionalized energy $\mathcal{F}(u)$ is bounded below by*

$$\mathcal{F}(u) \geq \frac{1}{4}\int_\Omega \left|\frac{\delta \mathcal{E}}{\delta u}\right|^2 - C. \tag{35}$$

Proof. Without loss of generality we may assume that $\eta \geq 1$ since if not we can add and subtract a constant, $\eta_0 > 0$,

$$\mathcal{F}(u) = \frac{1}{2}\left\|\frac{\delta \mathcal{E}}{\delta u}\right\|_{L^2}^2 - \int_\Omega (\eta + \eta_0) L\, \mathrm{dx} + \eta_0 \mathcal{E},$$

for which $\eta + \eta_0 \geq 1$ while the functional $\eta_0 \mathcal{E}(u)$ is bounded from below under the assumptions (18) and (21). Multiplying $\frac{\delta \mathcal{E}}{\delta u}$ by ηu, and integrating by parts, we have

$$\int_\Omega \frac{\delta \mathcal{E}}{\delta u} \eta u \, dx = \int_\Omega D_{\mathbf{p}} A(Du) \cdot D(\eta u) + \eta B_z(u, x) u \, dx. \tag{36}$$

Adding and subtracting the right- and left-hand sides of (36), respectively, to the functionalized energy yields the expression

$$\mathcal{F}(u) = \int_\Omega \frac{1}{2}\left(\frac{\delta\mathcal{E}}{\delta u}\right)^2 - \eta\frac{\delta\mathcal{E}}{\delta u}u + D_{\mathbf{p}}A(Du)\cdot D(\eta u) + \eta B_z u - \eta L\mathrm{d}x \tag{37}$$

Since $\eta \geq 0$, Young's inequalty implies that

$$\eta\frac{\delta\mathcal{E}}{\delta u}u \leq \frac{\eta}{4\|\eta\|_\infty}\left(\frac{\delta\mathcal{E}}{\delta u}\right)^2 + \eta\|\eta\|_\infty u^2 \leq \frac{1}{4}\left(\frac{\delta\mathcal{E}}{\delta u}\right)^2 + \eta\|\eta\|_\infty u^2, \tag{38}$$

and grouping terms we have

$$\begin{aligned}\mathcal{F}(u) \quad \geq \quad & \int_\Omega \Big[\frac{1}{4}\left(\frac{\delta\mathcal{E}}{\delta u}\right)^2 + \eta\left(B_z u - B - \|\eta\|_\infty u^2\right) - \\ & \eta\big(A(Du) - D_{\mathbf{p}}A(Du)\cdot Du\big) + uD_{\mathbf{p}}A\cdot D\eta\Big]\,\mathrm{d}x,\end{aligned} \tag{39}$$

To control the second line of (39) we Taylor expand $A(\mathbf{p})$,

$$A(\mathbf{p}_0) = A(\mathbf{p}) + D_{\mathbf{p}}A(\mathbf{p})\cdot(\mathbf{p}_0 - \mathbf{p}) + \frac{1}{2}(\mathbf{p}_0 - \mathbf{p})^t D^2_{\mathbf{p}}(\tilde{\mathbf{p}})(\mathbf{p}_0 - \mathbf{p}), \tag{40}$$

where $\tilde{\mathbf{p}}$ lies between $\mathbf{p}_0$ and $\mathbf{p}$, set $\mathbf{p}_0 = 0$, $\mathbf{p} = Du$, and use the convexity of A to obtain the lower bound

$$A(0) - \frac{\alpha}{2}|Du|^2 \geq A(Du) - D_{\mathbf{p}}A(Du)\cdot Du. \tag{41}$$

From condition (17) we have the bound

$$|D_{\mathbf{p}}A(\mathbf{p})| \leq |D_{\mathbf{p}}A(0)| + \mu|\mathbf{p}|, \tag{42}$$

and hence

$$\begin{aligned}|uD_{\mathbf{p}}A\cdot D\eta| \quad & \leq \quad C\|D\eta\|_\infty|u|\left(1 + \mu|Du|\right), \\ & \leq \quad \frac{\alpha}{4}|Du|^2 + C\frac{\mu^2\|D\eta\|^2_\infty}{\alpha}u^2.\end{aligned} \tag{43}$$

Bounding the second line of (39) by (41) and (43), and using $\eta \geq 1$, we see that the functionalized energy is bounded below by

$$\mathcal{F}(u) \geq \frac{1}{4}\left\|\frac{\delta\mathcal{E}}{\delta u}\right\|^2_{L^2} - C + \int_\Omega \eta(B_z u - B - \frac{1}{4}\beta u^2)\mathrm{d}x, \tag{44}$$

for any $\beta > 4\left(C\mu^2\|D\eta\|_\infty/\alpha + \|\eta\|_\infty\right)$. It remains to show that

$$h(z,x) \equiv B_z(z,x)z - B(z,x) - \frac{1}{4}\beta z^2, \tag{45}$$

is bounded below. We define

$$M := \sup_{x\in\Omega, |z|<z_0} |h(z,x)| < \infty \tag{46}$$

and observe from (21) that for $z \geq z_0$, h satisfies

$$h_z = (B_{zz} - \frac{1}{2}\beta)z > \frac{\beta z}{2}, \tag{47}$$

and hence

$$h(z,x) \geq \frac{\beta}{4}(z^2 - \mu^2) - M, \tag{48}$$

on $z > z_0$. Similar arguements for $z < -z_0$, and the bound (46) extend this inequality to all $x \in \Omega$ and $z \in \mathbb{R}$. Inserting this bound into (44) and integrating over Ω provides (35). □

□

The following Lemma establishes the H^2 coercivity of the functionalized energy $\mathcal{F}$.

Lemma 2. *Under the assumptions of Theorem 1, there exist constants $C_1 > 0$ and C_2 such that*

$$|\mathcal{F}(u)|^{\overline{p}} \geq C_1 \|u\|_{H^2} - C_2, \tag{49}$$

where $\overline{p} = \max\{p_1/2, 1\}$ for $p_1 \in \left(1, \frac{n}{n-2}\right)$ as in (19).

Proof. First, we claim that there exists $M > 0$, such that

$$\nabla_{\mathbf{p}} A(\mathbf{p}) \cdot \mathbf{p} \geq \frac{\alpha}{2} |\mathbf{p}|^2 - M. \tag{50}$$

Writing $\mathbf{p} = \mathbf{n} l$, where $\mathbf{n} = \frac{\mathbf{p}}{|\mathbf{p}|}$ and $l = |\mathbf{p}|$, then for a fixed $\mathbf{n}$

$$(D_{\mathbf{p}} A(\mathbf{p}) - D_{\mathbf{p}} A(0)) \cdot \mathbf{n} = \int_0^l \frac{\partial}{\partial s} D_{\mathbf{p}} A(s\mathbf{n}) \cdot \mathbf{n} \, \mathrm{d}s \tag{51}$$

$$= \int_0^l \mathbf{n}^t D^2_{\mathbf{p}} A(s\mathbf{n}) \mathbf{n} \, \mathrm{d}s \geq \alpha l. \tag{52}$$

Multiplying by l, we have

$$D_{\mathbf{p}} A(\mathbf{p}) \cdot \mathbf{p} \geq D_{\mathbf{p}} A(0) \cdot \mathbf{p} + \alpha |\mathbf{p}|^2 \geq \frac{\alpha}{2} |\mathbf{p}|^2 - \frac{|D_p A(0)|^2}{2\alpha^2}, \tag{53}$$

which establishes (50). Take $\eta = 1$ in (36) and apply (50) to obtain the bound

$$\frac{\alpha}{2} \int_\Omega |Du|^2 \, \mathrm{d}x \leq \int_\Omega u \frac{\delta \mathcal{E}}{\delta u} - B_z u \, \mathrm{d}x + M|\Omega|. \tag{54}$$

Using Young's inequality and adding $\frac{\alpha}{2}\|u\|^2_{L^2}$ to both sides leads to,

$$\frac{\alpha}{2} \|u\|^2_{H^1} \leq \frac{1}{2} \left\| \frac{\delta \mathcal{E}}{\delta u} \right\|^2_{L^2} - \int_\Omega \left[\left(B_z u - B - \frac{1+\alpha}{2} u^2 \right) + B \right] \mathrm{d}x + M|\Omega|. \tag{55}$$

For $\beta > 2(1+\alpha)$ the term in parenthesis is bounded from below by h, defined in (45), while form (48) and (21), both h and B are bounded below, so that

$$\frac{\alpha}{2} \|u\|^2_{H^1} \leq \frac{1}{2} \left\| \frac{\delta \mathcal{E}}{\delta u} \right\|^2_{L^2} + C, \tag{56}$$

for some $C > 0$. Applying the lower bound (35) on $\mathcal{F}$ to the right-hand side, we find there exist constants $C_1, C_2 > 0$, such that

$$\|u\|^2_{H^1} \leq C_1 \mathcal{F}(u) + C_2. \tag{57}$$

From condition (19), and the continuous embedding $H^1 \subset L^{2p_1}$, we may bound the L^2 norm of the derivative of the potential, B, in terms of the H^1 norm of u,

$$\|B_z(u, x)\|_{L^2} \leq \mu \left(|\Omega| + \|u\|^{p_1}_{L^{2p_1}} \right) \leq C \left(1 + \|u\|^{p_1}_{H^1} \right) \tag{58}$$

and from (57) we obtain the bound

$$\|B_z(u,x)\|_{L^2} \le C_1 \,|\mathcal{F}(u)|^{\frac{p_1}{2}} + C_2. \tag{59}$$

From the form of the first variation, (29), it follows that u is a weak solution of (32) with $f = \frac{\delta\mathcal{E}}{\delta u} - B_z(u,x)$, and from the H^2 regularity result (33) and the H^1 bound (57) which controls the mass of u, $\langle u\rangle$, we have the following H^2 estimate,

$$\|u\|_{H^2} \le C\left(\|B_z\|_{L^2} + \left\|\frac{\delta\mathcal{E}}{\delta u}\right\|_{L^2}\right). \tag{60}$$

Combining the estimate (59) and the lower bound (35) from Lemma 1, we obtain the H^2 coercivity, (49), of the functionalized energy. □

□

4.2. **Existence of the Minimizer.** With the results of Lemma 1 and Lemma 2 in hand, we complete the proof of Theorem 1. Since the functionalized energy is bounded below, there exists a minimizing sequence $\{u_\nu\} \in \mathcal{A}$ and numbers $m > -\infty$ and $M < \infty$, such that

$$M > F(u_\nu) \searrow m. \tag{61}$$

From the H^2 coercivity of $\mathcal{F}$ the sequence $\{u_\nu\}$ is bounded in H^2 and there exists a subsequence (without confusion, also labeled ν) and $\bar{u} \in H^2$, such that

$$u_\nu \rightharpoonup \bar{u} \text{ weakly in } H^2. \tag{62}$$

It remains to establish that $\bar{u} \in \mathcal{A}$ and the weak lower-semi-continuity of $\mathcal{F}$ in H^2, which together would imply

$$m = \liminf F(u_\nu) \ge F(\bar{u}), \tag{63}$$

and establish $\bar{u}$ as a minimizer. Both of these results are a consequence of the following Lemma, which shows that the Lagrangian L is L^1 continuous in the weak H^2 topology, and that its variational derivative $\dfrac{\delta\mathcal{E}}{\delta u}$ is L^2-weakly continuous in the weak H^2 topology.

Lemma 3. *Let the Lagrangian L be given by (16), subject to the conditions (17-21). If $u_\nu \rightharpoonup \bar{u}$ in H^2 weakly then the associated Lagrangian converges,*

$$L(Du_\nu, u_\nu, \cdot) \to L(D\bar{u}, \bar{u}, \cdot), \tag{64}$$

in L^1 and the variational derivative of $\mathcal{E}$ converges

$$\frac{\delta\mathcal{E}}{\delta u}(Du_\nu, u_\nu, \cdot) \rightharpoonup \frac{\delta\mathcal{E}}{\delta u}(D\bar{u}, \bar{u}, \cdot), \tag{65}$$

weakly in L^2.

Proof. Recalling the bound (42) we apply the mean value theorm to the variation in A to find

$$\begin{aligned} |A(Du_\nu) - A(D\bar{u})| &= |D_{\mathbf{p}}A(\tilde{\mathbf{p}}) \cdot (Du_\nu - D\bar{u})| && (66)\\ &\le C\,(1 + |\tilde{\mathbf{p}}|)\,|Du_\nu - D\bar{u}| && (67)\\ &\le C\,(1 + |Du_\nu| + |D\bar{u}|)\,|Du_\nu - D\bar{u}|. && (68) \end{aligned}$$

However $H^2 \subset\subset H^1$, so $u_\nu \to \bar{u}$ strongly in H^1 and $L^{\frac{2n}{n-2}}$. From the estimate above we find

$$\int_\Omega |A(Du_\nu) - A(D\bar{u})| \,\mathrm{d}x \le C\|Du_\nu - D\bar{u}\|_{L^2}\left(1 + \|Du_\nu\|_{L^2}\right), \tag{69}$$

which converges to zero since the sequence $\|Du_\nu\|_{L^2}$ is bounded. From the mean value theorem and (19) we have the estimate

$$|B(u_\nu, x) - B(\bar{u}, x)| \le \mu\,(1 + |u_\nu|^{p_1} + |\bar{u}|^{p_1})\,|u_\nu - \bar{u}|, \tag{70}$$

for $p_1 \in \left(0, \frac{n}{n-2}\right)$. However $\|u_\nu\|_{H^2}$ is uniformly bounded and hence so is $\|u_\nu\|_{L^\infty}$ for $n < 4$ and $\|u_\nu\|_{L^{\frac{2n}{n-4}}}$, for $n \ge 4$. In this later case, integrating (70) over Ω and using Hölder's inequality with the conjugate exponents $q_1 = \frac{2n}{n+2}$ and $q_2 = \frac{2n}{n-2}$ we have

$$\|B(u_\nu) - B(\bar{u})\|_{L^1} \le c\,(1 + \|u_\nu\|^{p_1}_{L^{p_1 q_1}} + \|\bar{u}\|^{p_1}_{L^{p_1 q_1}})\,\|u_\nu - \bar{u}\|_{L^{\frac{2n}{n-2}}}, \tag{71}$$

which converges to zero since $p_1 q_1 \le \dfrac{2n}{n-4}$ and hence $\|u_\nu\|_{L^{p_1 q_1}}$ is uniformly bounded. In the case $n < 4$ the estimates are easier, and in all cases we establish that $B(u_\nu)$ converges to $B(\bar{u})$ in L^1, which demonstrates the convergence of L.

From the formula (29) for the functional derivative of $\mathcal{E}$, it is sufficient to establish that $B_z(u_\nu, \cdot) \to B_z(\bar{u}, \cdot)$ in L^2 and

$$\nabla \cdot D_{\mathbf{p}} A(Du_\nu) \rightharpoonup \nabla \cdot D_{\mathbf{p}} A(D\bar{u}), \tag{72}$$

in L^2. Following the arguments which lead to (71), and using (20), we find

$$\|B_z(u_\nu) - B_z(\bar{u})\|_{L^2} \le c\,(1 + \|u_\nu\|^{p_2}_{L^{np_2}} + \|\bar{u}\|^{p_2}_{L^{np_2}})\,\|u_\nu - \bar{u}\|_{L^{\frac{2n}{n-2}}}, \tag{73}$$

where $p_2 \in \left(0, \frac{2}{n-4}\right]$ so that $np_2 \le \dfrac{2n}{n-4}$ and quantities within the parenthesis on the right-hand side are uniformly bounded, while the last term tends to zero. To address the weak convergence of the terms involving A, we observe that $u_\nu \to \bar{u}$ in H^1 and hence $Du_\nu \to D\bar{u}$ pointwise almost everywhere. In addition $D^2_{\mathbf{p}} A(\mathbf{p}) < \mu$, so that the sequence $\|D^2_{\mathbf{p}} A(Du_\nu)\|_{L^\infty}$ is uniformly bounded, and the Lesbegue dominated convergence theorem implies that

$$D^2_{\mathbf{p}} A(Du_\nu) \to D^2_{\mathbf{p}} A(D\bar{u}), \tag{74}$$

strongly in L^2. Because $D^2 u_\nu \rightharpoonup D^2 \bar{u}$ weakly in L^2, it follows that

$$\begin{aligned} \nabla \cdot D_{\mathbf{p}} A(Du_\nu) &= D^2_{\mathbf{p}} A(Du_\nu) : D^2_x u_\nu \rightharpoonup D^2_{\mathbf{p}}(Du_x \bar{u}) : D^2_x \bar{u}, & (75)\\ &= \nabla \cdot D_{\mathbf{p}} A(\bar{u}), & (76) \end{aligned}$$

weakly in L^2, which establishes (65). □

□

Proof of Theorem 1: We first establish that $\bar{u} \in \mathcal{A}$. We focus on the case $\mathcal{A} = \mathcal{A}_N$, for which the boundary condition is nonlinear and higher order. From integration by parts, for all $w, v \in H^2(\Omega)$ we have

$$\int_\Omega \nabla \cdot D_{\mathbf{p}}(Dw) v \,\mathrm{dx} = -\int_\Omega D_{\mathbf{p}}(Dw) \cdot Dv \,\mathrm{dx} + \int_{\partial\Omega} v D_{\mathbf{p}}(Dw) \cdot \vec{n} \,\mathrm{dS}. \tag{77}$$

If we take $w = u_\nu$ then boundary integral is zero, while from Lemma 3 we see that $\nabla \cdot D_{\mathbf{p}}(Du_\nu) \rightharpoonup \nabla \cdot D_{\mathbf{p}} A(D\bar{u})$ in L^2 and $u_\nu \to \bar{u}$ in H^1 so that the volume integrals converge, as $\nu \to \infty$, establishing

$$\int_\Omega \nabla \cdot D_{\mathbf{p}}(D\bar{u}) v \,\mathrm{dx} = -\int_\Omega D_{\mathbf{p}}(D\bar{u}) \cdot Dv \,\mathrm{dx}. \tag{78}$$

Comparing this result with $w = \bar{u}$ in (77) yields

$$\int_{\partial\Omega} v D_{\mathbf{p}}(D\bar{u}) \cdot \vec{n}\, \mathrm{dS} = 0, \tag{79}$$

for all $v \in H^2(\Omega)$ and hence $D_{\mathbf{p}}(D\bar{u}) \cdot \vec{n} = 0$ and $\bar{u} \in \mathcal{A}_N$.

Since weak convergence is lower-semi continuous, it follows that

$$\liminf \int_\Omega \left| \frac{\delta \mathcal{E}}{\delta u}(Du_\nu, u_\nu, x) \right|^2 \mathrm{d}x \geq \int_\Omega \left| \frac{\delta \mathcal{E}}{\delta u}(D\bar{u}, \bar{u}, x) \right|^2 \mathrm{d}x. \tag{80}$$

Moreover, η lies in L^∞ and the Lagrangians $L(Du_\nu, u_\nu, \cdot)$ converge in L^1, so that

$$\int_\Omega \eta L(Du_\nu, u_\nu, x)\mathrm{dx} \to \int_\Omega \eta L(D\bar{u}, \bar{u}, x)\mathrm{dx}. \tag{81}$$

Taken together these two convergence results establish the weak lower-semi-continuity of $\mathcal{F}$,

$$m = \liminf F(u_\nu) \geq F(\bar{u}). \tag{82}$$

The functionalized energy, $\mathcal{F}$, attains it global minima at $\bar{u}$, completing the proof of Theorem 1. □

5. **Critical Points of the Functionalized Lagrangian.** We examine the variational structure of the functionalized energy, and the relation between the critical points of $\mathcal{E}$ and $\mathcal{F}$.

5.1. **Variational Structure of the Functionalized Energy.** To examine the first variation of the functionalized energy, $\mathcal{F}$, we consider the restricted functional

$$i(\tau) = \mathcal{F}(\phi(\tau)), \tag{83}$$

where $\phi : (-\tau_0, \tau_0) \mapsto \mathcal{A}$ for some $\tau_0 > 0$ is smooth and satisfies $\phi(0) = u \in \mathcal{A}$ and $\phi'(0) = v \in \mathcal{A}'(u)$. We calculate the variation of $\mathcal{F}$ along ϕ,

$$i'(0) = \left(\mathcal{L}_\mathcal{E} v, \frac{\delta \mathcal{E}}{\delta u} \right)_{L^2} + \int_\Omega \left[\nabla \cdot (\eta D_{\mathbf{p}} A(Du)) - \eta B_z(u,x) \right] v\, \mathrm{dx}, \tag{84}$$

where $\mathcal{L}_\mathcal{E}$, the second variation of $\mathcal{E}$, is given in (31). Distributing the differential term in the volume integral and regrouping we define the weak critical points, $u \in \mathcal{C}^w_\mathcal{F} \subset \mathcal{A}$ of $\mathcal{F}$ to be the solutions of

$$\left((\mathcal{L}_\mathcal{E} - \eta) v, \frac{\delta \mathcal{E}}{\delta u} \right)_{L^2} = -\left(D\eta \cdot D_{\mathbf{p}} A(Du), v \right)_{L^2}, \qquad \forall v \in \mathcal{A}'. \tag{85}$$

In particular in the case that η is constant we have the inclusion $\mathcal{C}_\mathcal{E} \subset \mathcal{C}^w_\mathcal{F}$.

If in addition the critical point u lies in H^4 then integrating by parts in the inner product we find

$$i'(0) = \left(\frac{\delta \mathcal{F}}{\delta u}, v \right)_{L^2} + \int_{\partial\Omega} v D_u \frac{\delta \mathcal{E}}{\delta u} - \frac{\delta \mathcal{E}}{\delta u} D_u v\, \mathrm{dS}, \tag{86}$$

where the variational derivative of $\mathcal{F}$ takes the form

$$\frac{\delta \mathcal{F}}{\delta u} = \left(\mathcal{L}_\mathcal{E} - \eta \right) \frac{\delta \mathcal{E}}{\delta u}(u) + D\eta \cdot D_{\mathbf{p}} A(Du). \tag{87}$$

This motivates the definition of the strong critical points of $\mathcal{F}$,

$$\mathcal{C}_{\mathcal{F}} \equiv \left\{ u \in \mathcal{A}^{\mathcal{F}} \,\Big|\, \frac{\delta \mathcal{F}}{\delta u}(u) = 0 \right\}, \tag{88}$$

where $\mathcal{A}^{\mathcal{F}}_{0,N} = \mathcal{A}_{0,N} \cap H^4$, and

$$\mathcal{A}^{\mathcal{F}}_0(u) = \left\{ u \in \mathcal{A}_0 \cap H^4 \Big| \frac{\delta \mathcal{E}}{\delta u} = 0 \quad \text{on } \partial\Omega \right\}, \tag{89}$$

$$\mathcal{A}^{\mathcal{F}}_N(u) = \left\{ u \in \mathcal{A}_N \cap H^4 \Big| D_u \frac{\delta \mathcal{E}}{\delta u} = 0 \quad \text{on } \partial\Omega \right\}. \tag{90}$$

To characterize the critical points we investigate the second derivative of i at $\tau = 0$ which takes the form

$$\begin{aligned} i''(0) = {} & \|\mathcal{L}_{\mathcal{E}} v\|^2_{L^2} - \int_\Omega \eta(Dv D^2_{\mathbf{p}} A(Du) Dv + B_{zz}(u,x)v^2)\mathrm{dx} + \\ & \left(\frac{\delta \mathcal{E}}{\delta u}, \mathcal{L}_{\mathcal{E}} w\right)_{L^2} - \int_\Omega \eta(D_{\mathbf{p}} A(Du) Dw + B_z(u,x)w)\,\mathrm{dx} + \\ & \left(\frac{\delta \mathcal{E}}{\delta u}, -\nabla\cdot(D^3_{\mathbf{p}} A(Du)(Dv,Dv)) + B_{zzz}(u,x)v^2\right)_{L^2}, \end{aligned} \tag{91}$$

where $w = \phi''(0) \in \mathcal{A}''$. For the linear boundary conditions we have $\mathcal{A}'_0 = \mathcal{A}''_0$ and $\mathcal{A}'_{0,N} = \mathcal{A}''_{0,N}$. However for the case $\mathcal{A} = \mathcal{A}_N$ then

$$\mathcal{A}''_N(u,v) \equiv \left\{ w \in H^2 \Big| D_u w = -D^3_{\mathbf{p}} A(Du)(Dv,Dv,\vec{n}) \quad \text{on } \partial\Omega \right\}. \tag{92}$$

Integrating by parts on the terms involving η on the first and second lines of (91) yields

$$\begin{aligned} i''(0) = {} & ((\mathcal{L}_{\mathcal{E}} - \eta)v, \mathcal{L}_{\mathcal{E}} v)_{L^2} + \int_\Omega D\eta \cdot (v D^2_{\mathbf{p}} A(Du) Dv + w D_{\mathbf{p}} A(Du))\mathrm{dx} + \\ & \left(\frac{\delta \mathcal{E}}{\delta u}, (\mathcal{L}_{\mathcal{E}} - \eta) w\right)_{L^2} - \left(\frac{\delta \mathcal{E}}{\delta u}, \nabla\cdot(D^3_{\mathbf{p}} A(Du)(Dv,Dv)) - B_{zzz}(u,x)v^2\right)_{L^2}. \end{aligned} \tag{93}$$

We decompose $w = w_0 + w_v$ where $w_0 \in \mathcal{A}'$ is chosen to minimize $\|w - w_0\|_{H^2}$ and $w_v = w - w_0 \in \mathcal{A}''_N$ is determined by the boundary values of $v \in \mathcal{A}'_N$. In particular, $w_v = 0$ for $\mathcal{A} = \mathcal{A}_0$ or $\mathcal{A}_{0,N}$. Since $u \in \mathcal{C}^w_{\mathcal{F}}$ and $w_0 \in \mathcal{A}'$, the weak characterization of the critical points, (85), shows that the terms involving w_0 drop out, and (93) depends upon w only through w_v.

Indeed if u is a strong critical point of $\mathcal{F}$ then w may be eliminated from the formulation. Integration by parts shows that

$$\left((\mathcal{L}_{\mathcal{E}} - \eta)w, \frac{\delta \mathcal{E}}{\delta u}\right)_{L^2} = \left((\mathcal{L}_{\mathcal{E}} - \eta)\frac{\delta \mathcal{E}}{\delta u}, w\right)_{L^2} + \int_{\partial\Omega} w D_u \frac{\delta \mathcal{E}}{\delta u} - \frac{\delta \mathcal{E}}{\delta u} D_u w \,\mathrm{dS}, \tag{94}$$

however either $w = 0$ or $D_u \frac{\delta \mathcal{E}}{\delta u} = 0$ and the first boundary term is zero. The strong formulation of the critical point equation (87) permits us to rewrite the first term on the right-hand side of (94) so that the equality reads

$$\left((\mathcal{L}_{\mathcal{E}} - \eta)w, \frac{\delta \mathcal{E}}{\delta u}\right)_{L^2} + \int_\Omega w D\eta \cdot D_{\mathbf{p}} A(Du)\,\mathrm{dx} = -\int_{\partial\Omega} \frac{\delta \mathcal{E}}{\delta u} D_u w \,\mathrm{dS}. \tag{95}$$

Depending upon the admissible set $\mathcal{A}$, either $\frac{\delta \mathcal{E}}{\delta u} = 0$ or $w \in \mathcal{A}''_N$ and in this latter case we replace $D_u w$ with the boundary values from (92). This substitution eliminates the w terms from (93),

$$\begin{aligned} i''(0) &= ((\mathcal{L}_\mathcal{E} - \eta)v, \mathcal{L}_\mathcal{E} v)_{L^2} + \int_\Omega D\eta \cdot (v D^2_{\mathbf{p}} A(Du) Dv) \mathrm{dx} - \\ & \left(\frac{\delta \mathcal{E}}{\delta u}, \nabla \cdot (D^3_{\mathbf{p}} A(Du)(Dv, Dv)) - B_{zzz}(u,x) v^2 \right)_{L^2} + \\ & \int_{\partial\Omega} \frac{\delta \mathcal{E}}{\delta u} D^3_{\mathbf{p}} A(Du)(Dv, Dv, \mathbf{n}). \end{aligned} \tag{96}$$

Finally integrating the divergence in the second line of (96) yields the strong form of the second derivative of i, which is also the quadratic part, $Q_\mathcal{F}$ of $\mathcal{F}$, namely

$$\begin{aligned} Q_\mathcal{F}(v) &= ((\mathcal{L}_\mathcal{E} - \eta)v, \mathcal{L}_\mathcal{E} v)_{L^2} + \int_\Omega D\eta \cdot (v D^2_{\mathbf{p}} A(Du) Dv) \mathrm{dx} + \\ & \int_\Omega \left[D^3_{\mathbf{p}} A(Du) \left(Dv, Dv, D \frac{\delta \mathcal{E}}{\delta u} \right) + B_{zzz}(u,x) v^2 \frac{\delta \mathcal{E}}{\delta u} \right] \mathrm{dx}. \end{aligned} \tag{97}$$

5.2. **Saddle Points of $\mathcal{F}$.** For η constant, we see from the weak formulation of the variational derivative of $\mathcal{F}$, (85), that the critical points $\mathcal{C}_\mathcal{E}$ of $\mathcal{E}$, are inherited as weak critical point of $\mathcal{F}$. A natural question is whether the global minima of $\mathcal{F}$ is distinct from the critical points of $\mathcal{E}$, and more generally if these inherited critical points can be characterized. This we do in the following theorem.

Theorem 2. *In addition to the assumptions of Theorem 1, let the local balance, η, be constant, and let the admissible set $\mathcal{A}$ be either $\mathcal{A}_0$ or $\mathcal{A}_N$ where in the latter case the differential part of the Lagrangian, A, is restricted to be quadratic in $\mathbf{p}$, that is $D^3_{\mathbf{p}} A = 0$. Then for $\eta = 0$ the set $\mathcal{C}_\mathcal{E}$ is comprised of global minima of $\mathcal{F}$, however there exists a constant $0 < \underline{\eta}$ such that for all $\eta \geq \underline{\eta}$ the set $\mathcal{C}_\mathcal{E}$ is comprised of saddle points of $\mathcal{F}$, and the global minimizer of $\mathcal{F}$ is distinct from $\mathcal{C}_\mathcal{E}$.*

The first step in the proof is to develop uniform estimates on the L^∞ norm of the elements of $\mathcal{C}_\mathcal{E}$.

Proposition 2. *Under the assumptions of Theorem 1, there exists a constant $M > 0$ such that*

$$\|u\|_{H^2} + \|u\|_{L^\infty} \leq M, \tag{98}$$

for all $u \in \mathcal{C}_\mathcal{E}$.

Proof: Any $u \in \mathcal{C}_\mathcal{E}$ satisfies the critical point equation

$$\frac{\delta \mathcal{E}}{\delta u}(u) = -\nabla \cdot D_{\mathbf{p}} A(Du) + B_z(u,x) = 0. \tag{99}$$

Taking the L^2 inner product with u and integrating by parts give the equality

$$\int_\Omega D_p A(Du) \cdot Du + B_z(u,x) u \, dx = 0. \tag{100}$$

However the convexity bound (50) on A and the similar result

$$B_z(z,x) z \geq \beta z^2 - C, \tag{101}$$

which follows from (21) for some $C > 0$, shows that

$$\|u\|_{H^1} \leq M, \tag{102}$$

for some $M > 0$, establishing a uniform H^1 bound on $\mathcal{C}_{\mathcal{E}}$. From (58) we see that $B_z(u,x)$ is uniformly bounded in H^1 and hence from the H^2 regularity applied to the $\mathcal{E}$ critial point equation (99), we obtain a uniform H^2 bound on $\mathcal{C}_{\mathcal{E}}$. We can bootstrap these estimates by taking the inner product of (99) with $|u|^{2q}u$ for $q \geq 1$, After an integration by parts we obtain

$$\int_\Omega D_pA(Du) \cdot D\left(|u|^{2q}u\right) + B_z(u,x)|u|^{2q}u \,\mathrm{d}x = 0. \tag{103}$$

Using the differential identity

$$D(|u|^r u) = (r+1)|u|^r Du, \tag{104}$$

valid for $r \geq 1$, we can rewrite this equality as

$$\int_\Omega (2q+1)|u|^{2q} D_pA(Du) \cdot Du + B_z(u,x)|u|^{2q}u \,\mathrm{d}x = 0. \tag{105}$$

while from the convexity bounds we obtain

$$\int_\Omega \frac{(2q+1)\alpha}{2}|Du|^2|u|^{2q} + \beta|u|^{2(q+1)} - c|u|^{2q} \,\mathrm{d}x \leq 0, \tag{106}$$

for some $c > 0$. However using (104) we can re-write the first term as a pure derivative and use Young's inequality to absorb the last term into the power and a constant, obtaining

$$\int_\Omega \frac{(2q+1)\alpha}{2(q+1)^2}\left|D\left(|u|^q u\right)\right|^2 + \frac{\beta}{2}|u|^{2(q+1)} \,\mathrm{d}x \leq c^{q+1}|\Omega|, \tag{107}$$

for some $c > 0$ independent of $q \geq 1$. In particular dropping the first term on the left-hand side and taking the $2(q+1)$ root of the resulting inequality, we see that $\|u\|_{L^{2(q+1)}}$ is uniformly bounded, for all $u \in \mathcal{C}_{\mathcal{E}}$, independent of $q \geq 1$, and consequently $\|u\|_{L^\infty}$ is uniformly bounded. In particular $\|B_z(u,\cdot)\|_{L^2}$ is also uniformly bounded for $u \in \mathcal{C}_{\mathcal{E}}$, and hence from (99) and the H^2 regularity result of Proposition 1, the uniform H^2 bound on $\mathcal{C}_{\mathcal{E}}$ follows. □

Proof of Theorem 2: The first statement is obvious since for $\eta = 0$, $\mathcal{F} \geq 0$ and the minimum value $\mathcal{F} = 0$ is attained for all $u \in \mathcal{C}_{\mathcal{E}}$. We construct $\underline{\eta} > 0$ such that for all $\eta \geq \underline{\eta}$, the critical points $\mathcal{C}_{\mathcal{E}}$ are saddles of $\mathcal{F}$. For each $u \in \mathcal{C}_{\mathcal{E}}$ and $v \in \mathcal{A}'(u)$ we consider i as given by (83) and observe that η is constant, $\frac{\delta\mathcal{E}}{\delta u} = 0$, and $\mathcal{A}'' \subset \mathcal{A}'$ so that $w_v = 0$ in (93), which reduces to

$$i''(0) = \left((\mathcal{L}_{\mathcal{E}} - \eta)v, \mathcal{L}_{\mathcal{E}}v\right). \tag{108}$$

In particular, if $\mathcal{L}_{\mathcal{E}}$ has an eigenpair (v,λ) with $v \in \mathcal{A}'$ then

$$i''(0) = (\lambda^2 - \eta\lambda)\|v\|_{L^2}^2. \tag{109}$$

Since $\mathcal{L}_{\mathcal{E}}$ is self-adjoint on $\mathcal{A}'$, its spectrum is real and it suffices to construct $\underline{\eta} > 0$ such that $(0,\underline{\eta}) \cap \sigma(\mathcal{L}_{\mathcal{E}}) \neq \emptyset$ for all $u \in \mathcal{C}_{\mathcal{E}}$. From the Raleigh-Ritz characterization, the N'th eigenvalue of $\mathcal{L}_\mathcal{E}$ is given by

$$\lambda_N = \sup_{\dim V_N = N} \inf_{\substack{v \in V_N^\perp \\ \|v\|=1}} (\mathcal{L}_\mathcal{E} v, v)_{L^2}. \tag{110}$$

Define $\overline{B}$ by

$$\overline{B} \equiv \sup_{u \in \mathcal{C}_\mathcal{E}} \|B_{zz}(u,x)\|_{L^\infty}, \tag{111}$$

which is finite since the critical points of $\mathcal{E}$ are uniformly bounded in L^∞. For the case $\mathcal{A} = \mathcal{A}_0$ we introduce the operator

$$\overline{\mathcal{L}} = -\mu\Delta + \overline{B}, \tag{112}$$

from the boundedness of $D_p^2 A$, (17), we have

$$(\mathcal{L}_\mathcal{E} v, v)_{L^2} \leq \mu\|Dv\|_{L^2}^2 + \overline{B}\|v\|_{L^2}^2, \tag{113}$$

$$= \left(\overline{\mathcal{L}} v, v\right)_{L^2}. \tag{114}$$

Denoting N'th eigenvalue of $\overline{\mathcal{L}}$ by $\overline{\lambda}_N$, by comparing the two Raleigh-Ritz characterizations we see that $\lambda_N \leq \overline{\lambda}_N$. Similarly, denoting by $\underline{B}$ the uniform lower bound on $B(u,x)$ for $u \in \mathcal{C}_\mathcal{E}$, we introduce the operator $\underline{\mathcal{L}} = -\alpha\Delta + \underline{B}$, on Ω, and observe from the convexity of A, (18), that

$$(\mathcal{L}_\mathcal{E} v, v)_{L^2} \geq \alpha\|Dv\|_{L^2}^2 + \underline{B}\|v\|_{L^2}^2 = (\underline{\mathcal{L}} v, v)_{L^2}. \tag{115}$$

We deduce that $\underline{\lambda}_N \leq \lambda_N$, where $\underline{\lambda}_N$ is the N'th eigenvalue of $\underline{\mathcal{L}}$. Since $\underline{\lambda}_N$ and $\overline{\lambda}_N$ converge to ∞ as $N \to \infty$, we may pick N sufficiently large that $\underline{\lambda}_N > 0$ and then choose $\underline{\eta} > \overline{\lambda}_N$. It follows that for all $u \in \mathcal{C}_\mathcal{E}$, $\lambda_N \in [\underline{\lambda}_N, \overline{\lambda}_N] \subset (0, \underline{\eta})$. Hence $i''(0) < 0$ and since $\mathcal{L}_\mathcal{E}$ has arbitrarily large eigenvalues it follows that $i''(0) > 0$ if v is the associated eigenfunction and u is therefore a saddle of $\mathcal{F}$. In the case $\mathcal{A} = \mathcal{A}_N$ we define the operators

$$\overline{\mathcal{L}} v = -\nabla \cdot (D_\mathbf{p}^2 A(0) Dv) + \overline{B} v, \tag{116}$$

$$\underline{\mathcal{L}} v = -\nabla \cdot (D_\mathbf{p}^2 A(0) Dv) + \underline{B} v, \tag{117}$$

which are self-adjoint on $\mathcal{A}_N'$ and bound $\mathcal{L}_\mathcal{E}$ from above and below. The remainder of the proof is identical. □

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REFERENCES

[1] J.W. Cahn and J. E. Hilliard, Free energy of a nonuniform system. I. Interfacial energy, *J. Chem. Phys.* **28** 258-267 (1958).

[2] P. Canham, Minimum energy of bending as a possible explanation of biconcave shape of human red blood cell, J. Theor. Biol. **26** (1970) 61-81

[3] E. Crossland, M. Kamperman, M. Nedelcu, C. Ducati, U. Wiesner, D. Smilgies, G. Toombes, M. Hillmyer, S. Ludwigs, U. Steiner, H. Snaith, A Bicontinuous double gyroid hybrid solar cell, *Nano Letters* **9** (2009) 2807-2812.

[4] Qiang Du, Chun Liu, Rolf Ryham and Xiaoqiang Wang, A phase field formulation of the Willmore problem, *Nonlinearity* **18** 12491267 (2005).

[5] L.C. Evans:*Partial Differential Equations.* American Mathematical Society, Providence, R.I., (2000)

[6] N. Gavish, G. Hayrapetyan, K. Promislow, L. Yang, Curvature driven flow of bi-layer interfaces, *Physica D* submitted 2010.

[7] G. Gompper and M.Schick, Correlation between structural and interfacial properties of amphillic systems, *Phys. Rev. Lett.* **65** (1990) 1116-1119.

[8] W. Helfrich, Elastic properties of lipid bilayers - theory and possible experiments, *Zeitshcrift fur naturforschung C* **28** (1973) 693-703.

[9] William Hsu and Timothy Gierke, Ion transport and clustering in Nafion perfluorinated membranes, *J. Membrane Science* **13** (1983) 307-326.

[10] Kun-Mu Lee, Chih-Yu Hsu, Wei-Hao Chiu, Meng-Chin Tsui, Yung-Liang Tung, Song-Yeu Tsai, Kuo-Chuan Ho, Dye-sensitized solar cells with mirco-porous TiO_2 electrode and gel polymer electrolytes prepared by *in situ* cross-link reaction, *Solar Energy Materials & Solar cells* **93** 2003-2007(2009).

[11] Roger Moser, A higher order asymptotic problem related to phase transition, *SIAM Journal Math. Anal.* **37** 712736 (2005).

[12] L. Modica, The gradient theory of phase transitions and the minimal interface criterion, *Arch. Rational. Mech. Anal.* **98** 123-142.

[13] J. Peet, A. Heeger, and G. Bazan, "Plastic" Solar cells: Self-assembly of bulk hetrojunction nanomaterials by spontaneous phase separation, *Accounts of Chemical Research* **42** (2009) 1700-1708.

[14] K. Promislow and B. Wetton, PEM fuel cells: a mathematical overview, *SIAM Math. Analysis*, **70** 369-409 (2009).

[15] Matthias Röger and Reiner Schätzle, On a modified conjecture of De Giorgi, *Math. Z.* **254** (2006) 675-714.

[16] L. Rubatat, G. Gebel, O. Diat, Fibriallar structure of Nafion: Matching Fourier and real space studies of corresponding films and solutions, *Macromolecules* **2004**, 7772-7783.

[17] U. Schwarz and G. Gompper, Bicontinuous surfaces in self-assembled amphiphilic systems, pp 107-151, in *Morphology of Condensed Matter: Physics and Geometry of spatially complex systems*, K.R. Mecke and D. Stoyan (eds), Springer Lecture Notes in Physics, **600** (2002)

[18] P. Sternberg, The effect of a singular perturbation on nonconvex variational problems, *Arch. Rational Mech. Anal.* **101** (1988) 209-260.

[19] M. Struwe: *Variational Methods*. Springer-Verlag, Berlin, (1990).

E-mail address: kpromisl@math.msu.edu

E-mail address: hzhang@nicoholdings.com