

Lavrentiev Phenomenon in Microstructure Theory

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August 20, 1996

Abstract

A variational problem arising as a model in martensitic phase transformation including surface energy is studied. It explains the complex, multi-dimensional pattern of twin branching which is often observed in a martensitic phase near the austenite interface.

We prove that a Lavrentiev phenomenon can occur if the domain is a rectangle. We show that this phenomenon disappears under arbitrarily small shears of the domain. We also prove that other perturbations of the problem lead to an extinction of the Lavrentiev phenomenon.

1991 Mathematics Subject Classification: 49K40, 73S10.

Key words and phrases: Singular perturbation, Lavrentiev phenomenon, martensitic phase transformation.

1 Introduction

Phase transitions in solids often involve structure on a microscale. In martensitic phase transformation for example this is quite well understood. A common approach is by elastic energy minimization (see Ball and James [2, 3] for a geometrically nonlinear theory or Khachaturyan, Shatalov and Roitburd [10, 11, 19] for a geometrically linear theory). The stored energies are typically nonconvex (and not quasiconvex) and so the variational integrals involved are typically not lower semicontinuous. Therefore the minimum is not attained. However, there exist minimizing sequences, which involve finer and finer oscillations describing the microstructure in the solid.

Considering elastic energy alone one is capable of predicting many properties of the microstructure, for example the layering directions in twinned patterns or the lattice orientation of the different phases. However, other features such as lengthscales are still arbitrary. If also interfacial energy is incorporated into the model these can be determined, too. We consider two ways to represent interfacial energy. The first is by adding a singular perturbation involving higher order gradients, the second is by essentially adding the surface area of the interfaces.

In this paper we revisit a model which was introduced and analyzed by Kohn and Müller [12, 13, 14]. The model is as follows. Minimize

$$E^\varepsilon(u) = \int_{R_L} u_x^2 + (u_y^2 - 1)^2 + \varepsilon^2 u_{yy}^2 \, dx \, dy \quad (1.1)$$

subject to

$$u = 0 \text{ for } x = 0$$

where

$$R_L = (0, L) \times (0, 1).$$

The double-well potential $u_x^2 + (u_y^2 - 1)^2$ represents elastic energy of the

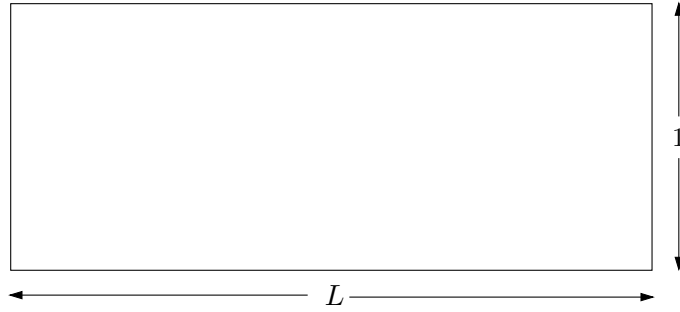


Figure 1: A rectangular domain ($\Omega = R_L$)

martensite, the preferred values $\nabla u = (0, \pm 1)$ being the stress-free states of two different variants of martensite. The higher-order term $\varepsilon^2 u_{yy}^2$ describes interfacial energy by singular perturbation. The boundary $x = 0$ represents the austenite–twinned-martensite interface. The boundary condition $u = 0$ for $x = 0$ refers to elastic compatibility with the austenite phase in the extreme case of complete rigidity of the austenite.

The variational problem (1.1) is closely related to the following one. Minimize

$$I^\varepsilon(u) = \int_{R_L} u_x^2 + \varepsilon |u_{yy}| \, dx \, dy \quad (1.2)$$

subject to

$$|u_y| = 1 \text{ a.e.}, \quad u = 0 \text{ for } x = 0.$$

(The precise class of admissible functions will be introduced in section 2.) Note that in both formulations (1.1) and (1.2) of the variational problem the surface terms consider only changes of u in y -direction. To simplify the presentation other components are neglected since the transition zones or interfaces, respectively, between the two variants of martensite are expected

to be essentially horizontal. Our results, in particular Theorem 2.3, remain valid also without this approximation.

There is no rigorous proof of a relationship between the two formulations of the problem. For a heuristic connection note that, following Modica [18],

$$\begin{aligned} \int_{x=x_0} (u_y^2 - 1)^2 + \varepsilon^2 u_{yy}^2 dy &\geq \int_{x=x_0} 2\varepsilon |u_y^2 - 1| |u_{yy}| dy \\ &= \int_{x=x_0} 2\varepsilon |H(u_y)_y| dy \end{aligned}$$

where $H(t)$ is a primitive of $|t^2 - 1|$. The inequality becomes sharp if $\varepsilon u_{yy} = \pm(u_y^2 - 1)$, i.e. if in the layer where u_y changes between ± 1 one has got the appropriate profile. Note that the unknowns of I^ε are the (sharp) interfaces where u_y changes its value between ± 1 , and $1/2 \int_0^1 |u_{yy}| dy$ counts the number of these changes along the segment $x = \text{const}$, $0 \leq y \leq 1$. We will present a striking difference between the two formulations of the problem, namely that a Lavrentiev phenomenon holds for the “sharp” formulation (1.2) but not for the “diffusional” one (1.1).

It was shown in [12, 13, 14] that for energy minimization of elastic and interfacial energy it is not enough to consider only a one-dimensional twinned pattern. On the contrary, in this situation it is necessary to study complex, two-dimensional patterns which are asymptotically self-similar. A rigorous analysis is performed in the context of formulation (1.2) of the variational problem. See also Schreiber [20] who extended many of the results to the situation of (1.1).

In this paper we show that for the variational problem (1.2) a “*Lavrentiev phenomenon*” occurs. Our main result is as follows. In the class $W^{1,\infty}(R_L)$ there is not even a function possessing finite energy in contrary to the class $H^1(R_L)$.

On the other hand, this Lavrentiev phenomenon does not occur if Ω is a

parallelogram. We prove this explicitly giving an example of a function in $W^{1,\infty}(\Omega)$ having finite energy.

Note that a rectangle is mapped onto a parallelogram by an arbitrarily small shear. Thus the behavior observed here depends on changes of the domain in a highly singular way. To our knowledge this example is the first where such a highly singular behavior of the Lavrentiev phenomenon on changes of the domain has been observed.

We show that this Lavrentiev phenomenon also vanishes if we consider the “diffusional” variational problem (1.1) instead of the “sharp” one (1.2). Furthermore, we prove that if we omit the surface area term in (1.2) and study the energy functional

$$I^\varepsilon(u) = \int_{R_L} u_x^2 dx dy$$

subject to

$$|u_y| = 1 \text{ a.e.}, \quad u = 0 \text{ for } x = 0$$

the Lavrentiev phenomenon also disappears. This shows that the introduction of surface energy into the model not only captures new physical features but also changes the problem in a fundamental way thus highlighting the importance of considering surface energy effects.

A refinement of our results would be question: Is the minimal value the same for functions chosen in H^1 or in $W^{1,\infty}$? Our results clearly show that this not the case for a rectangular domain and the “sharp” formulation since the first is finite, the latter is infinite. We expect that in case the domain is a parallelogram and/or for the “diffusional” formulation the minimal values are the same. But to our knowledge these are open questions.

In a general context the term Lavrentiev phenomenon is used to describe that the value of the minimum of a variational problem increases strictly if

the admissibility class $W^{1,p}(\Omega)$ is replaced by $W^{1,q}(\Omega)$ where Ω is a bounded domain and $1 \leq p < q$. Such effects were first observed by Lavrentiev [15]. There were refinements due to Mania [17] and Ball and Mizel [4]. See also Cesari [5] and Dacorogna [6]. In these works examples were presented where the energy of the absolute minimizer is different for the admissibility classes $W^{1,q}(\Omega)$ and $W^{1,p}(\Omega)$ for some or all p with $1 \leq p < q$. All of the treatments quoted above assume $q = \infty$ except for the work of Ball and Mizel where an example was presented with $q = 3$. All these studies consider one-dimensional problems. Connections between the Lavrentiev phenomenon in higher dimensions and cavitation were studied by Ball [1]. Numerical computations of the Lavrentiev phenomenon by truncation methods were recently performed by Li [16].

The Lavrentiev phenomenon is of great physical importance. Very often in the materials sciences it is important to know the maximum value of the gradients. If they are too big the approximation of the continuum model to the lattice model might no longer be valid. Furthermore, big gradients even on a very small set very often lead to fracture of the body or other effects. So in this case the model would have to be extended to account for these.

The structure of the paper is as follows. In section 2 we show that for the “sharp” variational problem (1.2) on a rectangular domain there is no Lipschitz function with finite energy and that this statement is not true if the domain is a parallelogram. In section 3 we consider two other changes to the variational problem, namely studying the “diffusional formulation” and omitting surface energy. We show that then there exist Lipschitz functions with finite energy.

We use C to denote generic constants which can vary from line to line.

Acknowledgements. It is a great pleasure to thank Professors J.M.

Ball, R.V. Kohn and S. Müller for many interesting discussions on microstructure and energy minimization. I thank Mrs. Tanya Smekal for the careful preparation of the figures. The hospitality of Courant Institute and the Institute for Advanced Study is gratefully acknowledged. This work is supported by an Individual Fellowship of the European Union (HCM Programme, contract no ERBCHBICT930744) which enabled the author to spend almost two years at Heriot-Watt University, Edinburgh.

2 The “sharp” formulation of the variational problem

In this section we study the minimization of the model energy

$$I^\varepsilon(u) = \int_{R_L} u_x^2 + \varepsilon |u_{yy}| \, dx \, dy$$

amongst all functions in the admissibility class

$$\mathcal{A}_0 = \{u \in H^1(R_L) : |u_y| = 1 \text{ a.e., } u_{yy} \text{ is a Radon measure on } R_L$$

$$\text{with finite mass, } u = 0 \text{ for } x = 0\}$$

where

$$R_L = (0, L) \times (0, 1).$$

To get an intuition for the condition that u_{yy} is a Radon measure the reader may think that u_y is ± 1 , respectively, on subsets of R_L which are separated by smooth curves. Then for each Borel set $A \subset R_L$ its distributional derivative satisfies

$$\int_A |u_{yy}|(x, y) \, dx \, dy = 2 \times (\text{length of the interfaces lying in } A).$$

This is the prototype of the Radon measure in our variational problem.

The theoretical reason for choosing Radon measures is that they have good compactness properties and guarantee existence of minimizers. For more background information on Radon measures see for example the monography [7].

Kohn and Müller proved in [13] that this problem has a minimizer using the direct method in the calculus of variations. They also showed the following result which plays the role of the Euler-Lagrange equation.

Lemma 2.1. (EQUIPARTITION OF ENERGY) *Let u be a minimizer of I^ε on \mathcal{A}_0 . Then there exists a constant λ (depending on ε , L , and u) such that*

$$\int_0^1 \varepsilon |u_{yy}|(x, y) dy - \int_0^1 u_x^2(x, y) dy = \lambda \quad (2.1)$$

for a.e. $x \in (0, L)$.

Furthermore, they derived the following scaling law:

Theorem 2.2. *There are constants $c, C > 0$ such that for ε sufficiently small*

$$c\varepsilon^{2/3}L^{1/3} \leq \min I^\varepsilon \leq C\varepsilon^{2/3}L^{1/3}. \quad (2.2)$$

We show that if we restrict the admissibility class to the set of Lipschitz functions

$$\begin{aligned} \mathcal{B}_0 &= \mathcal{A}_0 \cap W^{1,\infty}(R_L) \\ &= \{u \in W^{1,\infty}(R_L) : |u_y| = 1 \text{ a.e., } u_{yy} \text{ is a Radon measure on } R_L \\ &\quad \text{with finite mass, } u = 0 \text{ for } x = 0\} \end{aligned}$$

this statement is no longer true. In fact, we prove the following

Theorem 2.3. *If $\Omega = R_L$ then for all functions $u \in \mathcal{B}_0$ $I^\varepsilon(u) = \infty$.*

Remark 2.4. *It is easy to see that for all $p \in [1, \infty)$ the class*

$$\{u \in W^{1,p}(R_L) : |u_y| = 1 \text{ a.e.}, u_{yy} \text{ is a Radon measure on } R_L$$

$$\text{with finite mass, } u = 0 \text{ for } x = 0\}$$

*contains a function u such that $I^\varepsilon(u) < \infty$. An example for this is obtained by modifying **Example 3.1** below such that*

$$\begin{aligned} \theta &\in \left(\frac{1}{4}, \frac{1}{2}\right) && \text{if } 1 \leq p \leq 2, \\ \theta &\in \left(2^{p/(1-p)}, \frac{1}{2}\right) && \text{if } 2 < p < \infty. \end{aligned}$$

Note that

$$\begin{aligned} \int_{R_L} u_x^p dy dx &= \sum_{i=0}^{\infty} \int_{x_1}^L \int_0^{2^i} (2\theta)^{-pi} u_x^p 2^{-i} \theta^i dy dx \\ &= \sum_{i=0}^{\infty} 2^{-pi} \theta^{(1-p)i} \int_{x_1}^L \int_0^1 u_x^p dy dx \end{aligned}$$

and the series is convergent if and only if

$$\theta > 2^{p/(1-p)}.$$

Furthermore, note that

$$\begin{aligned} \int_{R_L} \varepsilon |u_{yy}| dy dx &= \varepsilon \sum_{i=0}^{\infty} \int_{x_1}^L \int_0^{2^i} 2^i |u_{yy}| 2^{-i} \theta^i dy dx \\ &= \varepsilon \sum_{i=0}^{\infty} (2\theta)^i \int_{x_1}^L \int_0^1 |u_{yy}| dy dx \end{aligned}$$

and the series is convergent if and only if

$$\theta < \frac{1}{2}.$$

Proof of Theorem 2.3. Assume that there is a constant $K > 0$ such that

$$|\nabla u| \leq K \quad \text{for a.e. } x \in R_L.$$

Then we have by the Cauchy-Schwarz inequality

$$u^2(l, y) = \left(\int_0^l 1 \cdot u_x(x, y) dx \right)^2 \leq \int_0^l 1^2 dx \cdot \int_0^l u_x^2(x, y) dx.$$

This implies the following Poincaré inequality

$$\int_0^1 u^2(l, y) dy \leq l \int_0^l \int_0^1 |\nabla u(x, y)|^2 dx dy \leq CK^2 l^2. \quad (2.3)$$

for all $l \in (0, L]$.

Next we use a “zig-zag” inequality which was proved by Kohn and Müller [13].

Lemma 2.5. *Let $f \in W^{1,\infty}(0, 1)$. Assume that $|f'| = 1$ a.e. and that f' changes sign N times. Then*

$$\int_0^1 f^2 dx \geq \frac{1}{12}(N + 1)^{-2} = \frac{1}{12} \left(\frac{1}{2} \int_0^1 |f''| dx + 1 \right)^{-2}.$$

Lemma 2.5 implies

$$\frac{1}{12} \left(\frac{1}{2} \int_0^1 |u_{yy}(l, y)| dy + 1 \right)^{-2} \leq \int_0^1 u^2(l, y) dy. \quad (2.4)$$

Combining (2.3) and (2.4) we get

$$\int_0^1 |u_{yy}(l, y)| dy \geq CK^{-1} l^{-1} - 2$$

where C is independent of K and l . After integration we have

$$\int_0^L \int_0^1 \varepsilon |u_{yy}(l, y)| dy dl \geq C \int_0^L l^{-1} dl - 2\varepsilon L = \infty.$$

This implies Theorem 2.3. \square

We now assume that the domain is a parallelogram. To simplify the presentation assume that the parallelogram has interior angles of $\pi/4$ and $3\pi/4$. But note that our method also works for other angles (except for $\pi/2$, of course). Set $\Omega = \{(x, y) : y < x < y + L, y \in (0, 1)\} =: P_L$. We consider

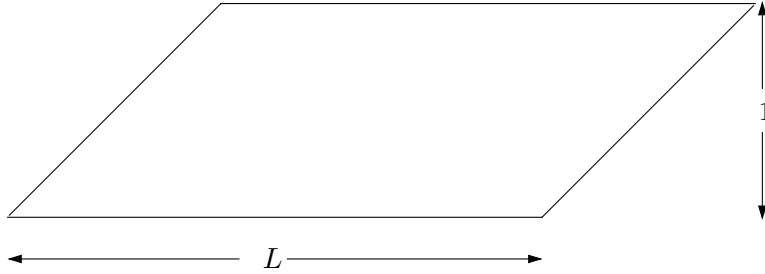


Figure 2: The domain is a parallelogram ($\Omega = P_L$)

the variational problem

$$I^\varepsilon(u) = \int_{P_L} u_x^2 + \varepsilon |u_{yy}| dx dy$$

amongst all functions in the admissibility class

$$\mathcal{A}_0 = \{u \in H^1(R_L) : |u_y| = 1 \text{ a.e., } u_{yy} \text{ is a Radon measure on } R_L$$

with finite mass, $u = 0$ for $x = y, 0 \leq x \leq 1\}$.

Furthermore, define

$$\mathcal{B}_0 = \mathcal{A}_0 \cap W^{1,\infty}(P_L).$$

The existence theorem of Kohn and Müller [13] applies to this case, too. Now Theorem 2.3 is no longer true, but we have the following result.

Theorem 2.6. *If $\Omega = P_L$ then there is a function $u \in \mathcal{B}_0$ such that $I^\varepsilon(u) < \infty$.*

Proof of Theorem 2.6. Choose the function $u(x, y) = x - y$. Then we have $u \in H^1(P_L)$, $u_y = -1$ on P_L , $u_{yy} = 0$ on P_L , and $u = 0$ if $x = y$, $0 \leq x \leq 1$. This implies $u \in \mathcal{B}_0$. Finally, we calculate

$$I^\varepsilon(u) = \int_{P_L} u_x^2 + \varepsilon |u_{yy}| dx dy = \int_{P_L} 1^2 dx dy = |P_L| < \infty. \quad \square$$

3 Other perturbations of the “sharp” formulation of the variational problem

In this section we consider other perturbations of the “sharp” formulation (1.2) of the variational problem and show that for them the Lavrentiev phenomenon observed in Section 2 disappears, i.e. there are Lipschitz functions with finite energy.

We first study the “diffusional” formulation (1.1) of the problem, i.e. we consider the model energy

$$E^\varepsilon(u) = \int_{\Omega} u_x^2 + (u_y^2 - 1)^2 + \varepsilon^2 u_{yy}^2 dx dy.$$

The class of admissible functions for $\Omega = R_L$ is

$$\mathcal{A}_1 = \{u \in H^2(R_L) : u = 0 \text{ for } x = 0\}$$

and for $\Omega = P_L$

$$\mathcal{A}_1 = \{u \in H^2(R_L) : u = 0 \text{ for } x = y, 0 \leq x \leq 1\}.$$

In analogy to section 2 we consider how the behavior of the problem changes by restricting the admissibility class to

$$\mathcal{B}_1 = \mathcal{A}_1 \cap W^{1,\infty}(\Omega).$$

We show that the Lavrentiev phenomenon observed in section 2 does not occur here. To this end for $\Omega = R_L$ consider the function $u = 0$. Note that $0 \in \mathcal{B}_1$ and calculate

$$E^\varepsilon(0) = \int_{R_L} 1^2 dx dy = |R_L| < \infty.$$

For $\Omega = P_L$ the same function and the same calculation as in section 2 provide an example of a function in \mathcal{B}_1 which has finite energy. We conclude that the Lavrentiev phenomenon does not occur for the “diffusional” formulation of the variational problem.

We finally consider the “sharp” formulation of the variational problem without surface energy terms on a rectangle ($\Omega = R_L$). Our goal is to show that Theorem 2.3 does not hold. To this end we have to show that there exists a function $u \in \mathcal{B}_0$ such that

$$I^0(u) < \infty.$$

(Recall that

$$\mathcal{B}_0 = \{u \in W^{1,\infty}(R_L) : |u_y| = 1 \text{ a.e., } u_{yy} \text{ is a Radon measure on } R_L$$

with finite mass, $u = 0$ for $x = 0\}$.)

To give such an example we revisit the microstructure given in the work of Kohn and Müller [12, 13, 14]. It turns out that this will give the desired example. However, we will have to choose the scaling parameter θ in the range $(91/2, 1)$ for which the surface energy would be infinite. But because we ignore surface energy we are allowed to do so.

Example 3.1. The microstructure is constructed as follows. First intro-

duce a function $\nu : [0, 1] \times [0, 1/2] \rightarrow \mathbb{R}$ defined as

$$\nu(x, y) = \begin{cases} y & \text{if } 0 \leq y \leq (x+1)/8, \\ (x+1)/4 - y & \text{if } (x+1)/8 \leq y \leq (x+3)/8, \\ y - 1/2 & \text{if } (x+3)/8 \leq y \leq 1/2. \end{cases}$$

Then ν is extended antiperiodically in y to $[0, 1] \times [0, 1]$ The function ν

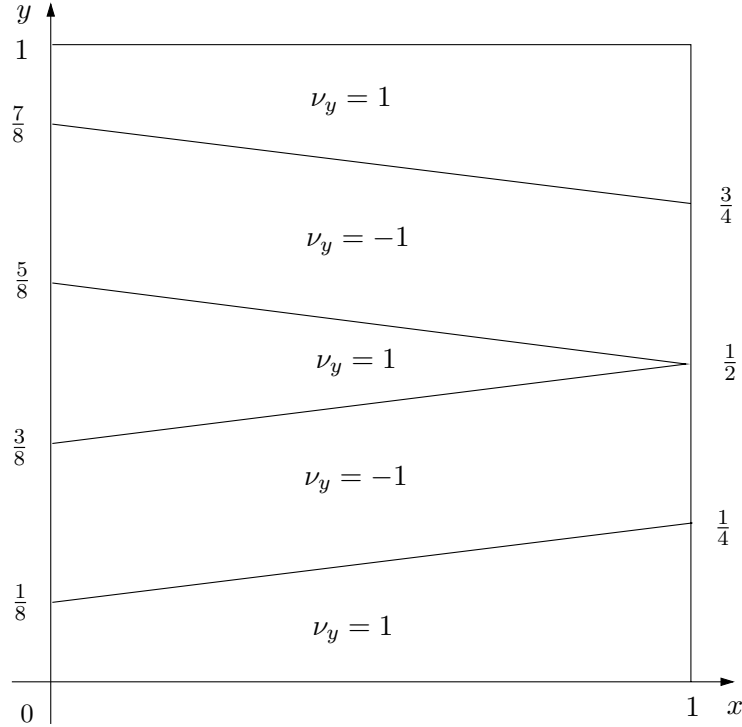


Figure 3: The function ν

satisfies

$$\begin{aligned} |\nu_y| &= 1 \quad \text{a.e.}, \\ \nu(x, y+1) &= \nu(x, y), \\ \nu(0, y) &= \frac{1}{2}\nu(1, 2y), \end{aligned}$$

$$\int_0^1 \int_0^1 \nu_x^2 + \varepsilon |\nu_{yy}| dx dy = \frac{1}{2} \left(\frac{1}{4} \right)^2 + 8\varepsilon.$$

Now choose $\theta \in (0, 1)$ and set

$$x_i = \theta^i L, \quad i = 0, 1, \dots$$

For $x \in [x_1, L]$ define

$$u(x, y) = \nu \left(\frac{x - x_1}{L - x_1}, y \right).$$

Extend u periodically from $[x_1, L] \times [0, 1]$ to $[x_1, L] \times \mathbb{R}$. Note that on $[x_1, L] \times \mathbb{R}$ u satisfies

$$|u| = 1 \quad \text{a.e.},$$

$$u(x, y + 1) = u(x, y),$$

$$u(x_1, y) = \frac{1}{2} u(L, 2y),$$

$$\int_{x_1}^L \int_0^1 u_x^2 + \varepsilon |u_{yy}| dy dx = \frac{1}{32} \frac{1}{L - x_1} + 8\varepsilon(L - x_1).$$

Then continue u to $(0, L] \times [0, 1]$ by

$$u(x, y) = 2^{-i} u(\theta^{-i} x, 2^i y) \quad \text{if } x \in [x_{i+1}, x_i].$$

Note that the resulting function is continuous. Obviously u can be extended continuously to $[0, L] \times [0, 1]$ by setting

$$u(0, y) = 0 \quad \text{for } 0 \leq y \leq 1.$$

Note that $u \in W^{1, \infty}(R_L)$ if and only if $\theta \in [1/2, 1)$. We calculate the energy of u as follows

$$I^0(u) = \sum_{i=0}^{\infty} \int_{x_{i+1}}^{x_i} \int_0^1 u_x^2 dy dx$$

$$= \sum_{i=0}^{\infty} \int_{x_1}^L \int_0^{2^i} (2\theta)^{-2i} u_x^2 2^{-i} \theta^i dy dx = \sum_{i=0}^{\infty} (4\theta)^{-i} \int_{x_1}^L \int_0^1 u_x^2 dy dx.$$

The last expression is finite if and only if $\theta \in (1/4, 1)$. Therefore we have $u \in \mathcal{B}_0$ and $I^0(u) < \infty$ if and only if $\theta \in [1/2, 1)$. This is the desired counterexample and we conclude that the problem without surface energy does not exhibit the Lavrentiev phenomenon.

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