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SHAPE DIFFERENTIATION OF STEADY-STATE REACTION-DIFFUSION PROBLEMS ARISING IN CHEMICAL ENGINEERING WITH NON-SMOOTH KINETICS WITH DEAD CORE

DAVID GÓMEZ-CASTRO

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Abstract. In this paper we consider an extension of the results in shape differentiation of semilinear equations with smooth nonlinearity presented by Díaz and Gómez-Castro [8], to the case in which the nonlinearities might be less smooth. Namely we show that Gateaux shape derivatives exists when the nonlinearity is only Lipschitz continuous, and we will give a definition of the derivative when the nonlinearity has a blow up. In this direction, we study the case of root-type nonlinearities.

1. Introduction

In this article we consider the shape differentiation of a family of diffusion-reaction problems introduced by Aris in the context of optimization of chemical reactors depending on the spatial domain (see [1]). It was later shown that the model can be rigorously deduced as a limit of different nonhomogeneous microscopic models (see [3, 4]). In particular we are interested in the solutions of the problem

$$\begin{gathered} -\Delta w + \beta(w) = f, \quad \text{in } \Omega, \\ w = 1, \quad \text{on } \partial\Omega, \end{gathered} \tag{1.1}$$

and their behaviour as we deform the domain Ω.

It will be sometimes useful to consider the change in variable $u = 1 - w$, $g(u) = \beta(1) - \beta(1-u)$ and $\widehat{f} = \beta(1) - f$, so that we have $u = 0$ on the boundary. After this change in variable we have that u is the solution of

$$\begin{gathered} -\Delta u + g(u) = \widehat{f}, \quad \text{in } \Omega, \\ u = 0, \quad \text{on } \partial\Omega. \end{gathered} \tag{1.2}$$

These functions will be sometimes denoted u_Ω, w_Ω when different domains are considered.

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In [8] (see also [15, 13, 14]) the authors showed that, if $\beta \in W^{2,\infty}(\mathbb{R})$ and $f \in L^2(\Omega)$, then the maps

$$\begin{aligned} W^{1,\infty}(\mathbb{R}^n,\mathbb{R}^n) &\to H_0^1(\Omega) \\ \theta &\mapsto u_{(I+\theta)\Omega} \circ (I+\theta) \\ W^{1,\infty}(\mathbb{R}^n,\mathbb{R}^n) &\to L^2(\mathbb{R}^n) \\ \theta &\mapsto u_{(I+\theta)\Omega}, \end{aligned}$$

where the extension by 0 is considered in $\mathbb{R}^n \setminus (1+\theta)\Omega$, are Fréchet differentiable at 0. Fixing $\theta \in W^{1,\infty}(\mathbb{R}^n,\mathbb{R}^n)$ it was shown in [8] that the directional derivative (the derivative of $u_\tau = u_{(I+\tau\theta)\Omega}$ with respect to τ, $\frac{du_\tau}{d\tau} = \frac{du_\tau}{d\tau}|_{\tau=0}$) is the solution of the problem

$$\begin{aligned} -\Delta \frac{du_\tau}{d\tau} + g'(u_\Omega)\frac{du_\tau}{d\tau} &= 0, \quad \text{in } \Omega, \\ \frac{du_\tau}{d\tau} &= -\nabla u_\Omega \cdot \theta, \quad \text{on } \partial\Omega. \end{aligned} \tag{1.3}$$

Notice that, since $u = 1-w$, we have that $\frac{du_\tau}{d\tau} = -\frac{dw_\tau}{d\tau}$. Hence, taking into account that $g'(u) = -\beta'(w)$, we have

$$\begin{aligned} -\Delta \frac{dw_\tau}{d\tau} + \beta'(w_\Omega)\frac{dw_\tau}{d\tau} &= 0, \quad \text{in } \Omega, \\ \frac{dw_\tau}{d\tau} &= -\nabla w_\Omega \cdot \theta, \quad \text{on } \partial\Omega. \end{aligned} \tag{1.4}$$

The aim of this paper is to extend this results to the case when $\beta \notin W^{2,\infty}$. First, we will show that, when $\beta \in W^{1,\infty}$, the Gateaux shape derivative exists. However, if β is not locally Lipschitz continuous, the solution of (1.1) might develop a region of positive measure

$$N_\Omega = \{x \in \Omega : w_\Omega(x) = 0\}. \tag{1.5}$$

This region, known as *dead core*, was studied at length in [5, 2]. It is a necessary condition for the existence of this region that $\beta'(w_\Omega) = +\infty$. Hence, equation (1.4) cannot be understood immediately in a standard way. In this setting, we will show that there exists a limit of the previous theory.

2. Statement of results

For the rest of the paper $\Omega \subset \mathbb{R}^n$ will be a fixed domain, of class $\mathcal{C}^2$, and $n \geq 2$.

2.1. **Existence and estimates of shape derivatives.**

Existence of Gateaux derivative when $\beta \in W^{1,\infty}$. In [8] the authors prove the existence of a shape derivative in the Fréchet sense when $\beta \in W^{2,\infty}(\mathbb{R})$. Nonetheless, as is it usually the case, the equation for the derivative is well defined in a straightforward way when $\beta \in W^{1,\infty}(\mathbb{R})$. In fact, the following result shows that, if $\beta \in W^{1,\infty}(\mathbb{R})$ rather than $W^{2,\infty}(\mathbb{R})$, then the shape derivative exists only in the Gateaux sense, which is weaker than the Fréchet sense.

Theorem 2.1. *Let $\theta \in W^{1,\infty}(\mathbb{R}^n,\mathbb{R}^n)$, $\beta \in W^{1,\infty}(\mathbb{R})$ be nondecreasing such that $\beta(0) = 0$ and $f \in H^1(\mathbb{R}^n)$. Then, the applications*

$$\begin{aligned} \mathbb{R} &\to L^2(\Omega) \\ \tau &\mapsto u_{(I+\tau\theta)\Omega} \circ (I+\tau\theta), \end{aligned}$$

and

$$\begin{aligned} \mathbb{R} &\to L^2(\mathbb{R}^n) \\ \tau &\mapsto u_{(I+\tau\theta)\Omega} \end{aligned}$$

are differentiable at 0. *Furthermore,* $\frac{du_\tau}{d\tau}|_{\tau=0}$ *is the unique solution of* (1.3).

Remark 2.2. In most cases, the process of homogenization mentioned in the introduction gives an homogeneous equation (1.1) in which β is the same as in the microscopic limit, and thus it is natural that β be singular. However, it sometimes happens that the limit kinetic is different. In the homogenization of problems with particles of critical size (see [9]) it turns out that the resulting kinetic in the macroscopic homogeneous equation (1.1) satisfies $\beta \in W^{1,\infty}$, even when the original kinetic of the microscopic problem was a general maximal monotone graph.

From $W^{2,\infty}$ *to* $W^{1,\infty} \cap \mathcal{C}^1$. Let us show that the shape derivative is continuously dependent on the nonlinearity, and thus that we can make a smooth transition from the Fréchet scenario presented in [8] to our current case. For the rest of the paper we will use the notation:

$$v = \frac{dw_\tau}{d\tau}\Big|_{\tau=0} \tag{2.1}$$

Lemma 2.3. *Let* $f \in L^2(\mathbb{R}^n)$, $\beta \in W^{1,\infty}(\mathbb{R})$ *be nondecreasing functions such that* $\beta(0) = 0$ *and let* $\beta_n \in W^{2,\infty}(\mathbb{R})$ *nondecreasing such that* $\beta_n(0) = 0$. *Let* w_n *be the unique solution of*

$$\begin{gathered} -\Delta w_n + \beta_n(w_n) = f \quad \text{in } \Omega, \\ w_n = 1 \quad \text{on } \partial\Omega. \end{gathered} \tag{2.2}$$

Then

$$\|w_n - w\|_{H^1(\Omega)} \le C\|\beta_n - \beta\|_{L^\infty} \tag{2.3}$$

$$\|w_n - w\|_{H^2(\Omega)} \le C(1 + \|\beta'\|_{L^\infty})\|\beta_n - \beta\|_{L^\infty}. \tag{2.4}$$

Furthermore, let $\beta \in C^1(\mathbb{R}) \cap W^{1,\infty}(\mathbb{R})$ *and* v_n *be the unique solution of*

$$\begin{gathered} -\Delta v_n + \beta_n'(w_n)v_n = 0 \quad \text{in } \Omega, \\ v_n + \nabla w_n \cdot \theta = 0 \quad \text{on } \partial\Omega. \end{gathered} \tag{2.5}$$

Then

$$v_n \rightharpoonup v \quad \text{in } H^1(\Omega). \tag{2.6}$$

Remark 2.4. In (2.3) the notation

$$\|\beta_n - \beta\|_{L^\infty} = \sup_{x\in\mathbb{R}} |\beta_n(x) - \beta(x)|$$

does not mean that either β_n or β are $L^\infty(\mathbb{R})$ functions themselves, but rather that their difference is pointwise bounded, and, in fact, this bound is destined to go 0 as $n \to +\infty$. We will use this notation throughout the paper.

Shape derivative with a dead core. We can prove that the shape derivative in the smooth case has, under some assumptions, a natural limit when β not smooth.

In some cases in the applications (see [5]) we can take β so that $\beta'(w_\Omega)$ has a blow up. It is common, specially in Chemical Engineering, that $\beta'(0) = +\infty$ and N_Ω exists (see [5]). In this case $\beta'(w_\Omega) = +\infty$ in N_Ω. Because of this fact, the natural behaviour of the weak solutions of (1.4) is $v = 0$ in N_Ω. We have the following result

Theorem 2.5. *Let β be nondecreasing, $\beta(0) = 0$, $\beta'(0) = +\infty$,*

$$\beta \in \mathcal{C}(\mathbb{R}) \cap \mathcal{C}^1(\mathbb{R} \setminus \{0\}),$$

and assume that $|N_\Omega| > 0$, $\theta \in W^{1,\infty}(\mathbb{R}^n, \mathbb{R}^n)$ and $0 \le f \le \beta(1)$. Then, there exists v a solution of

$$\begin{aligned} -\Delta v + \beta'(w_\Omega) v = 0 &\quad \Omega \setminus N_\Omega, \\ v = 0 &\quad \partial N_\Omega, \\ v = -\nabla w_\Omega \cdot \theta &\quad \partial\Omega, \end{aligned} \tag{2.7}$$

in the sense that $v \in H^1(\Omega)$, $v = 0$ in N_Ω, $v = -\nabla w_\Omega \cdot \theta$ in $L^2(\partial\Omega)$, $\beta'(w_\Omega)v^2 \in L^1(\Omega)$ and

$$\int_{\Omega \setminus N_\Omega} \nabla v \nabla \varphi + \int_{\Omega \setminus N_\Omega} \beta'(w) v \varphi = 0 \tag{2.8}$$

for every $\varphi \in W_c^{1,\infty}(\Omega \setminus N_\Omega)$. Furthermore, for $m \in \mathbb{N}$, consider β_m defined by

$$\beta_m'(s) = \min\{m, \beta'(s)\}, \quad \beta_m(0) = \beta(0) = 0,$$

and let w_m, v_m be the unique solutions of (2.2) and (2.5). Then,

$$v_m \rightharpoonup v, \quad \text{in } H^1(\Omega), \tag{2.9}$$

where v is a solution of (2.7).

The uniqueness of solutions of (2.7) when $\beta'(w_\Omega)$ blows up is by no means trivial. Problem (2.7) can be written in the following way:

$$-\Delta v + V v = f \tag{2.10}$$

where $V = \beta'(w_\Omega)$ may blow up as a power of the distance to a piece of the boundary. This kind of problems are common in Quantum Physics, although their mathematical treatment is not always rigorous (cf. [6, 7]).

In the next section we will show estimates on $\beta'(w_\Omega)$. Let us state here some uniqueness results depending on the different blow-up rates.

When the blow-up is subquadratic (i.e. not too rapid), by applying Hardy's inequality and the Lax-Migram theorem, we have the following result (see [6, 7]).

Corollary 2.6. *Let N_Ω have positive measure and $\beta'(w(x)) \le C d(x, N_\Omega)^{-2}$ for a.e. $x \in \Omega \setminus N_\Omega$. Then the solution v is unique.*

The study of solutions of problem (2.10) in Ω when $V \in L^1_{\rm loc}(\Omega)$ by many authors (see [11, 10] and the references therein). Existence and uniqueness of this problem in the case $V(x) \ge C d(x, \partial\Omega)^{-r}$ with $r > 2$ was proved in [10]. Applying these techniques one can show that

Corollary 2.7. *Let N_Ω have positive measure and $\beta'(w(x)) \ge C d(x, N_\Omega)^{-r}, r > 2$ for a.e. $x \in \Omega \setminus N_\Omega$. Then the solution v is unique.*

Similar techniques can be applied to the case $\beta'(w(x)) \ge C d(x, N_\Omega)^{-2}$. This will be the subject of a further paper.

2.2. **Estimates of w_Ω close to N_Ω.** Let us study the solution w_Ω on the proximity of the dead core and the blow up behaviour of $\beta'(w_\Omega)$. First, we present a known example

Example 2.8. Explicit radial solutions with dead core are known when $\beta(w) = |w|^{q-1}w$ $(0 < q < 1)$, Ω is a ball of large enough radius and f is radially symmetric. In this case it is known that N_Ω exists, has positive measure and

$$\frac{1}{C} d(x, N_\Omega)^{-2} \leq \beta'(w_\Omega) \leq C d(x, N_\Omega)^{-2}.$$

For the details see [5].

In fact, we present here a more general result to study the behaviour in the proximity of the dead core, based on estimates from [5].

Proposition 2.9. *Let $f = 0$, β be continuous, monotone increasing such that $\beta(0) = 0$, w be a solution of* (1.1) *that develops a dead core N_Ω of positive measure and $\partial N_\Omega \in \mathcal{C}^1$. Assume that*

$$G(t) = \sqrt{2}\Big(\int_0^t \beta(\tau)d\tau + \alpha t\Big)^{1/2}, \quad \text{where } \alpha = \max\big\{0, \min_{x\in\partial\Omega} H(x)\frac{\partial w}{\partial n}(x)\big\}, \tag{2.11}$$

is such that $\frac{1}{G} \in L^1(\mathbb{R})$. Then

$$w_\Omega(x) \leq \Psi^{-1}(d(x, N_\Omega)), \quad \text{where } \Psi(s) = \int_0^s \frac{dt}{G(t)}, \tag{2.12}$$

in a neighbourhood of N_Ω.

Example 2.10 (Root type reactions)**.** Let $f = 0$, $\beta(s) = \lambda|s|^{q-1}s$ with $0 < q < 1$ and Ω be convex such that N_Ω exists and $\partial N_\Omega \in \mathcal{C}^1$. Then

$$w_\Omega(x) \leq C d(x, N_\Omega)^{\frac{2}{1-q}}. \tag{2.13}$$

Furthermore

$$\beta'(w_\Omega(x)) \geq C d(x, N_\Omega)^{-2}. \tag{2.14}$$

3. Proof of Theorem 2.1

For the rest of this paper let us denote

$$u_\tau = u_{(I+\tau\theta)\Omega}. \tag{3.1}$$

Notice that $u_0 = u_\Omega$.

Let us define $U_\tau = u_{(I+\tau\theta)\Omega} \circ (I + \tau\theta) \in H_0^1(\Omega)$. Again $U_0 = u_0 = u_\Omega$. We have

$$\int_\Omega A_\tau \nabla U_\tau \nabla\varphi + \int_\Omega g(U_\tau)\varphi J_\tau = \int_\Omega f_\tau \varphi J_\tau, \tag{3.2}$$

where J_τ is the Jacobian of the transformation. $f_\tau = f \circ (I + \tau\theta)$ and A_τ is the corresponding diffusion matrix (see [8] for the explicit expression). Fortunately, $J_\tau \geq 0$ and, for τ small, we have that $\xi \cdot A_\tau \xi \geq A_0|\xi|^2$ for some $A_0 > 0$ constant. Considering the difference of the weak formulations of U_τ and $U_0 = u_\Omega$ we have

$$\begin{aligned} &\int_\Omega A_\tau \nabla(U_\tau - u_0)\nabla\varphi + \int_\Omega (g(U_\tau) - g(u_0))J_\tau\varphi \\ &= \int_\Omega (f_\tau J_\tau - f)\varphi + + \int_\Omega (I - A_\tau)\nabla u_0 \nabla\varphi + \int_\Omega (J_\tau - 1)g(u_0)\varphi. \end{aligned}$$

Hence, by the monotonicity of g, we have

$$\begin{aligned}&\|\nabla\big(\frac{U_\tau - u}{\tau}\big)\|_{L^2}\\&\le C\Big(\|\frac{f_\tau - f}{\tau}\|_{L^2} + \|\frac{A_\tau - I}{\tau}\|_{L^\infty}\|\nabla u_0\|_{L^2} + \|\frac{J_\tau - 1}{\tau}\|_{L^\infty}\|g(u_0)\|_{L^2}\Big)\end{aligned}$$

Since f_τ, A_τ and J_τ are differentiable at 0, there is weak $H_0^1(\Omega)$ limit. Hence, the limit is strong in $L^2(\Omega)$. Therefore, the function

$$u_\tau = U_\tau \circ (I + \tau\theta)^{-1} \tag{3.3}$$

is differentiable with respect to $\tau \in \mathbb{R}$ with images in $L^2(\Omega)$ at $\tau = 0$. Also

$$H_0^1(\Omega) \ni \frac{dU_\tau}{d\tau}\Big|_{\tau=0} = \frac{du_\tau}{d\tau}\Big|_{\tau=0} + \nabla u_0 \cdot \theta. \tag{3.4}$$

To characterize the derivative, we differentiate on the variational formulation

$$\int_{\mathbb{R}^n} f\varphi = \int_{\mathbb{R}^n} (-u_\tau \Delta\varphi + g(u_\tau)\varphi) \quad \forall \varphi \in \mathcal{C}_c^\infty(\Omega).$$

Considering the difference of the equations for u_τ and u_0 and diving by τ,

$$\begin{aligned}0 &= \int_{\mathbb{R}^n} \Big(-\frac{u_\tau - u_0}{\tau}\Delta\varphi + \frac{g(u_\tau) - g(u_0)}{\tau}\varphi\Big) &(3.5)\\&= \int_{\mathbb{R}^n} \frac{u_\tau - u_0}{\tau}\Big(-\Delta\varphi + \frac{g(u_\tau) - g(u_0)}{u_\tau - u_0}\varphi\Big). &(3.6)\end{aligned}$$

Notice that

$$\big|\frac{g(u_\tau) - g(u_0)}{u_\tau - u_0}\big| \le \|g'\|_{L^\infty}.$$

Therefore, up to a subsequence, $\frac{g(u_\tau)-g(u_0)}{u_\tau - u_0}$ converges weakly in $L^2(\Omega)$. On the other hand since $u_\tau \to u_0$ pointwise, again up to a subsequence, so

$$\frac{g(u_\tau) - g(u_0)}{u_\tau - u_0} \to g'(u_0) \quad \text{a.e. in } \Omega. \tag{3.7}$$

Via a Césaro mean argument we have that the weak L^2 limit and pointwise limit coincide. Hence, passing to the limit in $L^2(\Omega)$

$$0 = \int_\Omega \frac{du_\tau}{d\tau}\Big|_{\tau=0} (-\Delta\varphi + g'(u_0)\varphi), \quad \varphi \in \mathcal{C}_c^\infty(\Omega). \tag{3.8}$$

Therefore $\frac{du_\tau}{d\tau}$ is the unique solution of (1.3).

4. Proof of Lemma 2.3

By considering the difference of the weak formulations we have

$$\int_\Omega \nabla(w_m - w)\nabla\varphi + \int_\Omega (\beta_m(w_m) - \beta_m(w))\varphi = \int_\Omega (\beta(w) - \beta_m(w))\varphi.$$

Taking $\varphi = w_m - w$, and using the monotonicity of β_m we have

$$\|\nabla(w_m - w)\|_{L^2}^2 \le \|\beta_m - \beta\|_{L^\infty}\|w_m - w\|_{L^1(\Omega)}.$$

Using Poincaré inequality and the embedding $L^1 \hookrightarrow L^2$ we have

$$\|w_m - w\|_{L^2} \le C\|\beta_m - \beta\|_{L^\infty}.$$

By considering the equation

$$\|\Delta(w_m - w)\|_{L^2} = \|\beta(w) - \beta_m(w_m)\|_{L^2}$$

$$\begin{aligned} &\le \|\beta(w) - \beta(w_m)\|_{L^2} + \|\beta(w_m) - \beta_m(w_m)\|_{L^2} \\ &\le \|\beta'\|_{L^\infty} \|w_m - w\|_{L^2} + \|\beta_m - \beta\|_{L^\infty}. \end{aligned}$$

Hence, to deduce (2.4) we apply that

$$\|w_m - w\|_{H^2} \le C(\|\Delta(w_m - w)\|_{L^2} + \|w_m - w\|_{L^2}).$$

Considering the difference of the weak formulations of the problems for v_m and v we have

$$\begin{aligned} \int_\Omega \nabla(v_m - v)\nabla\varphi &= \int_\Omega (\beta'(w)v - \beta'_m(w_m)v_m)\varphi \\ &= \int_\Omega (\beta'(w) - \beta'_m(w_m))v_m\varphi + \int_\Omega \beta'(w)(v - v_m)\varphi \\ &= \int_\Omega (\beta'(w) - \beta'(w_m))v_m\varphi + \int_\Omega (\beta'(w_m) - \beta'_m(w_m))v_m\varphi \\ &\quad + \int_\Omega \beta'(w)(v - v_m)\varphi \end{aligned} \tag{4.1}$$

for all $\varphi \in H^1_0(\Omega)$. Considering the test function $\varphi = v_m - v + \nabla(w_m - w)\cdot\theta \in H^1_0(\Omega)$ we have, applying (2.4),

$$\begin{aligned} \int_\Omega |\nabla(v_m - v)|^2 &\le C(1 + \|w_m - w\|_{H^2})\Big((1 + \|\beta'(w)\|_{L^\infty})\|w_m - w\|_{H^2} \\ &\quad + \|v_m\|_{L^2}(\|\beta'_m + \beta'\|_{L^\infty} + \|\beta'(w_m) - \beta'(w)\|_{L^\infty})\Big). \end{aligned}$$

We cannot guaranty that $\|\beta'(w_m) - \beta'(w)\|_\infty$ goes to zero. However it is, indeed, bounded by $2\|\beta'\|_{L^\infty}$. On the other hand, taking into account the boundary condition

$$\begin{aligned} \|v_m - v\|_{L^2(\partial\Omega)} &\le C\|\nabla(w_m - w)\|_{L^2(\partial\Omega)} \\ &\le C\|w_m - w\|_{H^2(\Omega)} \le C\|\beta_m - \beta\|_{L^2} \to 0. \end{aligned} \tag{4.2}$$

Hence, there is a weak limit $\widehat{v} \in H^1(\Omega)$,

$$v_m - v \rightharpoonup \widehat{v} \quad \text{in } H^1(\Omega). \tag{4.3}$$

By (4.2) we have that $\widehat{v} \in H^1_0(\Omega)$. Taking into account (4.1) and the fact that $\beta'(w_m) \to \beta'(w)$ a.e. in Ω, have

$$\int_\Omega \nabla\widehat{v}\nabla\varphi + \int_\Omega \beta'(w)\widehat{v}\varphi = 0 \quad \forall\varphi \in H^1_0(\Omega). \tag{4.4}$$

Taking $\varphi = \widehat{v} \in H^1_0(\Omega)$ as a test function we deduce that $\widehat{v} = 0$.

5. Proof of Theorem 2.5

We start by pointing out that, from condition on f we have $0 \le w_m \le 1$. Since $\beta_m \nearrow \beta$ in $[0,1]$ we have w_m is pointwise decreasing (see [12]). Hence, there exists a pointwise limit w such that $w_m \searrow w$ a.e. in Ω. In particular $0 \le w \le 1$. By the Dominated Convergence Theorem we have

$$w_m \to w \text{ in } L^p(\Omega) \quad \forall 1 \le p < +\infty. \tag{5.1}$$

Let $U \subset \Omega$ be an open neighbourhood of $\partial\Omega$ such that $\overline{U} \cap N_\Omega = \emptyset$ and $\partial U \in \mathcal{C}^2$. Then

$$\underline{w}_U = \inf_U w > 0. \tag{5.2}$$

We have that $w_m \geq w \geq \underline{w}_U$. We have that $\beta \in \mathcal{C}^1([\underline{w}_U, 1])$ and, hence, $\beta_m \to \beta$ in $\mathcal{C}^1([\underline{w}_U, 1])$. Therefore

$$\beta_m(w_m) \to \beta(w) \text{ in } L^p(\Omega \setminus \overline{U}) \quad \forall 1 \leq p < +\infty, \tag{5.3}$$

Since $\|w_m\|_{H^1} \leq C(1 + \|\beta_m(w_m)\|_{L^2} + \|f\|_{L^2})$, we have $w_m \rightharpoonup w$ in $H^1(\Omega)$, and thus w is the unique solution of (1.1). Applying this,

$$\Delta w_m = \beta_m(w_m) - f \to \beta(w) - f = \Delta w \text{ in } L^p(\Omega \setminus \overline{U}). \tag{5.4}$$

Thus

$$\|w_m - w\|_{H^2(\Omega \setminus \overline{U})} \leq C(\|\Delta(w_m - w)\|_{L^2(\Omega\setminus\overline{U})} + \|w_m - w\|_{L^2(\Omega\setminus\overline{U})}) \to 0. \tag{5.5}$$

Hence $w_m \to w$ in $H^2(\Omega \setminus \overline{U})$. In particular

$$\nabla w_m \to \nabla w \text{ in } H^{1/2}(\partial\Omega)^n.$$

Since $\beta_m' \in L^\infty(\mathbb{R})$ we take the "shape derivative" v_m solution of (2.5), which is well defined. Let us find their limit.

Let us show that

$$\beta_m'(w_m) \to \beta'(w) \text{ a.e. in } \Omega. \tag{5.6}$$

First, let $x \notin N_\Omega$. Then β is C^1 in $w(x)$. Therefore $\beta'(w_m(x)) \to \beta'(w(x))$. Hence, the sequence $\beta'(w_m(x))$ is bounded, so $\beta'(w_m(x)) \leq m_0$ for some m_0 large. Thus $\beta_m'(w_m(x)) = \beta'(w_m(x))$ for $m \geq m_0$. Hence the convergence is proved for $x \notin N_\Omega$. Let $x \in N_\Omega$. Then $\beta'(w(x)) = +\infty$. Since $w_m(x) \to w(x)$, it follows then $\beta'(w_m(x)) \to +\infty$. In this case, we have

$$\beta_m'(w_m(x)) = \beta(w_m(x)) \wedge m \to +\infty = \beta(w(x)).$$

This completes the proof of (5.6).

Let us show that sequence (v_m) is bounded in $H^1(\Omega)$. There exist two open sets $U_0, U_1 \subset \Omega$ such that $\partial\Omega \subset U_1, N_\Omega \subset U_0$, $U_0 \cap U_1 = \emptyset$. There also exists a smooth transition function Ψ such that $\Psi = 0$ in U_0 and $\Psi = 1$ in U_1. Let us define $g_m = \Psi \nabla w_m \cdot \theta \in H^1(\Omega)$. Then $\varphi = v_m + g_m \in H_0^1(\Omega)$ and it can be used as a test function in the weak formulation. Hence

$$\int_\Omega \nabla v_m \nabla (v_m + g_m) + \int_\Omega \beta_m'(w_m) v_m (v_m + g_m) = 0.$$

Therefore, through standard arguments,

$$\begin{aligned}
&\int_\Omega |\nabla v_m|^2 + \int_\Omega \beta_m'(w_m) v_m^2 \\
&= -\int_\Omega \nabla v_m \nabla g_m - \int_\Omega \beta_m'(w_m) v_m g_m \\
&\leq \Big(\int_\Omega |\nabla v_m|^2\Big)^{1/2} \Big(\int_\Omega |\nabla g_m|^2\Big)^{1/2} + \Big(\int_\Omega \beta_m'(w_m) v_m^2\Big)^{1/2} \Big(\int_\Omega \beta_m'(w_m) g_m^2\Big)^{1/2} \\
&\leq \frac{1}{2}\Big(\int_\Omega |\nabla v_m|^2 + \int_\Omega \beta_m'(w_m) v_m^2\Big) + C\Big(\int_\Omega |\nabla g_m|^2 + \int_\Omega \beta_m'(w_m) g_m^2\Big).
\end{aligned}$$

Since $\beta_m'(w_m)$ is uniformly bounded in $L^\infty(\Omega \setminus \overline{U_0})$ we have that the sequence is bounded:

$$\Big(\int_\Omega |\nabla v_m|^2 + \int_\Omega \beta_m'(w_m) v_m^2\Big) \leq C\Big(\int_\Omega |\nabla g_m|^2 + \int_\Omega \beta_m'(w_m) g_m^2\Big) \leq C.$$

In particular, there exists $v \in H^1(\Omega)$ such that, up to a subsequence, $v_m \rightharpoonup v$ in $H^1(\Omega)$. Also, by Fatou's lemma,

$$\int_\Omega \beta'(w)v^2 \le C. \tag{5.7}$$

Since $\beta'(w) = +\infty$ in N_Ω we have that $v = 0$ a.e. in N_Ω. For $\varphi \in W_c^{1,\infty}(\Omega \setminus N_\Omega)$ we have

$$\int_{\Omega\setminus N_\Omega} \nabla v_m \nabla \varphi + \int_{\Omega\setminus N_\Omega} \beta_m'(w_m) v_m \varphi = 0. \tag{5.8}$$

Let us consider the compact subset $K = \operatorname{supp}\varphi \subset \Omega \setminus N_\Omega$.

Let us show that $\beta'(w_m) \to \beta'(w)$ in $L^2(K)$. We have $0 < \underline{w}_K \le w \le w_m$ in K. By the Dominated Convergence Theorem we have that $\beta_m'(w_m) \to \beta'(w)$ strongly in $L^p(K)$ for $1 \le p < +\infty$. Hence, by passing to the limit we deduce that

$$\int_{\Omega\setminus N_\Omega} \nabla v \nabla \varphi + \int_{\Omega\setminus N_\Omega} \beta'(w) v \varphi = 0. \tag{5.9}$$

This completes the proof.

6. Proof of Proposition 2.9

Let us consider $x_0 \in \partial N_\Omega$ and

$$W(t) = w_\Omega(x_0 + tn(x_0)) \tag{6.1}$$

where $n(x_0)$ represents the normal vector to ∂N_Ω at x_0. By [5, Theorem 1.24], we have

$$\frac{1}{2}|\nabla w_\Omega(x)|^2 \le \int_0^{w_\Omega(x)} \beta(s)ds + \alpha w_\Omega(x) \tag{6.2}$$

for all $x \in \overline{\Omega}$. Hence

$$\begin{aligned} \frac{dW}{dt} &\le |\frac{dW}{dt}| = |\nabla w_\Omega(x_0 + tn(x_0)) \cdot n(x_0)| \\ &\le |\nabla w_\Omega(x_0 + tn(x_0))| \le G(w_\Omega(x_0 + tn(x_0))) \\ &= G(W(t)). \end{aligned}$$

Thus, W is a solution of the ordinary differential inequality

$$\begin{gathered} \frac{dW}{dt}(t) \le G(W(t)), \\ W(0) = 0. \end{gathered} \tag{6.3}$$

Let us consider W_ε, the solution of

$$\begin{gathered} \frac{dW_\varepsilon}{dt}(t) = G(W_\varepsilon(t)), \\ v_\varepsilon(0) = \varepsilon. \end{gathered} \tag{6.4}$$

This problem has a unique smooth solution, since $G \in \mathcal{C}^1(\mathbb{R} \setminus \{0\}) \cap \mathcal{C}(\mathbb{R})$ is strictly increasing and $G(0) = 0$. In fact, solving this simply separable O.D.E., we obtain

$$W_\varepsilon(t) = \Psi^{-1}(t + \Psi(\varepsilon)). \tag{6.5}$$

By the monotonicity of G we have

$$W(t) \le W_\varepsilon(t) \quad \forall t \ge 0. \tag{6.6}$$

Passing to the limit as $\varepsilon \to 0$ in (6.5) we have

$$W(t) \le \Psi^{-1}(t). \tag{6.7}$$

Hence, since we can parametrize a neighbourhood of ∂N_Ω by $(x,t) \in \partial N_\Omega \times (-\lambda_0, \lambda_0) \mapsto x + tn(x)$, we deduce that

$$w(x) \le \Psi^{-1}(d(x, N_\Omega)) \tag{6.8}$$

at least in a neighbournood of ∂N_Ω. This proves the proposition.

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David Gómez-Castro
Instituto de Matemática Interdisciplinar, Universidad Complutense de Madrid, Plaza de las Ciencias 3, 28040 Madrid, Spain
E-mail address: dgcastro@ucm.es