SHAPE DIFFERENTIATION OF A STEADY-STATE REACTION-DIFFUSION PROBLEM ARISING IN CHEMICAL ENGINEERING: THE CASE OF NON-SMOOTH KINETIC WITH DEAD CORE

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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 in Díaz, J.I., Gómez-Castro, D.: An Application of Shape Differentiation to the Effectiveness of a Steady State Reaction-Diffusion Problem Arising in Chemical Engineering. Electron. J. Differ. Equations. 22, 31—45 (2015) to the case in which the nonlinearities might be less smooth. Namely we will 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 will study the case of root-type nonlinearities.

1. Introduction

In this paper 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 will be interested in the solutions of problem

\[ \begin{align*}
-\Delta w + \beta(w) &= f, & \text{in } \Omega, \\
w &= 1, & \text{on } \partial \Omega,
\end{align*} \tag{1.1} \]

and their behaviour as we deform the domain \( \Omega \).

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

\[ \begin{align*}
-\Delta u + g(u) &= \hat{f}, & \text{in } \Omega, \\
u &= 0, & \text{on } \partial \Omega.
\end{align*} \tag{1.2} \]

These functions will be sometimes denoted \( u_\Omega, w_\Omega \) 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

$$W^{1,\infty}(\mathbb{R}^n, \mathbb{R}^n) \to H^1_0(\Omega)$$

$$\theta \mapsto u_{(I+\theta)\Omega}$$

$$W^{1,\infty}(\mathbb{R}^n, \mathbb{R}^n) \to L^2(\mathbb{R}^n)$$

$$\theta \mapsto u_{(I+\theta)\Omega},$$

where the extension by 0 is considered in $\mathbb{R}^n \setminus \Omega$, 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 $\tau$, $\frac{du_\tau}{d\tau} = \frac{du_\tau}{d\tau}|_{\tau=0}$) is the solution of the following problem

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

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 that

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

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

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

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 $C^2$, and $n \geq 2$.

2.1. Existence and estimates of shape derivatives.

2.1.1. 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

$$\mathbb{R} \to L^2(\Omega)$$

$$\tau \mapsto u_{(I+\tau\theta)\Omega} \circ (I + \tau\theta),$$

...
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and

\[ \begin{align*}
\mathbb{R} & \rightarrow L^2(\mathbb{R}^n) \\
\tau & \mapsto u_{(1+\tau \theta)\Omega}
\end{align*} \]

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

**Remark 2.2.** In most case, the process of homogenization mentioned in the introduction gives an homogeneous equation (1.1) in which \( \beta \) is the same as in the microscopic limit, and thus it is natural that \( \beta \) 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.

2.1.2. From \( W^{2,\infty} \) to \( W^{1,\infty} \cap C^1 \). 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:

\[ v = \frac{dw}{d\tau}|_{\tau=0} \tag{2.1} \]

**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

\[ \begin{align*}
-\Delta w_n + \beta_n(w_n) &= f & \Omega, \\
w_n &= 1 & \partial\Omega.
\end{align*} \tag{2.2} \]

Then

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

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

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

\[ \begin{align*}
-\Delta v_n + \beta_n'(w_n)v_n &= 0 & \Omega, \\
v_n + \nabla w_n \cdot \theta &= 0 & \partial\Omega.
\end{align*} \tag{2.5} \]

Then

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

**Remark 2.4.** In (2.3) the notation

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

does mean that either \( \beta_n \) or \( \beta \) 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.
2.1.3. 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 $\beta$ not smooth.

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

**Theorem 2.5.** Let $\beta$ be nondecreasing, $\beta(0) = 0$, $\beta'(0) = +\infty$, \[ \beta \in C(\mathbb{R}) \cap C^1(\mathbb{R} \setminus \{0\}), \]
and assume that $|N_\Omega| > 0$, $\theta \in W^{1,\infty}(\mathbb{R}^n, \mathbb{R}^n)$ and $0 \leq f \leq \beta(1)$. Then, there exists $v$ a solution of

\[
\begin{cases}
-\Delta v + \beta'(w_\Omega)v = 0 & \Omega \setminus N_\Omega, \\
v = 0 & \partial N_\Omega, \\
v = -\nabla w_\Omega \cdot \theta & \partial \Omega,
\end{cases}
\]

(2.7)
in the sense that $v \in H^1(\Omega)$, $v = 0$ in $N_\Omega$, $v = -\nabla w_\Omega \cdot \theta$ in $L^2(\partial \Omega)$, $\beta'(w_\Omega)v^2 \in L^1(\Omega)$ and

\[
\int_{\Omega \setminus N_\Omega} \nabla v \nabla \varphi + \int_{\Omega \setminus N_\Omega} \beta'(w)v \varphi = 0
\]

(2.8)
for every $\varphi \in W^{1,\infty}_c(\Omega \setminus N_\Omega)$. Furthermore, for $m \in \mathbb{N}$, consider $\beta_m$ 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,

\[
v_m \rightharpoonup v, \quad \text{in } H^1(\Omega),
\]

(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:

\[- \Delta v + Vv = f\]

(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 blows is subquadratic (i.e. not too rapid), by applying Hardy’s inequality and the Lax-Migmag theorem, we have the following result (see [6, 7]).

**Corollary 2.6.** Let $N_\Omega$ have positive measure and $\beta'(u(x)) \leq Cd(x, N_\Omega)^{-2}$ for a.e. $x \in \Omega \setminus N_\Omega$. Then the solution $v$ is unique.
The study of solutions of problem (2.10) in $\Omega$ when $V \in L^1_{loc}(\Omega)$ by many authors (see [11] and the references therein). Existence and uniqueness of this problem in the case $V(x) \geq Cd(x, \partial \Omega)^{-r}$ with $r > 2$ was proved in [10]. Applying these techniques one can show that

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

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

### 2.2. Estimates of $w_\Omega$ close to $N_\Omega$.

Let us study the solution $w_\Omega$ 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 $\beta(w) = |w|^{q-1}w$ ($0 < q < 1$), $\Omega$ is a ball of large enough radius and $f$ is radially symmetric. In this case it is known that $N_\Omega$ exists, has positive measure and

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

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 $f = 0$, $\beta$ be continuous, monotone increasing such that $\beta(0) = 0$, $w$ be a solution of (1.1) that develops a dead core $N_\Omega$ of positive measure and $\partial N_\Omega \in C^1$. Assume that

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

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

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

in a neighbourhood of $N_\Omega$.

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

$$w_\Omega(x) \leq Cd(x, N_\Omega)^{-\frac{2}{q}}.$$  \hspace{1cm} (2.13)

Furthermore

$$\beta'(w_\Omega(x)) \geq Cd(x, N_\Omega)^{-2}.$$  \hspace{1cm} (2.14)

### 3. Proof of Theorem 2.1

For the rest of the paper let us note

$$u_\tau = u(t+\tau \theta)\Omega.$$  \hspace{1cm} (3.1)

Notice that $u_0 = u_\Omega$. 
Let us define $U_\tau = u_{(I+\tau\theta)\circ (I+\tau\theta)} \in H^1_0(\Omega)$. Again $U_0 = u_0 = u_\Omega$. We have that

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

where $J_\tau$ is the Jacobian of the transformation. $f_\tau = f \circ (I + \tau \theta)$ and $A_\tau$ is the corresponding diffusion matrix (see [8] for the explicit expression). Fortunately, $J_\tau \geq 0$ and, for $\tau$ 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 $U_\tau$ and $U_0$ we have that

$$
\int_\Omega A_\tau \nabla (U_\tau - u_0) \nabla \varphi + \int_\Omega (g(U_\tau) - g(u_0)) \varphi J_\tau = \int_\Omega (f_\tau - f) \varphi + \int_\Omega (I - A_\tau) \nabla u_0 \nabla \varphi + \int_\Omega (J_\tau - 1) g(u_0) \varphi.
$$

Hence, due to the monotonicity of $g$, we have that

$$
\left\| \nabla \left( \frac{U_\tau - u_0}{\tau} \right) \right\|_{L^2} \leq C \left( \left\| \frac{f_\tau - f}{\tau} \right\|_{L^2} + \left\| \frac{A_\tau - I}{\tau} \right\|_{L^\infty} \left\| \nabla u_0 \right\|_{L^2} + \left\| \frac{J_\tau - 1}{\tau} \right\|_{L^\infty} \left\| g(u_0) \right\|_{L^2} \right)
$$

Since $f_\tau, A_\tau$ and $J_\tau$ are differentiable at 0, there is weak $H^1_0(\Omega)$ limit. Hence, the limit is strong in $L^2(\Omega)$. Therefore, the function

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

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

$$
H^1_0(\Omega) \ni \frac{dU_\tau}{d\tau} \bigg|_{\tau=0} = \frac{du_\tau}{d\tau} \bigg|_{\tau=0} + \nabla u_0 \cdot \theta.
$$

To characterize the derivative, we differentenciate on the variational formulation

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

Considering the difference of the equations for $u_\tau$ and $u_0$ and diving by $\tau$

$$
0 = \int_{\mathbb{R}^n} \left( -\frac{u_\tau - u_0}{\tau} \Delta \varphi + \frac{g(u_\tau) - g(u_0)}{\tau} \varphi \right)
$$

and

$$
= \int_{\mathbb{R}^n} \frac{u_\tau - u_0}{\tau} \left( -\Delta \varphi + \frac{g(u_\tau) - g(u_0)}{u_\tau - u_0} \varphi \right).
$$

Notice that

$$
\left| \frac{g(u_\tau) - g(u_0)}{u_\tau - u_0} \right| \leq \left\| g' \right\|_{L^\infty}.
$$

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

$$
\frac{g(u_\tau) - g(u_0)}{u_\tau - u_0} \to g'(u_0) \quad \text{a.e. in } \Omega.
$$
Via a Césaro mean argument we have that the weak $L^2$ limit and pointwise limit coincide. Hence, passing to the limit in $L^2(\Omega)$

$$0 = \int_{\Omega} \left. \frac{d u_\tau}{d \tau} \right|_{\tau = 0} (-\Delta \varphi + g'(u_0)\varphi), \quad \varphi \in C^\infty_c(\Omega). \quad (3.8)$$

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

4. PROOF OF LEMMA 2.3

By considering the difference of the weak formulations we have that

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

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

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

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

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

By considering the equation

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

Hence, to deduce (3.4) we apply that

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

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

$$\int_{\Omega} \nabla(v_m - v)\nabla \varphi = \int_{\Omega} (\beta'(w)v - \beta'_m(w_m)v_m)\varphi$$

$$= \int_{\Omega} (\beta'(w) - \beta'_m(w_m))v_m\varphi + \int_{\Omega} \beta'(w)(v - v_m)\varphi$$

$$= \int_{\Omega} (\beta'(w) - \beta'_m(w_m))v_m\varphi + \int_{\Omega} (\beta'(w_m) - \beta'_m(w_m))v_m\varphi$$

$$+ \int_{\Omega} \beta'(w)(v - v_m)\varphi \quad (4.1)$$

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)

$$\int_{\Omega} |\nabla(v_m - v)|^2 \leq C(1 + \|w_m - w\|_{H^2})$$

$$\times \left( (1 + \|\beta'(w)\|_{L^\infty})\|w_m - w\|_{H^2} + \|v_m\|_{L^2}(\|\beta'_m + \beta'\|_{L^\infty} + \|\beta'(w_m) - \beta'(w)\|_{L^\infty}) \right).$$
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
\[
\|v_m - v\|_{L^2(\partial \Omega)} \leq C\|\nabla (w_m - w)\|_{L^2(\partial \Omega)} \leq C\|w_m - w\|_{H^2(\Omega)} \leq C\|\beta_m - \beta\|_{L^2} \to 0. \tag{4.2}
\]
Hence, there is a weak limit \(\hat{v} \in H^1(\Omega)\)
\[
v_m - v \rightharpoonup \hat{v} \text{ in } H^1(\Omega). \tag{4.3}
\]
Due to (4.2) we have that \(\hat{v} \in H^1_0(\Omega)\). Taking into account (4.1) and the fact that \(\beta'(w_m) \to \beta'(w)\) a.e. in \(\Omega\), have that
\[
\int_\Omega \nabla \hat{v} \nabla \varphi + \int_\Omega \beta'(w)\hat{v}\varphi = 0 \quad \forall \varphi \in H^1_0(\Omega). \tag{4.4}
\]
Taking \(\varphi = \hat{v} \in H^1_0(\Omega)\) as a test function we deduce that \(\hat{v} = 0\). \(\Box\)

## 5. Proof of Theorem 2.5

We start by pointing out that, due to the condition on \(f\) we have that \(0 \leq w_m \leq 1\). Since \(\beta_m \not\to \beta\) in \([0, 1]\) we have \(w_m\) is pointwise decreasing (see [12]). Hence, there exists a pointwise limit \(w\) such that \(w_m \rightharpoonup w\) a.e. in \(\Omega\). In particular \(0 \leq w \leq 1\). Due to the Dominated Convergence Theorem we have that
\[
w_m \to w \text{ in } L^p(\Omega) \quad \forall 1 \leq p < +\infty. \tag{5.1}
\]
Let \(U \subset \Omega\) be an open neighbourhood of \(\partial \Omega\) such that \(\overline{U} \cap N_\Omega = \emptyset\) and \(\partial U \in C^2\). Then
\[
w_U = \inf_U w > 0. \tag{5.2}
\]
We have that \(w_m \geq w \geq w_U\). We have that \(\beta \in C^1([w_U, 1])\) and, hence, \(\beta_m \to \beta\) in \(C^1([w_U, 1])\). 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 that \(w_m \to w\) in \(H^1(\Omega)\), and thus that \(w\) 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
\[
w_m \to w \text{ in } H^2(\Omega \setminus \overline{U}).
\]
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 we show that \(\beta_m'(w_m) \to \beta'(w)\) a.e. in \(\Omega\).
\[
\beta_m'(w_m) \to \beta'(w) \text{ a.e. in } \Omega. \tag{5.6}
\]
First, let \(x \notin N_\Omega\). Then \(\beta\) 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 \(\beta_m'(w_m(x)) = \beta'(w_m(x)) \text{ for } m \geq m_0\). Hence the convergence is proved for \(x \notin N_\Omega\).
Let $x \in N_\Omega$. Then $\beta'(w(x)) = +\infty$. Since $w_m(x) \to w(x)$ then $\beta'(w_m(x)) \to +\infty$. In that case, we have that
\[
\beta'_m(w_m(x)) = \beta(w_m(x)) \land m \to +\infty = \beta(w(x)).
\]
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 $\Psi$ 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 $v_m + g_m \in H^1(\Omega)$ 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
\[
\int_{\Omega} |\nabla v_m|^2 + \int_{\Omega} \beta'_m(w_m)v_m^2 = -\int_{\Omega} \nabla v_m \nabla g_m - \int_{\Omega} \beta'_m(w_m)v_m g_m \leq \left( \int_{\Omega} |\nabla v_m|^2 \right)^{\frac{1}{2}} \left( \int_{\Omega} |\nabla g_m|^2 \right)^{\frac{1}{2}} + \left( \int_{\Omega} \beta'_m(w_m)v_m^2 \right)^{\frac{1}{2}} \left( \int_{\Omega} \beta'_m(w_m)g_m^2 \right)^{\frac{1}{2}} \leq \frac{1}{2} \left( \int_{\Omega} |\nabla v_m|^2 + \int_{\Omega} \beta'_m(w_m)v_m^2 \right) + C \left( \int_{\Omega} |\nabla g_m|^2 + \int_{\Omega} \beta'_m(w_m)g_m^2 \right).
\]
Since $\beta'_m(w_m)$ is uniformly bounded in $L^\infty(\Omega \setminus \overline{U_0})$ we have that the sequence is bounded:
\[
\left( \int_{\Omega} |\nabla v_m|^2 + \int_{\Omega} \beta'_m(w_m)v_m^2 \right) \leq C \left( \int_{\Omega} |\nabla g_m|^2 + \int_{\Omega} \beta'_m(w_m)g_m^2 \right) \leq C.
\]
In particular, there exists $v \in H^1(\Omega)$ such that, up to a subsequence,
\[
v_m \rightharpoonup v \text{ in } H^1(\Omega).
\]
Also, due to Fatou’s lemma
\[
\int_{\Omega} \beta'(w)v^2 \leq C. \tag{5.7}
\]
Since $\beta'(w) = +\infty$ in $N_\Omega$ we have that $v = 0$ a.e. in $N_\Omega$. For $\varphi \in W^{1,\infty}_c(\Omega \setminus N_\Omega)$ we have that
\[
\int_{\Omega \setminus N_\Omega} \nabla v_m \nabla \varphi + \int_{\Omega \setminus N_\Omega} \beta'_m(w_m)v_m \varphi = 0. \tag{5.8}
\]
Let us consider the compact subset $K = \text{supp}\varphi \subset \Omega \setminus N_\Omega$. Let us show that $\beta'(w_m) \to \beta'(w)$ in $L^2(K)$. We have $0 < w_K \leq w \leq w_m$ in $K$. Due to the Dominated Convergence Theorem we have that $\beta'_m(w_m) \to \beta'(w)$ strongly in $L^p(K)$ for $1 \leq p < +\infty$.

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. \[\square\]
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 \( \partial N_\Omega \) at \( x_0 \). Due to Theorem 1.24 in [5], we have that
\[
\frac{1}{2} |\nabla w_\Omega(x)|^2 \leq \int_0^{w_\Omega(x)} \beta(s) ds + \alpha w_\Omega(x) \tag{6.2}
\]
for all \( x \in \overline{\Omega} \). Hence
\[
\frac{dW}{dt} \leq |\nabla w_\Omega(x_0 + tn(x_0)) \cdot n(x_0)|
\leq |\nabla w_\Omega(x_0 + tn(x_0))| \leq G(w_\Omega(x_0 + tn(x_0)))
= G(W(t)).
\]
Thus, \( W \) is a solution of the following Ordinary Differential Inequality
\[
\begin{cases}
\frac{dW}{dt}(t) \leq G(W(t)), \\
W(0) = 0.
\end{cases} \tag{6.3}
\]
Let us consider \( W_\varepsilon \) the solution of
\[
\begin{cases}
\frac{dW_\varepsilon}{dt}(t) = G(W_\varepsilon(t)), \\
v_\varepsilon(0) = \varepsilon.
\end{cases} \tag{6.4}
\]
This problem has a unique smooth solution, since \( G \in C^1(\mathbb{R} \setminus \{0\}) \cap C(\mathbb{R}) \) is strictly increasing and \( G(0) = 0 \). In fact, solving this simply separable O.D.E., we obtain that
\[
W_\varepsilon(t) = \Psi^{-1}(t + \Psi(\varepsilon)). \tag{6.5}
\]
Due to the monotonicity of \( G \) we have that
\[
W(t) \leq W_\varepsilon(t) \quad \forall t \geq 0. \tag{6.6}
\]
Passing to the limit as \( \varepsilon \to 0 \) in (6.5), we have that
\[
W(t) \leq \Psi^{-1}(t). \tag{6.7}
\]
Hence, since we can parametrize a neighbourhood of \( \partial N_\Omega \) by \( (x, t) \in \partial N_\Omega \times (-\lambda_0, \lambda_0) \mapsto x + tn(x) \), we deduce that
\[
w(x) \leq \Psi^{-1}(d(x, N_\Omega)) \tag{6.8}
\]
at least in a neighbourhood of \( \partial N_\Omega \). This proves the result. \( \square \)

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References

[1] R. Aris and W. Strieder. *Variational Methods Applied to Problems of Diffusion and Reaction*, volume 24 of *Springer Tracts in Natural Philosophy*. Springer-Verlag, New York, 1973.

[2] C. Bandle, R. Sperb, and I. Stakgold. Diffusion and reaction with monotone kinetics. *Nonlinear Analysis: Theory, Methods and Applications*, 8(4):321–333, 1984.

[3] C. Conca, J. I. Díaz, A. Liñán, and C. Timoteo. Homogenization in Chemical Reactive Flows. *Electronic Journal of Differential Equations*, 40:1–22, 2004.

[4] J. Díaz, D. Gómez-Castro, A. Podolskii, and T. Shaposhnikova. On the asymptotic limit of the effectiveness of reaction–diffusion equations in periodically structured media. *Journal of Mathematical Analysis and Applications*, 455(2):1597–1613, 2017.

[5] J. I. Díaz. *Nonlinear Partial Differential Equations and Free Boundaries*. Pitman, London, 1985.

[6] J. I. Díaz. On the ambiguous treatment of the Schrödinger equation for the infinite potential well and an alternative via flat solutions: The one-dimensional case. *Interfaces and Free Boundaries*, 17(3):333–351, 2015.

[7] J. I. Díaz. On the ambiguous treatment of the Schrödinger equation for the infinite potential well and an alternative via singular potentials: the multi-dimensional case. *SeMA Journal*, 17(3):333–351, 2017.

[8] J. I. Díaz and D. Gómez-Castro. An Application of Shape Differentiation to the Effectiveness of a Steady State Reaction-Diffusion Problem Arising in Chemical Engineering. *Electronic Journal of Differential Equations*, 22:31–45, 2015.

[9] J. I. Díaz, D. Gómez-Castro, A. V. Podol’skii, and T. A. Shaposhnikova. Characterizing the strange term in critical size homogenization: quasilinear equations with a nonlinear boundary condition involving a general maximal monotone graph. *Advances in Nonlinear Analysis*, To appear, 2017.

[10] J. I. Díaz, D. Gómez-Castro, J. M. Rakotoson, and R. Temam. Linear diffusion with singular absorption potential and/or unbounded convective flow: the weighted space approach. To appear.

[11] J. I. Díaz and J. M. Rakotoson. On very weak solutions of semi-linear elliptic equations in the framework of weighted spaces with respect to the distance to the boundary. *Discrete and Continuous Dynamical Systems*, 27(3):1037–1058, 2010.

[12] L. C. Evans. *Partial Differential Equations*. American Mathematical Society, Providence, Rhode Island, 1998.

[13] A. Henrot and M. Pierre. *Optimization des Formes: Un analyse géométrique*. Springer, 2005.

[14] O. Pironneau. *Optimal Shape Design for Elliptic Equations*. Springer Series in Computational Physics. Springer-Verlag, Berlin, 1984.

[15] J. Simon. Differentiation with respect to the domain in boundary value problems. *Numerical Functional Analysis and Optimization*, 2(7-8):649–687, 1980.

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