OPTIMAL POTENTIALS FOR PROBLEMS WITH CHANGING SIGN DATA

GIUSEPPE BUTTAZZO, FAUSTINO MAESTRE, BOZHIDAR VELICHKOV

Abstract. We consider optimal control problems where the state equation is an elliptic PDE of a Schrödinger type, governed by the Laplace operator $-\Delta$ with the addition of a potential V, and the control is the potential V itself, that may vary in a suitable admissible class. In a previous paper (Ref. [10]) an existence result was established under a monotonicity assumption on the cost functional, which occurs if the data do not change sign. In the present paper this sign assumption is removed and the existence of an optimal potential is still valid. Several numerical simulations, made by `FreeFem++`, are shown.

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1. Introduction and statement of the problem

In the present paper we consider optimization problems of the form

$$\min\left\{\int_D g(x)u(x)\,dx \ : \ -\Delta u + Vu = f,\ u\in H^1_0(D),\ V\in\mathcal{V}\right\}. \tag{1.1}$$

Here D is a fixed bounded domain of $\mathbb{R}^d$, f and g are two given functions in $L^2(D)$, and the potential V may vary in the admissible class $\mathcal{V}$ which is described below. Problem (1.1) is then an optimal control problem where $H^1_0(D)$ is the space of states, $\mathcal{V}$ is the set of admissible controls, $-\Delta u + Vu = f$ is the state equation, and $\int_D g(x)u(x)\,dx$ is the cost functional.

Problems of this form have been considered in [10] under some assumptions on the admissible class $\mathcal{V}$. In particular, the admissible class $\mathcal{V}$ was taken of the form

$$\mathcal{V} = \left\{V : D\to[0,+\infty] \ : \ V \text{ Lebesgue measurable}, \int_D \Psi(V)\,dx \le 1\right\}, \tag{1.2}$$

with a function Ψ satisfying some appropriate qualitative conditions. For instance, in order to approximate shape optimization problems with Dirichlet condition on the free boundary, the choice

$$\Psi(s) = e^{-\alpha s}$$

with α small, was proposed. More precisely, as $\alpha\to 0$ the problems with the parameter α were shown to Γ-converge to the shape optimization problem with a volume constraint $|\Omega|\le 1$ being Ω the shape variable. The existence of an optimal potential V_{opt} was shown under the key assumption (see Theorem 4.1 of [10]) to have a cost functional depending on the potential V in a monotonically increasing way. This occurs, by the maximum principle, when $f\ge 0$ and $g\le 0$ (or symmetrically, when $f\le 0$ and $g\ge 0$), and in this case the constraint is saturated, that is $\int_D \Psi(V_{opt})\,dx = 1$.

When the data f and g are allowed to change sign, the structure of the proof above is not valid any more and the question of the existence of an optimal potential was open. Similar questions arise for shape optimization problems, where again the monotonicity of the cost plays a crucial role.

The case of shape optimization problems with changing sign data was recently considered in [11] where a new approach was proposed, allowing to obtain the existence of optimal shapes in a larger framework allowing general functions f and g. We adopt here an approach similar

to the one of [11], adapted to the case of potentials. Of course, when f and g may change sign, the constraint does not need to be saturated, in the sense that it is possible to have some situations in which there is an optimal potential V_{opt} such that $\int_D \Psi(V_{opt})\,dx < 1$.

Problems of the kind considered here naturally appear in variational problems with uncertainty, where the right-hand side f is only known up to a probability P on $L^2(D)$ (see for instance [11] for the shape optimization framework). Other kinds of uncertainties can be treated by the so-called *worst case analysis*; in the case of shape optimization problems we refer for this topic to [2], to [3] and to the references therein.

We stress the fact that the assumption that the cost function is linear with respect the state variable u is crucial; otherwise simple examples show that an optimal shape or an optimal potential may not exist (see for instance [6], [8] and [9]) and the optimal solution only exists in a relaxed sense in the space of capacitary measures, introduced in [12]. The assumption that D is bounded is also crucial, since the characterization of the relaxed formulation of Dirichlet problems is available under this assumption (see for instance [6], [12]). In the case of spectral optimization problems the case $D = \mathbb{R}^d$ has been studied and the existence of optimal domains has been obtained in several situations (see [4], [5] and [14]); even if it is not the goal of the present paper, it would be interesting to generalize the existence of optimal potentials to the case D unbounded, this would require additional tools that are at the moment unavailable.

The paper is organized as follows. In Section 2 we give the precise statement of the existence result (Theorem 2.5) and its proof. In Section 3 we provide some necessary conditions (Proposition 3.5 and Proposition 3.6) the optimal potentials have to fulfill. Finally, in Section 4 we provide several numerical simulations that show the optimal potentials in some two dimensional cases.

2. Existence of optimal potentials

In this section we consider the optimization problem (1.1) in the admissible class $\mathcal{V}$ defined in (1.2). On the function $\Psi : [0, +\infty] \to [0, +\infty]$ we assume that:

(i) Ψ is strictly decreasing;
(ii) there exist $p > 1$ such that the function $s \mapsto \Psi^{-1}(s^p)$ is convex.

For instance the following functions:

(1) $\Psi(s) = s^{-p}$, for any $p > 0$,
(2) $\Psi(s) = e^{-\alpha s}$, for any $\alpha > 0$,

satisfy the assumptions (i) and (ii) above. Moreover, we will also assume that the admissible class $\mathcal{V}$ is nonempty. We notice that this is equivalent to the assumption that $|D|\Psi(+\infty) \le 1$. Indeed, if $\mathcal{V}$ is nonempty, then the monotonicity assumption (i) implies that $|D|\Psi(+\infty) \le 1$. On the other hand, if $|D|\Psi(+\infty) \le 1$, then the potential $V \equiv +\infty$ belongs to the class $\mathcal{V}$.

Capacitary measures. The relaxed form of the optimization problem (1.1) is expressed in terms of the so called capacitary measures. In this subsection we briefly recall the definition and the main properties of these measures. For all the details about capacitary measures and their use in optimization problems we refer to the book [6].

A *capacitary measure* μ is a nonnegative Borel measure on D, possibly taking the value $+\infty$, that vanishes on all sets of capacity zero (here the capacity is intended with respect to the H^1 norm). In particular, if two functions are in the same class of equivalence of $H^1_0(D)$, then they are also in the same class of equivalence of $L^2(\mu)$. Thus the space $H^1_0(D) \cap L^2(\mu)$ is a well-defined Hilbert space endowed with the norm

$$\|u\| = \Big(\|\nabla u\|^2_{L^2(D)} + \|u\|^2_{L^2(\mu)} \Big)^{1/2}.$$

We say that $u \in H^1_0(D) \cap L^2(\mu)$ is a solution of the problem

$$-\Delta u + \mu u = f, \qquad u \in H^1_0(D) \cap L^2(\mu),$$

for a function $f \in L^2(D)$, if

$$\int_D \nabla u \nabla \phi \, dx + \int_D u\phi \, d\mu = \int_D f\phi \, dx \qquad \forall \phi \in H^1_0(D) \cap L^2(\mu), \tag{2.1}$$

or equivalently, if u is the (unique, due to the strict convexity of the functional) minimizer in $H^1_0(D) \cap L^2(\mu)$ of the functional

$$H^1_0(D) \cap L^2(\mu) \ni u \mapsto \frac{1}{2}\int_D |\nabla u|^2 \, dx + \frac{1}{2}\int_D u^2 \, d\mu - \int_D uf \, dx.$$

We define the associated resolvent operator $R_\mu : L^2(D) \to L^2(D)$ as $R_\mu(f) := u \in H^1_0(D) \cap L^2(\mu)$ and we notice that R_μ is a compact positive self-adjoint operator.

Analogously, for every function F in the dual space $(H^1_0(D) \cap L^2(\mu))'$ we can define the solution $u = R_\mu(F)$ of the problem

$$-\Delta u + \mu u = F, \qquad u \in H^1_0(D) \cap L^2(\mu),$$

in a weak sense or, equivalently, as the minimizer of the functional

$$H^1_0(D) \cap L^2(\mu) \ni u \mapsto \frac{1}{2}\int_D |\nabla u|^2 \, dx + \frac{1}{2}\int_D u^2 \, d\mu - F(u).$$

Remark 2.1. We notice that, if $\nu_1 \le \mu$ and $\nu_2 \le \mu$ are two capacitary measures and $f_1, f_2 \in L^2(\mu)$ are two given functions, then the functional $F : H^1_0(D) \cap L^2(\mu) \to \mathbb{R}$ defined by

$$F(u) = \int_D uf_1 \, d\nu_1 - \int_D uf_2 \, d\nu_2,$$

is in the dual space $\big(H^1_0(D) \cap L^2(\mu)\big)'$ and so the solution $R_\mu(f_1\nu_1 - f_2\nu_2)$ does exists.

Remark 2.2. The linear functional $R_\mu : \big(H^1_0(D) \cap L^2(\mu)\big)' \to H^1_0(D) \cap L^2(\mu)$ defined above remains symmetric, that is, for every $F_1, F_2 \in \big(H^1_0(D) \cap L^2(\mu)\big)'$ we have

$$\int_D F_1 R_\mu(F_2) \, dx = \int_D \nabla R_\mu(F_1) \cdot \nabla R_\mu(F_2) \, dx + \int_D R_\mu(F_1) R_\mu(F_2) \, d\mu = \int_D R_\mu(F_1) F_2 \, dx,$$

where slightly abusing the notation we have set $\int_D F_1 R_\mu(F_2) \, dx := F_1(R_\mu(F_2))$.

The γ-convergence. The space of capacitary measures over a domain D of finite Lebesgue measure can be endowed with the structure of a metric space, whose distance d_γ is appositely designed to treat optimization problems involving solutions of PDEs; the convergence with respect to this metric is called γ-convergence. The main properties of the γ-convergence (see for example [6] for more details) are the following:

- The space of capacitary measures endowed with distance d_γ is a compact metric space.
- If a sequence of capacitary measures $(\mu_n)_{n\in\mathbb{N}}$ γ-converges to the capacitary measure μ, then for every $f \in L^2(D)$ the sequence of solutions $R_{\mu_n}(f)$ converges to $R_\mu(f)$ strongly in $L^2(D)$ and $H^1_0(D)$.
- The non-negative potentials, that is the capacitary measures absolutely continuous with respect to the Lebesgue measure, are dense in the metric space of all capacitary measures.

The admissible class of potentials and its relaxation. Let us first specify the action of a potential $V \in \mathcal{V}$ on the state equation

$$-\Delta u + Vu = f, \qquad u \in H^1_0(D) \cap L^2(V).$$

By this we mean the equation (2.1), where the capacitary measure μ associated to V is defined as:

$$\mu(A) = \begin{cases} \int_A V(x) \, dx & \text{if } \operatorname{cap}\big(A \cap \{V = +\infty\}\big) = 0 \\ +\infty & \text{if } \operatorname{cap}\big(A \cap \{V = +\infty\}\big) > 0, \end{cases}$$

which implies $u = 0$ quasi-everywhere on the set $\{V = +\infty\}$. Slightly abusing the terminology in the following we identify μ and V.

Let us denote by $\overline{\mathcal{V}}$ the family of capacitary measures μ obtained as limits (with respect to the γ-distance) of sequences (V_n) of potentials in $\mathcal{V}$. These measures can be written as $\mu = V + \mu^s$, where $V \in \mathcal{V}$ and μ^s is singular with respect to the Lebesgue measure and with $\mu^s\big(\{V = +\infty\}\big) = 0$. This fact is non-trivial, so we give the proof in the following Lemma.

Lemma 2.3. *Let $D \subset \mathbb{R}^d$ be a bounded open set and let Ψ satisfy the assumptions i) and ii) above. Then every $\mu \in \overline{\mathcal{V}}$ is of the form $\mu = V + \mu^s$ with $V \in \mathcal{V}$, and μ^s singular with respect to the Lebesgue measure and with $\mu^s\big(\{V = +\infty\}\big) = 0$.*

Proof. Let $V_n \in \mathcal{V}$ be a given sequence. Then, $v_n = \big(\Psi(V_n)\big)^{1/p}$ is a bounded sequence in $L^p(D)$ and so, up to a subsequence, v_n converges weakly in $L^p(D)$ to some nonnegative function v. Let $W = \Psi^{-1}(v^p)$. Notice that by the weak lower semicontinuity of the L^p norm and the fact that $\Psi(W) = v^p$ we get that $\int_D \Psi(W)\,dx \le 1$.

Moreover, since the γ-convergence is compact, we may assume that, up to a subsequence, V_n γ-converges to a capacitary measure μ. By the definition of γ-convergence, we have that for any $u \in H^1_0(D)$, there is a sequence $u_n \in H^1_0(D)$ which converges to u in $L^2(D)$ and is such that

$$\begin{aligned}\int_D |\nabla u|^2\,dx + \int_D u^2\,d\mu &= \lim_{n\to\infty} \int_D |\nabla u_n|^2\,dx + \int_D u_n^2 V_n\,dx \\ &\ge \lim_{n\to\infty} \int_D |\nabla u_n|^2\,dx + \int_D u_n^2 \Psi^{-1}(v_n^p)\,dx \\ &\ge \int_D |\nabla u|^2\,dx + \int_D u^2 \Psi^{-1}(v^p)\,dx \\ &= \int_D |\nabla u|^2\,dx + \int_D u^2 W\,dx,\end{aligned}$$

where the inequality above is due to the strong-weak lower semicontinuity of integral functionals (see for instance Theorem 2.3.1 of [7]), which follows by the assumptions made on the function Ψ. Thus, for any $u \in H^1_0(D)$, we have

$$\int_D u^2\,d\mu \ge \int_D u^2 W\,dx,$$

which gives $W \le \mu$. If we now write $\mu = V + \mu^s$ with μ^s singular with respect to the Lebesgue measure and with $\mu^s\big(\{V = +\infty\}\big) = 0$, by the monotonicity of Ψ and by the fact that $W \le V$ we obtain

$$\int_D \Psi(V)\,dx \le \int_D \Psi(W)\,dx \le 1,$$

which shows that $V \in \mathcal{V}$. □

Existence of optimal potentials. The relaxed problem associated to (1.1) is

$$\min\left\{ \int_D g(x)u(x)\,dx \ :\ -\Delta u + \mu u = f,\ u \in H^1_0(D) \cap L^2(\mu),\ \mu \in \overline{\mathcal{V}} \right\}. \tag{2.2}$$

Since the class of capacitary measures is known to be compact with respect to the γ convergence, the relaxed problem (2.2) admits a solution $\mu \in \overline{\mathcal{V}}$. We aim to show that we can actually find a solution in the original admissible class $\mathcal{V}$. We start by a lemma which shows that the cost functional is analytic.

Lemma 2.4. *Suppose that μ and ν are two capacitary measures such that $\nu \le \mu$. Then the function*

$$\phi(t) := \int_D R_{\mu+t\nu}(f) g\,dx$$

is analytic on $(-1,+\infty)$ *and, for every* $t\in(-1,1)$,

$$\phi(t)=\int_D R_\mu(f)g\,dx+\sum_{k=1}^{\infty}(-1)^k t^k\int_D R_\mu(f)g_k\,d\nu, \tag{2.3}$$

where $g_1=R_\mu(g)$ *and, for* $k\geq 1$, $g_{k+1}=R_\mu(g_k\nu)$.

Proof. We set for the sake of simplicity $u_t:=R_{\mu+t\nu}(f)$. Now, since $L^2(\mu)=L^2(\mu+t\nu)$ for $t\in(-1,+\infty)$, we have that $u_t=R_\mu(f-t\nu u_t)$, where the right-hand side is well defined, again by Remark 2.1. We first claim that for every $n\geq 1$ we have

$$\phi(t)=\int_D R_\mu(f)g\,dx+\sum_{k=1}^{n}(-1)^k t^k\int_D R_\mu(f)g_k\,d\nu+(-1)^{n+1}t^{n+1}\int_D u_t g_{n+1}\,d\nu. \tag{2.4}$$

We argue by induction. The claim for $n=1$ holds, since by Remark 2.2 we have

$$\begin{aligned}\phi(t)&=\int_D R_\mu(f-t\nu u_t)g\,dx=\int_D (f-t\nu u_t)R_\mu(g)=\int_D fR_\mu(g)\,dx-t\int_D u_tR_\mu(g)\,d\nu\\&=\int_D fR_\mu(g)\,dx-t\int_D R_\mu(f-t\nu u_t)R_\mu(g)\,d\nu\\&=\int_D fR_\mu(g)\,dx-t\int_D R_\mu(f)R_\mu(g)\,d\nu+t^2\int_D R_\mu(\nu u_t)R_\mu(g)\,d\nu\\&=\int_D fR_\mu(g)\,dx-t\int_D R_\mu(f)R_\mu(g)\,d\nu+t^2\int_D R_\mu(R_\mu(g)\nu)u_t\,d\nu.\end{aligned}$$

In order to get the claim for every n, we notice that

$$\int_D u_tg_{n+1}\,d\nu=\int_D R_\mu(f-t\nu u_t)g_{n+1}\,d\nu=\int_D R_\mu(f)g_{n+1}\,d\nu-t\int_D u_tR_\mu(g_{n+1}\nu)\,d\nu,$$

which, together with the relation $g_{n+2}=R_\mu(g_{n+1}\nu)$, concludes the proof of (2.4).

We now claim that for every $n\geq 1$ we have $\|g_{n+1}\|_{L^2(\mu)}\leq\|g_n\|_{L^2(\mu)}$. Indeed, by the defintion of $g_{n+1}=R_\mu(g_n\nu)$ we get that

$$\begin{aligned}\|g_{n+1}\|^2_{L^2(\mu)}&\leq\int_D|\nabla g_{n+1}|^2\,dx+\int_D g_{n+1}^2\,d\mu=\int_D g_ng_{n+1}\,d\nu\\&\leq\|g_{n+1}\|_{L^2(\nu)}\|g_n\|_{L^2(\nu)}\leq\|g_{n+1}\|_{L^2(\mu)}\|g_n\|_{L^2(\mu)},\end{aligned}$$

where in the last inequality we used that $\nu\leq\mu$. In particular, this implies that the radius of convergence of the series in the right-hand side of (2.3) is at least one.

We now claim that ϕ is analytic on $(-1,1)$ and that (2.3) holds for $t\in(-1,1)$. Indeed, it is sufficient to estimate the last term in the right-hand side of the Taylor expansion (2.4). To do so, we notice that for every $\delta\in(0,1)$ and $|t|\leq 1-\delta$ we have that $\mu+t\nu\geq\delta\mu$ and

$$\delta\|u_t\|^2_{L^2(\mu)}\leq\int_D|\nabla u_t|^2\,dx+\int_D u_t^2\,d(\mu+t\nu)=\int_D u_tf\,dx\leq\|u_t\|_{L^2}\|f\|_{L^2}\leq C\|\nabla u_t\|_{L^2}\|f\|_{L^2},$$

where C is the constant from the Poincaré inequality on D. We deduce that

$$\|\nabla u_t\|_{L^2}\leq C\|f\|_{L^2}\qquad\text{and}\qquad\|u_t\|_{L^2(\mu)}\leq\frac{C\|f\|_{L^2}}{\sqrt{\delta}},$$

and we can estimate the error in (2.4) as

$$\int_D u_tg_{n+1}\,d\nu\leq\|u_t\|_{L^2(\mu)}\|g_{n+1}\|_{L^2(\mu)}\leq\frac{C\|f\|_{L^2}}{\sqrt{\delta}}\|g_1\|_{L^2(\mu)},$$

which implies that (2.3) holds for $t\in(-1,1)$. In order to conclude the proof of the lemma, it is sufficient to notice that, by the same argument as above, the function ϕ is analytic on every interval $\left(\frac{n-1}{2},\frac{n+1}{2}\right)$, $n\in\mathbb{N}$. □

We are now in a position to prove the existence of an optimal potential in the original class $\mathcal{V}$.

Theorem 2.5. *Let $D \subset \mathbb{R}^d$ be a bounded open set and let Ψ satisfy the assumptions i) and ii) above. Then, for every $f, g \in L^2(D)$, the optimization problem* (1.1) *has a solution.*

Proof. Let $\mu \in \overline{\mathcal{V}}$ be a solution of the relaxed problem (2.2). Then, by Lemma 2.3 μ is of the form $V + \mu_s$, where $V \in \mathcal{V}$, μ^s singular with respect to the Lebesgue measure and $\mu^s\big(\{V = +\infty\}\big) = 0$. Notice that we can assume

$$\{R_\mu(f) = 0\} \cap \{R_\mu(g) = 0\} = \{V = +\infty\},$$

by setting $\mu = +\infty$ on the set $\{R_\mu(f) = 0\} \cap \{R_\mu(f) = 0\}$. This capacitary measure is still admissible by the monotonicity of the function Ψ and has the same cost functional. Now, by the optimality of μ and Lemma 2.4, with $\nu = \varphi\mu^s$ for some continuous function $0 \le \varphi \le 1$, we get that the function $\phi(t)$ attains its minimum for $t = 0$. Thus,

$$\phi'(0) = \int_D R_\mu(f) R_\mu(g) \varphi \, d\mu_s = 0,$$

and since φ is arbitrary we get

$$R_\mu(f) R_\mu(g) = 0 \quad \mu^s - \text{almost everywhere}.$$

Now let $\nu_f := 1_{\{R_\mu(f) \neq 0\}} \mu^s$ and $\nu_g := 1_{\{R_\mu(g) \neq 0\}} \mu^s$. Thus $\mu_s = \nu_f + \nu_g$.

Applying again Lemma 2.4, this time to $\nu = \nu_g$ (and also to $\nu = \nu_f$), we obtain that $R_\mu(f)\, d\nu_g \equiv 0$ (and analogously $R_\mu(g)\, d\nu_f \equiv 0$) and so, the analytic function ϕ is identically zero. In particular,

$$\int_D R_\mu(f) g \, dx = \int_D R_{\mu + t\nu_g}(f) g \, dx, \quad \text{for every} \quad t \ge 0.$$

Thus, $\mu + t\nu_g$ is still optimal and applying again Lemma 2.4 to $\mu + t\nu_g$ and ν_f we get that

$$\int_D R_\mu(f) g \, dx = \int_D R_{(\mu + t\nu_g) + t\nu_f}(f) g \, dx = \int_D R_{\mu + t\mu_s}(f) g \, dx, \quad \text{for every} \quad t \ge 0.$$

Passing to the limit as $t \to \infty$, we get that $\mu + t\mu^s$ γ-converges to the measure $V = \mu + (+\infty)\mu^s = \mu + (+\infty) 1_{\{R_\mu(f) R_\mu(g) = 0\}}$, which belongs to the admissible class $\mathcal{V}$. Thus, V is a solution of the original problem (1.1). □

3. Necessary conditions of optimality

We start by a Lemma which applies to a general optimal capacitary measure μ.

Lemma 3.1. *Let μ be a capacitary measure in the bounded domain $D \subset \mathbb{R}^d$. Then, there is a constant C, depending only on D, such that if $\varphi : D \to \mathbb{R}$ satisfies $\|\varphi\|_{L^\infty} \le C$, then the function $\varepsilon \mapsto \int_D R_{\mu + \varepsilon\varphi}(f) g \, dx$ is differentiable in zero and*

$$\frac{d}{d\varepsilon}\Big|_{\varepsilon = 0} \int_D R_{\mu + \varepsilon\varphi}(f) g \, dx = -\int_D R_\mu(f) R_\mu(g) \varphi(x) \, dx. \tag{3.1}$$

Proof. For every $\varepsilon > 0$ let $\mu_\varepsilon = \mu + \varepsilon\varphi$. Let $u = R_\mu(f)$ and u_ε denote the solutions of

$$\begin{aligned} &-\Delta u + \mu u = f \text{ in } D, \qquad u \in H^1_0(D) \cap L^2(\mu), \\ &-\Delta u_\varepsilon + \mu_\varepsilon u_\varepsilon = f \text{ in } D, \qquad u_\varepsilon \in H^1_0(D) \cap L^2(\mu_\varepsilon), \end{aligned}$$

where we notice that in order to have a solution of the second equation we have to choose C to be smaller than the first eigenvalue of the Dirichlet Laplacian on the domain D. Thus, $H^1_0(D) \cap L^2(\mu_\varepsilon) = H^1_0(D) \cap L^2(\mu)$ and, setting $w_\varepsilon = (u_\varepsilon - u)/\varepsilon$, we have

$$-\Delta w_\varepsilon + \mu w_\varepsilon = -\varphi u_\varepsilon, \qquad w_\varepsilon \in H^1_0(D) \cap L^2(\mu), \tag{3.2}$$

and

$$\frac{1}{\varepsilon}\left(\int_D R_{\mu + \varepsilon\varphi}(f) g \, dx - \int_D R_\mu(f) g \, dx \right) = \int_D g(x) w_\varepsilon(x) \, dx \, .$$

Since μ_ε is γ-converging to μ we have that u_ε tends to u in $L^2(D)$ and, by (3.2) we obtain that w_ε tends to w in $L^2(D)$, where w solves

$$-\Delta w + \mu w = -\varphi u \quad \text{in} \quad D, \qquad u \in H^1_0(D) \cap L^2(\mu)\ .$$

Since the resolvent operator R_μ of $-\Delta + \mu$ is self-adjoint, we have

$$\frac{d}{d\varepsilon}\Big|_{\varepsilon=0} \int_D R_{\mu+\varepsilon\varphi}(f) g\, dx = \int_D g(x) w(x)\, dx = \int_D g(x) R_\mu(-\varphi u)\, dx = -\int_D R_\mu(g)\varphi u\, dx,$$

which concludes the proof. □

The above Lemma allows us to deduce several optimality conditions for both the solutions of the relaxed problem (2.2) and of the original problem (1.1).

Proposition 3.2. *Suppose that μ is a solution of the relaxed optimization problem* (2.2) *on the bounded domain $D \subset \mathbb{R}^d$. Then*

$$R_\mu(f) R_\mu(g) \le 0 \quad \textit{a.e. on } D. \tag{3.3}$$

Moreover, the above inequality holds quasi-everywhere on D.

Proof. Let μ be a solution of the relaxed optimization problem (2.2). In particular, $\mu \in \overline{\mathcal{V}}$, so there is a sequence $V_n \in \mathcal{V}$ which γ-converges to μ. Let $\varphi : D \to \mathbb{R}^+$ be a bounded non-negative function and $\varepsilon \ge 0$. By the monotonicity of Ψ, we have that $\int_D \Psi(V_n + \varepsilon\varphi)\, dx \le \int_D \Psi(V_n)\, dx \le 1$. Thus $V_n + \varepsilon\varphi \in \mathcal{V}$. Now since $V_n + \varepsilon\varphi$ γ-converges to $\mu + \varepsilon\varphi$, we get that $\mu + \varepsilon\varphi \in \overline{\mathcal{V}}$. In particular, we have that

$$\frac{d}{d\varepsilon}\Big|_{\varepsilon=0} \int_D R_{\mu+\varepsilon\varphi}(f) g\, dx = \int_D g(x) w(x)\, dx = -\int_D R_\mu(g) R_\mu(f)\varphi\, dx \ge 0,$$

and since φ is arbitrary, we obtain (3.3). Finally, the last claim is a consequence of a standard argument since $R_\mu(f)$ and $R_\mu(g)$ are Sobolev functions. □

Remark 3.3 (An optimality condition for the optimal potentials). Proposition 3.2 allows us to obtain the following necessary condition for a potential V solution of the optimization problem (1.1), whose existence follows from Theorem 2.5. We have

$$R_V(f) R_V(g) \le 0 \quad \text{a.e. on} \quad D. \tag{3.4}$$

Indeed, the optimal potential V solves also the relaxed problem (2.2), hence Proposition 3.2 applies.

Saturation of the constraint. Let $V \in \mathcal{V}$ be a solution of (1.1). In general, one cannot expect that the constraint $\int_D \Psi(V)\, dx \le 1$ is saturated (see for example [11] for the case of shape optimization problems). In this case however, we may obtain that the optimal potential V can be reduced to be a domain Ω, that is $V = 0$ on Ω and $V = +\infty$ on Ω^c. Indeed, suppose that $\int_D \Psi(V)\, dx < 1$, consider the set $\{\delta \le V \le 1/\delta\}$ for some $\delta \ge 0$, and a bounded function $\varphi : \{\delta \le V \le 1/\delta\} \to \mathbb{R}$. Thus, for ε small enough, the function $V + \varepsilon\varphi$ is admissible. Now since δ and φ are arbitrary, we get by Lemma 3.1

$$R_V(f) R_V(g) = 0 \quad \text{a.e. on} \quad \{0 < V < +\infty\}. \tag{3.5}$$

Now, arguing as in the proof of Theorem 2.5 we get that the potential $+\infty \cdot V$ (see (3.6)) is also a solution of (1.1). We also notice that $+\infty \cdot V$ can be replaced by a quasi-open set. Indeed, by the general theory of Sobolev spaces on measurable domains (see [6]), we know there is a quasi-open set $\Omega \subset \{V = 0\}$ (the inclusion holds up to a set of zero capacity) such that $H^1_0(\Omega) = H^1_0(\{V = 0\})$, which means that the potentials

$$+\infty \cdot V := \begin{cases} 0 & \text{on } \{V = 0\} \\ +\infty & \text{on } \{V > 0\} \end{cases} \qquad \text{and} \qquad V_\Omega := \begin{cases} 0 & \text{on } \Omega \\ +\infty & \text{on } \Omega^c \end{cases} \tag{3.6}$$

generate the same Sobolev space and so have the same cost functional, while the constraint (1.2) remains clearly satisfied by V_Ω that is

$$\int_D gR_{V_\Omega}(f)\,dx = \int_D gR_V(f)\,dx \qquad \text{and} \qquad \int_D \Psi(V_\Omega)\,dx \le \int_D \Psi(V)\,dx. \tag{3.7}$$

This fact have several important consequences, which we describe below.

Remark 3.4. Let Ψ be the function describing the admissible constraint $\mathcal{V}$ in (1.2). Then we consider two cases:

• If $\Psi(0) = +\infty$, which occurs for instance in the case $\Psi(s) = s^{-p}$ with $p > 0$, then (see Proposition 3.5 below) we obtain that either there exists an optimal potential V which saturates the constraint, or $V \equiv +\infty$ is a solution (corresponding to the domain $\Omega = \emptyset$).

• On the contrary, if $\Psi(0) < +\infty$, which for instance occurs in the case $\Psi(s) = e^{-\alpha s}$ with $\alpha > 0$, we have (see Proposition 3.6 below) that either an optimal potential V saturates the constraint, or we have an optimal solution which is a domain, that is a potential V assuming only the values 0 and $+\infty$.

We now give the precise statements of the results in the Remark above.

Proposition 3.5. *Suppose that $\Psi : [0,+\infty] \to [0,+\infty]$ satisfies the conditions (i) and (ii), and is such that $\Psi(0) = +\infty$. Suppose, moreover, that the minimum value of* (1.1) *is non-zero. Then for every solution V of* (1.1) *the constraint is saturated, $\int_D \Psi(V)\,dx = 1$. Moreover, if Ψ is differentiable with $\Psi' < 0$, then there is a non-zero Lagrange multiplier $\Lambda \in \mathbb{R}$ such that*

$$R_V(f)R_V(g) = \Lambda\Psi'(V) \quad \textit{a.e. on the set} \quad \{0 < V < +\infty\}.$$

Proof. Let V be an optimal potential, for which the constraint is not saturated, and let Ω be as in (3.6). Then V_Ω is still a solution of (1.1). On the other hand, again by (3.7), $\int_{\{V=0\}} \Psi(0)\,dx \le \int_D \Psi(+\infty \cdot V)\,dx \le 1$ and, since $\Psi(0) = +\infty$, we get that $|\{V = 0\}| = 0$. This means that $\Omega = \emptyset$ and thus the minimum value of (1.1) is zero, which concludes the proof of the first part of the Proposition. For the last claim, it is sufficient to notice that on the set $\{0 < V < +\infty\}$ the constraint is differentiable, so the existence of the Lagrange multiplier on this set follows by a classical result. □

Proposition 3.6. *Suppose that $\Psi : [0,+\infty] \to [0,+\infty]$ satisfies the conditions (i) and (ii), and is such that $\Psi(0) < +\infty$. Let V be a solution of* (1.1) *for which the constraint is not saturated: $\int_D \Psi(V)\,dx < 1$. Then the quasi-open set Ω from* (3.6) *solves the shape optimization problem*

$$\min\Big\{\int_D gR_\Omega(f)\,dx \ : \ \Omega \subset D,\ |\Omega| \le C_\Psi\Big\}, \quad \textit{where} \quad C_\Psi := \frac{1 - |D|\Psi(+\infty)}{\Psi(0) - \Psi(+\infty)}. \tag{3.8}$$

Proof. The fact that Ω solves (3.8) follows since V_Ω is a solution (1.1), which in turn is a consequence of (3.7). Notice that the constraint $|\Omega| \le C_\Psi$ corresponds to the bound

$$1 \ge \int_D \Psi(V_\Omega)\,dx = |\Omega|\Psi(0) + |D \setminus \Omega|\Psi(+\infty). \qquad \square$$

4. Some numerical simulations

In this section we present and show a numerical method in order to solve a problem of the kind of (1.1). We would like to introduce some numerical experiments which let us understand some qualitative properties of the optimizers and underline the phenomenon of the non saturation of the volume constraint.

We start showing how to get a gradient descent direction. Later we describe an algorithm for the optimization problem and finally we show some numerical experiments for some function g and different choices of the function f which have non-constant sign, and diverse functions $\Psi(V) = \exp(-\alpha V)/m$ for different values of $\alpha > 0$ and $m \in (0,1)$ in order to impose different volume constraints.

4.1. **First derivative.** Our goal is to solve numerically minimization problems of the form (1.1):

$$\min\Big\{\int_D g(x)u(x)\,dx \;:\; \int_D e^{-\alpha V(x)}\,dx \le m\Big\}, \tag{4.1}$$

where $\alpha > 0$ and $m > 0$ are given, u is the solution of the state equation

$$-\Delta u + Vu = f \quad \text{in} \quad D, \qquad u = 0 \quad \text{on} \quad \partial D, \tag{4.2}$$

and the optimal potential $V : D \to [0, +\infty]$ is a Lebesgue measurable function. In the case of shape optimization problems a domain $\Omega \subset D$ is associated to the potential V_Ω defined in (3.6), so that

$$|\Omega| = \int_D e^{-\alpha V_\Omega(x)}\,dx.$$

We start with the computation of the derivative of the cost functional (4.1) with respect to V, in order to apply a optimization algorithms (see, for instance, [1] and [15]). This part is standard but we consider the computation of the derivative is necessary in order to apply the optimization algorithms in the next section. We show it for completeness.

Let us assume V and V' two admissible potentials and let us compute *formally* the derivative of the cost functional

$$I(V) = \int_D g(x)u(x)\,dx$$

at the position V in the direction V'. By applying Lemma 3.1 we obtain

$$\frac{dI(V)}{dV}\cdot V' = \int_D V'(x)u(x)p(x)\,dx, \tag{4.3}$$

where p is the unique solution of the adjoint equation

$$-\Delta p + Vp = -g \quad \text{in} \quad D, \qquad p = 0 \quad \text{on} \quad \partial D. \tag{4.4}$$

Then, taking into account formula (4.3), in order to apply a gradient descent method it is enough to take the direction

$$V'(x) = -u(x)p(x).$$

In order to take into account the volume constraint on V, we introduce the Lagrange multiplier $\lambda \in \mathbb{R}$ and the functional

$$I_\lambda(V) = I(V) + \lambda \int_D e^{-\alpha V(x)}\,dx$$

and therefore,

$$\frac{dI_\lambda(V)}{dV}\cdot V' = \int_D V'(x)\left(u(x)p(x) - \lambda\alpha e^{-\alpha V(x)}\right)dx, \tag{4.5}$$

where the multiplier λ is determined in order to ensure the constraint $\int e^{-\alpha V(x)}\,dx \le m$.

Thus, a general gradient algorithm to solve numerically the extremal problem (4.1) - (4.2) is the following:

- Initialization: choose an admissible V_0;
- for $k \ge 0$, iterate until convergence as follows:
  - compute u_k solution of (4.2) and p_k solution of (4.4), both corresponding to $V = V_k$;
  - compute the associated descent direction V_k' given by (4.5) associated to u_k and p_k;
  - update the potential V_k:

    $$V_{k+1} = V_k + \eta_k V_k',$$

    with η_k small enough to ensure the decrease of the cost function.

4.2. **Numerical Simulations.** For our numerical experiments we decided to use the free software FreeFEM++ v 3.50 (see [13] and `http://www.freefem.org`), complemented with the library NLopt (see `http://ab-initio.mit.edu/wiki/index.php/NLopt`) with the use of the Method of Moving Asymptotes (MMA) as optimizing routing (see [16]). MMA is a method for non-linear programming in general and structural optimization in particular, having very effective results for this kind of problems. Moreover, this effective method has relevant results in problems of different nature, in [3] MMA is applied by the authors to a close problem having very interesting results. The MMA technique is a gradient method based on a spatial type of convex approximation where in each iteration a strictly convex approximation subproblem is generated. For the implementation of this algorithm the main required data are the initialization V_0, the associated routines to the cost and volume function and the associated routines to the gradient of the cost and volume function using the adjoint state (we will use the derivatives computed in the previous Subsection 4.1). The admissible potentials V take values in $[0, +\infty]$ but from the numerical point of view it is advisable to constrain V to take values on a bounded interval $[0, V_{max}]$, with V_{max} large enough. These data are required for the algorithm too. We observe that, when V takes its maximal value V_{max}, the state u is very small and practically vanishes, according to the well-posed character of the extremal problem and the state equation. This is consistent with the necessary conditions of optimality obtained in Section 3.

We show the numerical result for some experiments. We have made the simulations in the two dimensional case and we have chosen $D = (0, 1) \times (0, 1)$. The optimization criterion we consider is the minimization of the average solution $u = R_V(f)$ on D for a given right-hand side f, where the potential V varies in the admissible class

$$\mathcal{V} = \left\{ V \geq 0, \ \int_D e^{-\alpha V(x)} \, dx \leq m \right\}.$$

Therefore, in the following we take $g = 1$ and we consider various choices for f and for the parameters α and m. It has to be noticed that, if $f \geq 0$, by the maximum principle all the solutions u are nonnegative, so that the optimization problem has the trivial solution $V = +\infty$ for which the corresponding state is $u = 0$.

We use a P_2-Lagrange finite element approximations for u and p, solutions of the state and co-state equations (4.2) and (4.4) respectively, and P_0-Lagrange finite element approximations for the potential V. In our simulations we have considered $V_{max} = 10^4$ and a regular mesh of 200×200 elements, see Figure 1 left. We analyze different cases. For the optimal potential representation we use a grey scale, where black corresponds to 0 value and white to V_{max}.

The first case we consider is when $f(x, y) = -(1 + 10x)$ (see Figure 1 right) and $m = 0.2$. We expect that the optimal potential consists of a quasi-ellipsoid-shape placed on the region where the values of the function f are smaller. For this case we make two different experiments for various values of the parameter α related to the volume constraint. In Figure 2 left, we have used $\alpha = 0.01$ while in Figure 2 right we have used $\alpha = 3.10^{-4}$. We can observe that in the first case the optimal potential V_{opt} is distributed on all the domain D, while in the second case (when α is small enough) the optimal potential is very close to an optimal shape.

In the subsequent numerical experiments we fix $\alpha = 3.10^{-4}$ in order to recover optimal shapes, and we consider various functions f for the right-hand side of the state equation, where f changes its sign.

In Figure 3 we show the cost evolution in the Example 1, case $\alpha = 3.10^{-4}$ (the figure for the other examples are similar). With this picture we observe the convergence history to a minimum. The lack of strict convexity of the problem does not guarantee the uniqueness of solution for the optimization problem, and the possible existence of local minima. From the numerical point of view, in order to avoid these local minima we have run the problem for different initial values of V, but for all the cases the algorithm recover the same optimal solution.

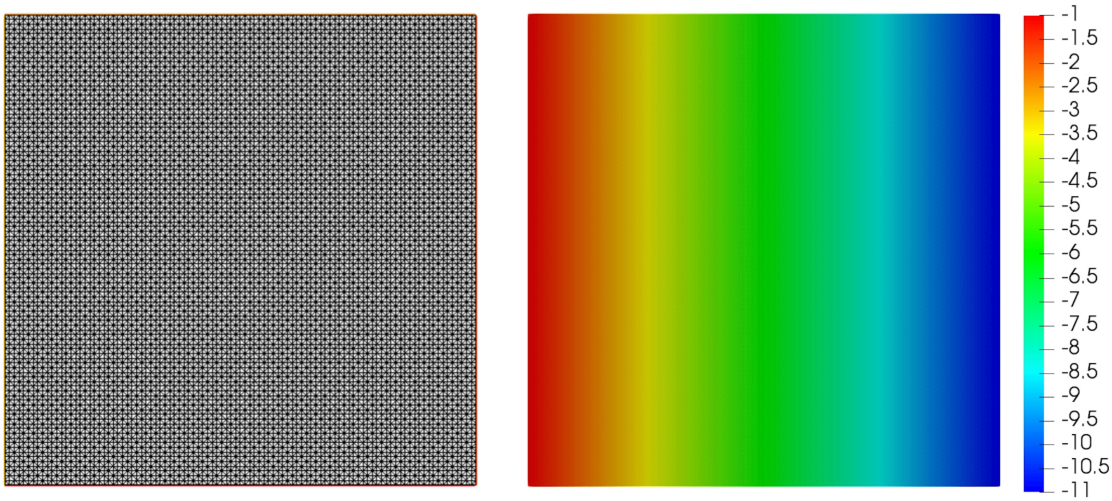

FIGURE 1. To the left: the domain D and its triangulation; number of nodes: 40401; number of triangles: 80000. To the right: the right-hand side function $f(x, y) = -(1 + 10x)$.

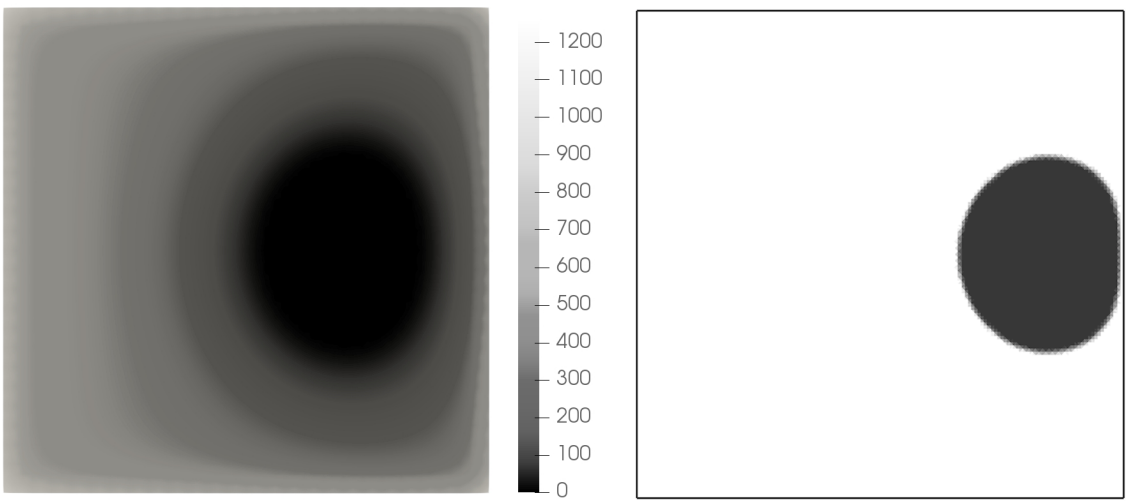

FIGURE 2. Example 1 – The optimal potential V_{opt} for volume constraint $m = 0.2 = m_{opt}$. Case $\alpha = 0.01$ (left) and $\alpha = 3.10^{-4}$ (right).

For the Example 2 we consider the right-hand side function:

$$f(x, y) = \begin{cases} -1 & \text{if } y - 1.4x \geq 0.3 \\ 1 & \text{if } y - 1.4x < 0.3 \end{cases}$$

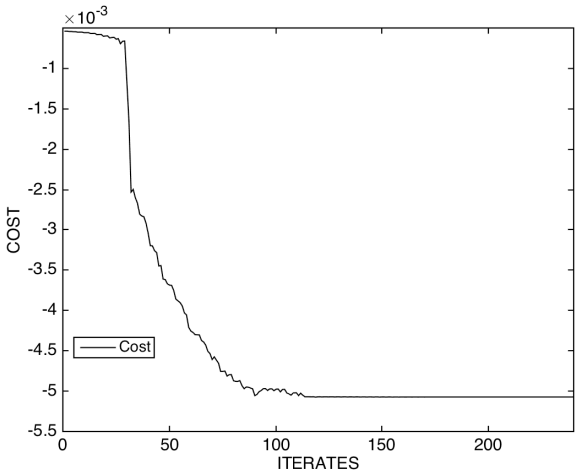

FIGURE 3. Cost evolution for Example 1, case $\alpha = 3.10^{-4}$.

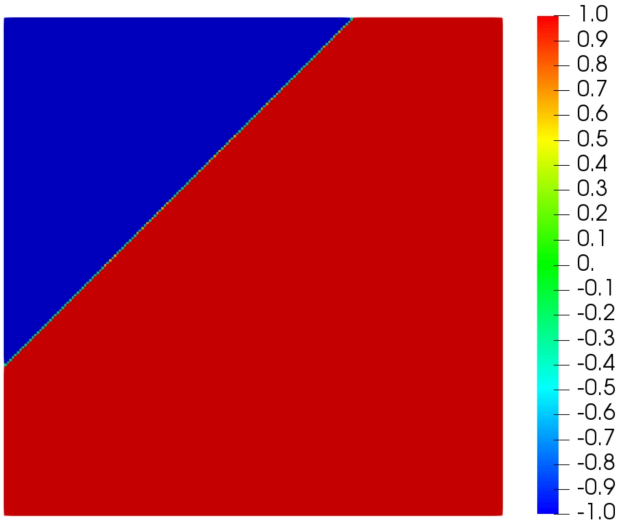

FIGURE 4. The right-hand side function $f(x, y) = -1$ if $y - 1.4x \geq 0.3$, and $f(x, y) = 1$ if $y - 1.4x < 0.3$

negative on a corner of the domain D, and positive on the rest (see Figure 4). In this case, we make two simulations with volume constraints $m = 0.2$ (small volume) and $m = 0.45$ (larger volume). In both cases we observe that the optimal shapes are placed near the corner where the function f is negative (see Figure 5). However, in the case of small volume constraint the optimal domain Ω_{opt} has volume equal to m (saturation of the constraint, see Figure 5 left), while in the case of larger m the optimal domain satisfies $|\Omega_{opt}| < m$ (see Figure 5 right). For instance, in the case under consideration, the optimal domain uses only 0.33276 of the volume, of the 0.45 available.

For the Example 3 the right-hand side function which we consider is a characteristic function which takes the values 1 on a centered non-symmetric cross and -1 on the rest of the domain D (see Figure 6 left). In this case we have imposed a volume constraint $m = 0.45$ and we observe (see Figure 6 right) that the optimal shape is made of four small balls of different sizes at the corners of the square domain outside of the cross and the volume constraint is saturated.

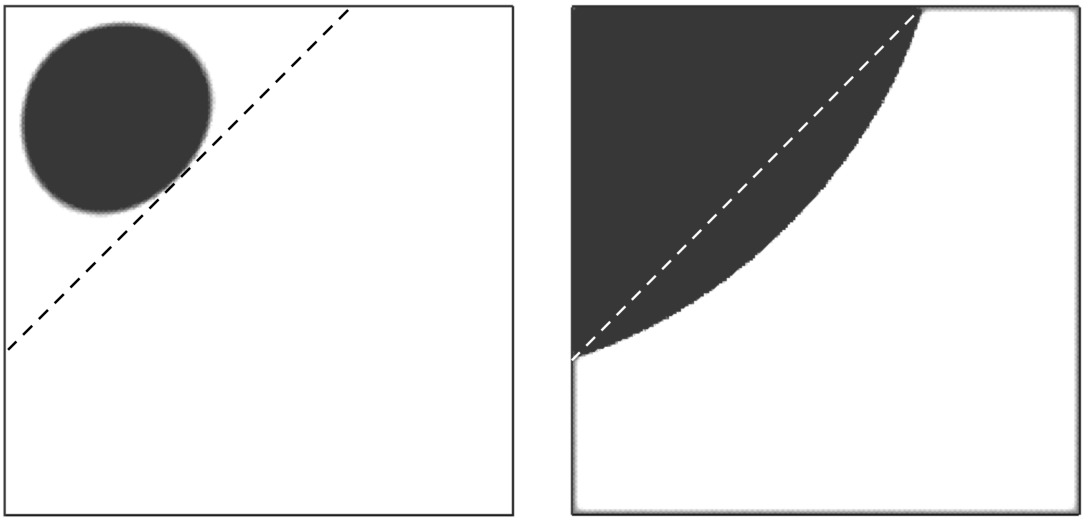

FIGURE 5. Example 2 – Optimal potential V_{opt}. Case: $m = 0.2$ (left), $m = 0.45$ occupied volume 0.33276 (right).

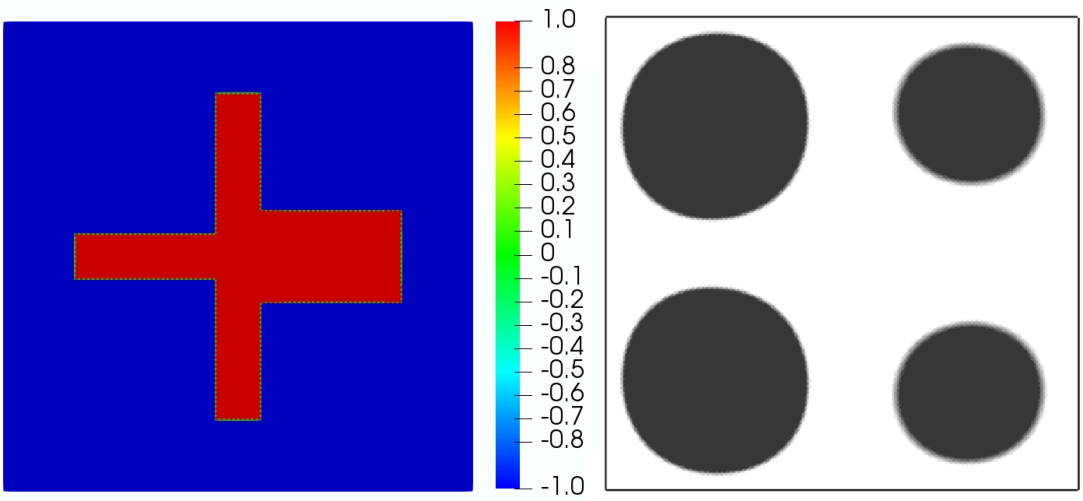

FIGURE 6. Example 3 – The right-hand side function f (left) and the optimal potential V_{opt} (right). The volume $m = 0.45$ is all occupied.

Finally, in the Example 4 we consider for the right-hand side f the reverse case of the Example 3. We consider a characteristic function, which on a centered non-symmetric cross takes the value -1 and 1 on the rest of the domain (see Figure 7 left). For this simulation the results give an optimal shape that is placed around the cross, including regions where f is negative but also small areas around the cross where f is positive. The volume constraint in this case is not saturated using 0.378404 of the $m = 0.5$ available.

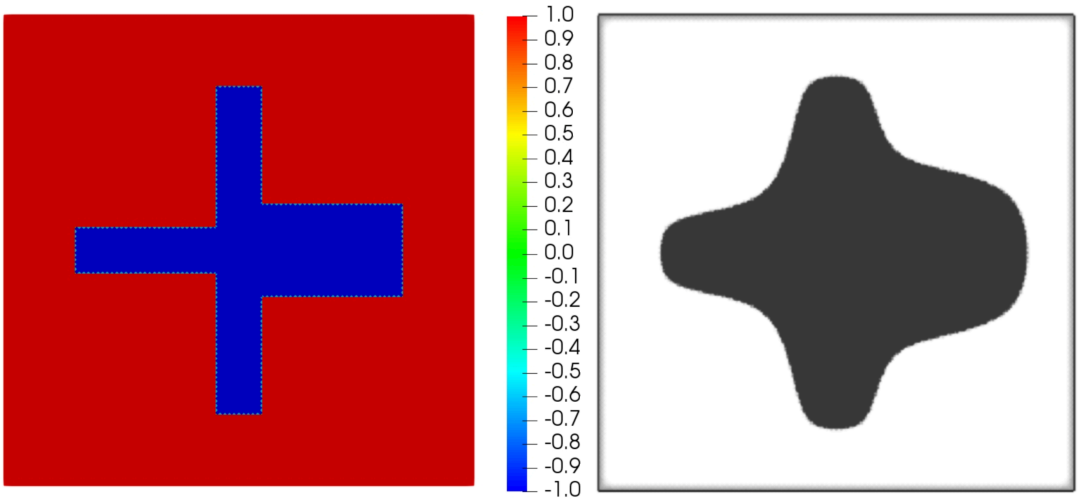

FIGURE 7. Example 4 – The right-hand side function f (left) and the optimal potential V_{opt} (right). The occupied volume is 0.378404 of the $m = 0.5$ available.

In conclusion, according to the previous results we have shown the numerical evidence that the optimization problems in the form of (1.1) admit optimal solutions when the data f and g are allowed to change sign. We can observe that in order to approximate the shape optimization problem with Dirichlet condition on the free boundary, taking the function $\Psi(s) = e^{-\alpha s}$, with α small enough, is a good choice in order to obtain optimal shapes. Moreover, we can observe that the optimal shapes are located mostly in areas where the sign of f is negative but they may in some cases occupy also small regions where f is positive. Finally, the optimal domains may not always saturate the volume constraint.

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Giuseppe Buttazzo:
Dipartimento di Matematica, Università di Pisa
Largo B. Pontecorvo 5, 56127 Pisa - ITALY
`buttazzo@dm.unipi.it`
`http://www.dm.unipi.it/pages/buttazzo/`

Faustino Maestre Caballero:
Dpto. Ecuaciones Diferenciales y Análisis Numérico, Universidad de Sevilla
C/ Tarfia s/n. Aptdo 1160, 41080 Sevilla - SPAIN
`fmaestre@us.es`
`http://personal.us.es/fmaestre`

Bozhidar Velichkov:
Laboratoire Jean Kuntzmann (LJK), Université Grenoble Alpes
Bâtiment IMAG, 700 Avenue Centrale, 38401 Saint-Martin-d'Hères - FRANCE
`bozhidar.velichkov@univ-grenoble-alpes.fr`
`http://www.velichkov.it`