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Article

# Dual Variational Formulations for a Large Class of Non-Convex Models in the Calculus of Variations

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**Abstract:** This article develops dual variational formulations for a large class of models in variational optimization. The results are established through basic tools of functional analysis, convex analysis and duality theory. The main duality principle is developed as an application to a Ginzburg-Landau type system in superconductivity in the absence of a magnetic field. In the first sections, we develop new general dual convex variational formulations, more specifically, dual formulations with a large region of convexity around the critical points which are suitable for the non-convex optimization for a large class of models in physics and engineering. Finally, in the last section we present some numerical results concerning the generalized method of lines applied to a Ginzburg-Landau type equation.

## 1. Introduction

In this section we establish a dual formulation for a large class of models in non-convex optimization.

The main duality principle is applied to the Ginzburg-Landau system in superconductivity in an absence of a magnetic field.

Such results are based on the works of J.J. Telega and W.R. Bielski [2,3,13,14] and on a D.C. optimization approach developed in Toland [15].

About the other references, details on the Sobolev spaces involved are found in [1]. Related results on convex analysis and duality theory are addressed in [5–7,9,12]. Finally, similar models on the superconductivity physics may be found in [4,11].

**Remark 1.1.** *It is worth highlighting, we may generically denote*

$$\int_{\Omega} [(-\gamma \nabla^2 + K I_d)^{-1} v^*] v^* dx$$

*simply by*

$$\int_{\Omega} \frac{(v^*)^2}{-\gamma \nabla^2 + K} dx,$$

*where  $I_d$  denotes a concerning identity operator.*

*Other similar notations may be used along this text as their indicated meaning are sufficiently clear.*

*Also,  $\nabla^2$  denotes the Laplace operator and for real constants  $K_2 > 0$  and  $K_1 > 0$ , the notation  $K_2 \gg K_1$  means that  $K_2 > 0$  is much larger than  $K_1 > 0$ .*

*Finally, we adopt the standard Einstein convention of summing up repeated indices, unless otherwise indicated.*

In order to clarify the notation, here we introduce the definition of topological dual space.

**Definition 1.2** (Topological dual spaces). *Let  $U$  be a Banach space. We shall define its dual topological space, as the set of all linear continuous functionals defined on  $U$ . We suppose such a dual space of  $U$ , may be represented by another Banach space  $U^*$ , through a bilinear form  $\langle \cdot, \cdot \rangle_U : U \times U^* \rightarrow \mathbb{R}$  (here we are referring*

to standard representations of dual spaces of Sobolev and Lebesgue spaces). Thus, given  $f : U \rightarrow \mathbb{R}$  linear and continuous, we assume the existence of a unique  $u^* \in U^*$  such that

$$f(u) = \langle u, u^* \rangle_U, \forall u \in U. \quad (1)$$

The norm of  $f$ , denoted by  $\|f\|_{U^*}$ , is defined as

$$\|f\|_{U^*} = \sup_{u \in U} \{ |\langle u, u^* \rangle_U| : \|u\|_U \leq 1 \} \equiv \|u^*\|_{U^*}. \quad (2)$$

At this point we start to describe the primal and dual variational formulations.

Let  $\Omega \subset \mathbb{R}^3$  be an open, bounded, connected set with a regular (Lipschitzian) boundary denoted by  $\partial\Omega$ .

Firstly we emphasize that, for the Banach space  $Y = Y^* = L^2(\Omega)$ , we have

$$\langle v, v^* \rangle_{L^2} = \int_{\Omega} v v^* dx, \forall v, v^* \in L^2(\Omega).$$

For the primal formulation we consider the functional  $J : U \rightarrow \mathbb{R}$  where

$$\begin{aligned} J(u) &= \frac{\gamma}{2} \int_{\Omega} \nabla u \cdot \nabla u dx \\ &\quad + \frac{\alpha}{2} \int_{\Omega} (u^2 - \beta)^2 dx - \langle u, f \rangle_{L^2}. \end{aligned} \quad (3)$$

Here we assume  $\alpha > 0, \beta > 0, \gamma > 0, U = W_0^{1,2}(\Omega), f \in L^2(\Omega)$ . Moreover we denote

$$Y = Y^* = L^2(\Omega).$$

Define also  $G_1 : U \rightarrow \mathbb{R}$  by

$$G_1(u) = \frac{\gamma}{2} \int_{\Omega} \nabla u \cdot \nabla u dx,$$

$G_2 : U \times Y \rightarrow \mathbb{R}$  by

$$G_2(u, v) = \frac{\alpha}{2} \int_{\Omega} (u^2 - \beta + v)^2 dx + \frac{K}{2} \int_{\Omega} u^2 dx,$$

and  $F : U \rightarrow \mathbb{R}$  by

$$F(u) = \frac{K}{2} \int_{\Omega} u^2 dx,$$

where  $K \gg \gamma$ .

It is worth highlighting that in such a case

$$J(u) = G_1(u) + G_2(u, 0) - F(u) - \langle u, f \rangle_{L^2}, \forall u \in U.$$

Furthermore, define the following specific polar functionals specified, namely,  $G_1^* : [Y^*]^2 \rightarrow \mathbb{R}$  by

$$\begin{aligned} G_1^*(v_1^* + z^*) &= \sup_{u \in U} \{ \langle u, v_1^* + z^* \rangle_{L^2} - G_1(u) \} \\ &= \frac{1}{2} \int_{\Omega} [(-\gamma \nabla^2)^{-1}(v_1^* + z^*)](v_1^* + z^*) dx, \end{aligned} \quad (4)$$

$G_2^* : [Y^*]^2 \rightarrow \mathbb{R}$  by

$$\begin{aligned} G_2^*(v_2^*, v_0^*) &= \sup_{(u,v) \in U \times Y} \{ \langle u, v_2^* \rangle_{L^2} + \langle v, v_0^* \rangle_{L^2} - G_2(u, v) \} \\ &= \frac{1}{2} \int_{\Omega} \frac{(v_2^*)^2}{2v_0^* + K} dx \\ &\quad + \frac{1}{2\alpha} \int_{\Omega} (v_0^*)^2 dx + \beta \int_{\Omega} v_0^* dx, \end{aligned} \quad (5)$$

if  $v_0^* \in B^*$  where

$$B^* = \{v_0^* \in Y^* : 2v_0^* + K > K/2 \text{ in } \Omega\}.$$

At this point, we give more details about this calculation.

Observe that

$$\begin{aligned} G_2^*(v_2^*, v_0^*) &= \sup_{(u,v) \in U \times Y} \{ \langle u, v_2^* \rangle_{L^2} + \langle v, v_0^* \rangle_{L^2} - G_2(u, v) \} \\ &= \sup_{(u,v) \in U \times Y} \left\{ \langle u, v_2^* \rangle_{L^2} + \langle v, v_0^* \rangle_{L^2} - \frac{\alpha}{2} \int_{\Omega} (u^2 - \beta + v)^2 dx - \frac{K}{2} \int_{\Omega} u^2 dx \right\}. \end{aligned} \quad (6)$$

Defining  $w = u^2 - \beta + v$ , we have  $v = w - u^2 + \beta$ , so that

$$\begin{aligned} &G_2^*(v_2^*, v_0^*) \\ &= \sup_{(u,v) \in U \times Y} \left\{ \langle u, v_2^* \rangle_{L^2} + \langle v, v_0^* \rangle_{L^2} - \frac{\alpha}{2} \int_{\Omega} (u^2 - \beta + v)^2 dx - \frac{K}{2} \int_{\Omega} u^2 dx \right\} \\ &= \sup_{(u,w) \in U \times Y} \left\{ \langle u, v_2^* \rangle_{L^2} + \langle w - u^2 + \beta, v_0^* \rangle_{L^2} - \frac{\alpha}{2} \int_{\Omega} (w)^2 dx - \frac{K}{2} \int_{\Omega} u^2 dx \right\} \\ &= \langle \tilde{u}, v_2^* \rangle_{L^2} + \langle \tilde{w} - \tilde{u}^2 + \beta, v_0^* \rangle_{L^2} - \frac{\alpha}{2} \int_{\Omega} (\tilde{w})^2 dx - \frac{K}{2} \int_{\Omega} \tilde{u}^2 dx, \end{aligned} \quad (7)$$

where  $(\tilde{u}, \tilde{w})$  are solution of equations (optimality conditions for such a quadratic optimization problem)

$$v_0^* - \alpha \tilde{w} = 0,$$

and

$$v_2^* - (2v_0^* + K)\tilde{u} = 0,$$

and therefore

$$\tilde{w} = \frac{v_0^*}{\alpha},$$

and

$$\tilde{u} = \frac{v_2^*}{2v_0^* + K}.$$

Replacing such results into (7) we obtain

$$\begin{aligned} G^*(v_1^*, v_0^*) &= \frac{1}{2} \int_{\Omega} \frac{(v_2^*)^2}{2v_0^* + K} dx \\ &\quad + \frac{1}{2\alpha} \int_{\Omega} (v_0^*)^2 dx + \beta \int_{\Omega} v_0^* dx, \end{aligned} \quad (8)$$

if  $v_0^* \in B^*$ .

Finally,  $F^* : Y^* \rightarrow \mathbb{R}$  is defined by

$$\begin{aligned} F^*(z^*) &= \sup_{u \in U} \{ \langle u, z^* \rangle_{L^2} - F(u) \} \\ &= \frac{1}{2K} \int_{\Omega} (z^*)^2 dx. \end{aligned} \quad (9)$$

Define also

$$A^* = \{v^* = (v_1^*, v_2^*, v_0^*) \in [Y^*]^2 \times B^* : v_1^* + v_2^* - f = 0, \text{ in } \Omega\},$$

$J^* : [Y^*]^4 \rightarrow \mathbb{R}$  by

$$J^*(v^*, z^*) = -G_1^*(v_1^* + z^*) - G_2^*(v_2^*, v_0^*) + F^*(z^*)$$

and  $J_1^* : [Y^*]^4 \times U \rightarrow \mathbb{R}$  by

$$J_1^*(v^*, z^*, u) = J^*(v^*, z^*) + \langle u, v_1^* + v_2^* - f \rangle_{L^2}.$$

## 2. The main duality principle, a convex dual formulation and the concerning proximal primal functional

Our main result is summarized by the following theorem.

**Theorem 2.1.** *Considering the definitions and statements in the last section, suppose also  $(\hat{v}^*, \hat{z}^*, u_0) \in [Y^*]^2 \times B^* \times Y^* \times U$  is such that*

$$\delta J_1^*(\hat{v}^*, \hat{z}^*, u_0) = \mathbf{0}.$$

*Under such hypotheses, we have*

$$\begin{aligned} \delta J(u_0) &= \mathbf{0}, \\ \hat{v}^* &\in A^* \end{aligned}$$

and

$$\begin{aligned} J(u_0) &= \inf_{u \in U} \left\{ J(u) + \frac{K}{2} \int_{\Omega} |u - u_0|^2 dx \right\} \\ &= J^*(\hat{v}^*, \hat{z}^*) \\ &= \sup_{v^* \in A^*} \{ J^*(v^*, \hat{z}^*) \}. \end{aligned} \quad (10)$$

**Proof.** Since

$$\delta J_1^*(\hat{v}^*, \hat{z}^*, u_0) = \mathbf{0}$$

from the variation in  $v_1^*$  we obtain

$$-\frac{(\hat{v}_1^* + \hat{z}^*)}{-\gamma \nabla^2} + u_0 = 0 \text{ in } \Omega,$$

so that

$$\hat{v}_1^* + \hat{z}^* = -\gamma \nabla^2 u_0.$$

From the variation in  $v_2^*$  we obtain

$$-\frac{\hat{v}_2^*}{2\hat{v}_0^* + K} + u_0 = 0, \text{ in } \Omega.$$

From the variation in  $v_0^*$  we also obtain

$$\frac{(\hat{v}_2^*)^2}{(2\hat{v}_0^* + K)^2} - \frac{\hat{v}_0^*}{\alpha} - \beta = 0$$

and therefore,

$$\hat{v}_0^* = \alpha(u_0^2 - \beta).$$

From the variation in  $u$  we get

$$\hat{v}_1^* + \hat{v}_2^* - f = 0, \text{ in } \Omega$$

and thus

$$\hat{v}^* \in A^*.$$

Finally, from the variation in  $z^*$ , we obtain

$$-\frac{(\hat{v}_1^* + \hat{z}^*)}{-\gamma \nabla^2} + \frac{\hat{z}^*}{K} = 0, \text{ in } \Omega.$$

so that

$$-u_0 + \frac{\hat{z}^*}{K} = 0,$$

that is,

$$\hat{z}^* = Ku_0 \text{ in } \Omega.$$

From such results and  $\hat{v}^* \in A^*$  we get

$$\begin{aligned} 0 &= \hat{v}_1^* + \hat{v}_2^* - f \\ &= -\gamma \nabla^2 u_0 - \hat{z}^* + 2(v_0^*)u_0 + Ku_0 - f \\ &= -\gamma \nabla^2 u_0 + 2\alpha(u_0^2 - \beta)u_0 - f, \end{aligned} \quad (11)$$

so that

$$\delta J(u_0) = 0.$$

Also from this and from the Legendre transform proprieties we have

$$\begin{aligned} G_1^*(\hat{v}_1^* + \hat{z}^*) &= \langle u_0, \hat{v}_1^* + \hat{z}^* \rangle_{L^2} - G_1(u_0), \\ G_2^*(\hat{v}_2^*, \hat{v}_0^*) &= \langle u_0, \hat{v}_2^* \rangle_{L^2} + \langle 0, v_0^* \rangle_{L^2} - G_2(u_0, 0), \\ F^*(\hat{z}^*) &= \langle u_0, \hat{z}^* \rangle_{L^2} - F(u_0) \end{aligned}$$

and thus we obtain

$$\begin{aligned} J^*(\hat{v}^*, \hat{z}^*) &= -G_1^*(\hat{v}_1^* + \hat{z}^*) - G_2^*(\hat{v}_2^*, \hat{v}_0^*) + F^*(\hat{z}^*) \\ &= -\langle u_0, \hat{v}_1^* + \hat{v}_2^* \rangle + G_1(u_0) + G_2(u_0, 0) - F(u_0) \\ &= -\langle u_0, f \rangle_{L^2} + G_1(u_0) + G_2(u_0, 0) - F(u_0) \\ &= J(u_0). \end{aligned} \quad (12)$$

Summarizing, we have got

$$J^*(\hat{v}^*, \hat{z}^*) = J(u_0). \quad (13)$$

On the other hand

$$\begin{aligned}
 J^*(\hat{v}^*, \hat{z}^*) &= -G_1^*(\hat{v}_1^* + \hat{z}^*) - G_2^*(\hat{v}_2^*, \hat{v}_0^*) + F^*(\hat{z}^*) \\
 &\leq -\langle u, \hat{v}_1^* + \hat{z}^* \rangle_{L^2} - \langle u, \hat{v}_2^* \rangle_{L^2} - \langle 0, \hat{v}_0^* \rangle_{L^2} + G_1(u) + G_2(u, 0) + F^*(\hat{z}^*) \\
 &= -\langle u, f \rangle_{L^2} + G_1(u) + G_2(u, 0) - \langle u, \hat{z}^* \rangle_{L^2} + F^*(\hat{z}^*) \\
 &= -\langle u, f \rangle_{L^2} + G_1(u) + G_2(u, 0) - F(u) + F(u) - \langle u, \hat{z}^* \rangle_{L^2} + F^*(\hat{z}^*) \\
 &= J(u) + \frac{K}{2} \int_{\Omega} u^2 dx - \langle u, \hat{z}^* \rangle_{L^2} + F^*(\hat{z}^*) \\
 &= J(u) + \frac{K}{2} \int_{\Omega} u^2 dx - K \langle u, u_0 \rangle_{L^2} + \frac{K}{2} \int_{\Omega} u_0^2 dx \\
 &= J(u) + \frac{K}{2} \int_{\Omega} |u - u_0|^2 dx, \quad \forall u \in U.
 \end{aligned} \tag{14}$$

Finally by a simple computation we may obtain the Hessian

$$\left\{ \frac{\partial^2 J^*(v^*, z^*)}{\partial (v^*)^2} \right\} < \mathbf{0}$$

in  $[Y^*]^2 \times B^* \times Y^*$ , so that we may infer that  $J^*$  is concave in  $v^*$  in  $[Y^*]^2 \times B^* \times Y^*$ .

Therefore, from this, (13) and (14), we have

$$\begin{aligned}
 J(u_0) &= \inf_{u \in U} \left\{ J(u) + \frac{K}{2} \int_{\Omega} |u - u_0|^2 dx \right\} \\
 &= J^*(\hat{v}^*, \hat{z}^*) \\
 &= \sup_{v^* \in A^*} \{ J^*(v^*, \hat{z}^*) \}.
 \end{aligned} \tag{15}$$

The proof is complete.  $\square$

### 3. A primal dual variational formulation

In this section we develop a more general primal dual variational formulation suitable for a large class of models in non-convex optimization.

Consider again  $U = W_0^{1,2}(\Omega)$  and let  $G : U \rightarrow \mathbb{R}$  and  $F : U \rightarrow \mathbb{R}$  be three times Fréchet differentiable functionals. Let  $J : U \rightarrow \mathbb{R}$  be defined by

$$J(u) = G(u) - F(u), \quad \forall u \in U.$$

Assume  $u_0 \in U$  is such that

$$\delta J(u_0) = \mathbf{0}$$

and

$$\delta^2 J(u_0) > \mathbf{0}.$$

Denoting  $v^* = (v_1^*, v_2^*)$ , define  $J^* : U \times Y^* \times Y^* \rightarrow \mathbb{R}$  by

$$J^*(u, v^*) = \frac{1}{2} \|v_1^* - G'(u)\|_2^2 + \frac{1}{2} \|v_2^* - F'(u)\|_2^2 + \frac{1}{2} \|v_1^* - v_2^*\|_2^2 \tag{16}$$

Denoting  $L_1^*(u, v^*) = v_1^* - G'(u)$  and  $L_2^*(u, v^*) = v_2^* - F'(u)$ , define also

$$C^* = \left\{ (u, v^*) \in U \times Y^* \times Y^* : \|L_1^*(u, v_1^*)\|_{\infty} \leq \frac{1}{K} \text{ and } \|L_2^*(u, v_1^*)\|_{\infty} \leq \frac{1}{K} \right\},$$

for an appropriate  $K > 0$  to be specified.

Observe that in  $C^*$  the Hessian of  $J^*$  is given by

$$\{\delta^2 J^*(u, v^*)\} = \begin{Bmatrix} G''(u)^2 + F''(u)^2 + \mathcal{O}(1/K) & -G''(u) & -F''(u) \\ -G''(u) & 2 & -1 \\ -F''(u) & -1 & 2 \end{Bmatrix}, \quad (17)$$

Observe also that

$$\det \left\{ \frac{\partial^2 J^*(u, v^*)}{\partial v_1^* \partial v_2^*} \right\} = 3,$$

and

$$\det\{\delta^2 J^*(u, v^*)\} = (G''(u) - F''(u))^2 + \mathcal{O}(1/K) = (\delta^2 J(u))^2 + \mathcal{O}(1/K).$$

Define now

$$\hat{v}_1^* = G'(u_0),$$

$$\hat{v}_2^* = F'(u_0),$$

so that

$$\hat{v}_1^* - \hat{v}_2^* = \mathbf{0}.$$

From this we may infer that  $(u_0, \hat{v}_1^*, \hat{v}_2^*) \in C^*$  and

$$J^*(u_0, \hat{v}^*) = 0 = \min_{(u, v^*) \in C^*} J^*(u, v^*).$$

Moreover, for  $K > 0$  sufficiently big,  $J^*$  is convex in a neighborhood of  $(u_0, \hat{v}^*)$ .

Therefore, in the last lines, we have proven the following theorem.

**Theorem 3.1.** *Under the statements and definitions of the last lines, there exist  $r_0 > 0$  and  $r_1 > 0$  such that*

$$J(u_0) = \min_{u \in B_{r_0}(u_0)} J(u)$$

and  $(u_0, \hat{v}_1^*, \hat{v}_2^*) \in C^*$  is such that

$$J^*(u_0, \hat{v}^*) = 0 = \min_{(u, v^*) \in U \times [Y^*]^2} J^*(u, v^*).$$

Moreover,  $J^*$  is convex in

$$B_{r_1}(u_0, \hat{v}^*).$$

#### 4. One more duality principle and a concerning primal dual variational formulation

In this section we establish a new duality principle and a related primal dual formulation.

The results are based on the approach of Toland, [15].

##### 4.1. Introduction

Let  $\Omega \subset \mathbb{R}^3$  be an open, bounded, connected set with a regular (Lipschitzian) boundary denoted by  $\partial\Omega$ .

Let  $J : V \rightarrow \mathbb{R}$  be a functional such that

$$J(u) = G(u) - F(u), \forall u \in V,$$

where  $V = W_0^{1,2}(\Omega)$ .



Suppose  $G, F$  are both three times Fréchet differentiable convex functionals such that

$$\frac{\partial^2 G(u)}{\partial u^2} > 0$$

and

$$\frac{\partial^2 F(u)}{\partial u^2} > 0$$

$\forall u \in V$ .

Assume also there exists  $\alpha_1 \in \mathbb{R}$  such that

$$\alpha_1 = \inf_{u \in V} J(u).$$

Moreover, suppose that if  $\{u_n\} \subset V$  is such that

$$\|u_n\|_V \rightarrow \infty$$

then

$$J(u_n) \rightarrow +\infty, \text{ as } n \rightarrow \infty.$$

At this point we define  $J^{**} : V \rightarrow \mathbb{R}$  by

$$J^{**}(u) = \sup_{(v^*, \alpha) \in H^*} \{\langle u, v^* \rangle + \alpha\},$$

where

$$H^* = \{(v^*, \alpha) \in V^* \times \mathbb{R} : \langle v, v^* \rangle_V + \alpha \leq F(v), \forall v \in V\}.$$

Observe that  $(0, \alpha_1) \in H^*$ , so that

$$J^{**}(u) \geq \alpha_1 = \inf_{u \in V} J(u).$$

On the other hand, clearly we have

$$J^{**}(u) \leq J(u), \forall u \in V,$$

so that we have got

$$\alpha_1 = \inf_{u \in V} J(u) = \inf_{u \in V} J^{**}(u).$$

Let  $u \in V$ .

Since  $J$  is strongly continuous, there exist  $\delta > 0$  and  $A > 0$  such that,

$$\alpha_1 \leq J^{**}(v) \leq J(v) \leq A, \forall v \in B_\delta(u).$$

From this, considering that  $J^{**}$  is convex on  $V$ , we may infer that  $J^{**}$  is continuous at  $u$ ,  $\forall u \in V$ .

Hence  $J^{**}$  is strongly lower semi-continuous on  $V$ , and since  $J^{**}$  is convex we may infer that  $J^{**}$  is weakly lower semi-continuous on  $V$ .

Let  $\{u_n\} \subset V$  be a sequence such that

$$\alpha_1 \leq J(u_n) < \alpha_1 + \frac{1}{n}, \forall n \in \mathbb{N}.$$

Hence

$$\alpha_1 = \lim_{n \rightarrow \infty} J(u_n) = \inf_{u \in V} J(u) = \inf_{u \in V} J^{**}(u).$$

Suppose there exists a subsequence  $\{u_{n_k}\}$  of  $\{u_n\}$  such that

$$\|u_{n_k}\|_V \rightarrow \infty, \text{ as } k \rightarrow \infty.$$

From the hypothesis we have

$$J(u_{n_k}) \rightarrow +\infty, \text{ as } k \rightarrow \infty,$$

which contradicts

$$\alpha_1 \in \mathbb{R}.$$

Therefore there exists  $K > 0$  such that

$$\|u_n\|_V \leq K, \forall u \in V.$$

Since  $V$  is reflexive, from this and the Katutani Theorem, there exists a subsequence  $\{u_{n_k}\}$  of  $\{u_n\}$  and  $u_0 \in V$  such that

$$u_{n_k} \rightharpoonup u_0, \text{ weakly in } V.$$

Consequently, from this and considering that  $J^{**}$  is weakly lower semi-continuous, we have got

$$\alpha_1 = \liminf_{k \rightarrow \infty} J^{**}(u_{n_k}) \geq J^{**}(u_0),$$

so that

$$J^{**}(u_0) = \min_{u \in V} J^{**}(u).$$

Define  $G^*, F^* : V^* \rightarrow \mathbb{R}$  by

$$G^*(v^*) = \sup_{u \in V} \{\langle u, v^* \rangle_V - G(u)\},$$

and

$$F^*(v^*) = \sup_{u \in V} \{\langle u, v^* \rangle_V - F(u)\}.$$

Defining also  $J^* : V \rightarrow \mathbb{R}$  by

$$J^*(v^*) = F^*(v^*) - G^*(v^*),$$

from the results in [15], we may obtain

$$\inf_{u \in V} J(u) = \inf_{v^* \in V^*} J^*(v^*),$$

so that

$$\begin{aligned} J^{**}(u_0) &= \inf_{u \in V} J^{**}(u) \\ &= \inf_{u \in V} J(u) = \inf_{v^* \in V^*} J^*(v^*). \end{aligned} \quad (18)$$

Suppose now there exists  $\hat{u} \in V$  such that

$$J(\hat{u}) = \inf_{u \in V} J(u).$$

From the standard necessary conditions, we have

$$\delta J(\hat{u}) = \mathbf{0},$$

so that

$$\frac{\partial G(\hat{u})}{\partial u} - \frac{\partial F(\hat{u})}{\partial u} = \mathbf{0}.$$

Define now

$$v_0^* = \frac{\partial F(\hat{u})}{\partial u}.$$

From these last two equations we obtain

$$v_0^* = \frac{\partial G(\hat{u})}{\partial u}.$$

From such results and the Legendre transform properties, we have

$$\hat{u} = \frac{\partial F^*(v_0^*)}{\partial v^*},$$

$$\hat{u} = \frac{\partial G^*(v_0^*)}{\partial v^*},$$

so that

$$\delta J^*(v_0^*) = \frac{\partial F^*(v_0^*)}{\partial v^*} - \frac{\partial G^*(v_0^*)}{\partial v^*} = \hat{u} - \hat{u} = \mathbf{0},$$

$$G^*(v_0^*) = \langle \hat{u}, v_0^* \rangle_V - G(\hat{u})$$

and

$$F^*(v_0^*) = \langle \hat{u}, v_0^* \rangle_V - F(\hat{u})$$

so that

$$\begin{aligned} \inf_{u \in V} J(u) &= J(\hat{u}) \\ &= G(\hat{u}) - F(\hat{u}) \\ &= \inf_{v^* \in V^*} J^*(v^*) \\ &= F^*(v_0^*) - G^*(v_0^*) \\ &= J^*(v_0^*). \end{aligned} \tag{19}$$

#### 4.2. The main duality principle and a related primal dual variational formulation

Considering these last statements and results, we may prove the following theorem.

**Theorem 4.1.** Let  $\Omega \subset \mathbb{R}^3$  be an open, bounded, connected set with a regular (Lipschitzian) boundary denoted by  $\partial\Omega$ .

Let  $J : V \rightarrow \mathbb{R}$  be a functional such that

$$J(u) = G(u) - F(u), \forall u \in V,$$

where  $V = W_0^{1,2}(\Omega)$ .

Suppose  $G, F$  are both three times Fréchet differentiable functionals such that there exists  $K > 0$  such that

$$\frac{\partial^2 G(u)}{\partial u^2} + K > 0$$

and

$$\frac{\partial^2 F(u)}{\partial u^2} + K > 0$$

$\forall u \in V$ .

Assume also there exists  $u_0 \in V$  and  $\alpha_1 \in \mathbb{R}$  such that

$$\alpha_1 = \inf_{u \in V} J(u) = J(u_0).$$

Assume  $K_3 > 0$  is such that

$$\|u_0\|_\infty < K_3.$$

Define

$$\tilde{V} = \{u \in V : \|u\|_\infty \leq K_3\}.$$

Assume  $K_1 > 0$  is such that if  $u \in \tilde{V}$  then

$$\max \{ \|F'(u)\|_\infty, \|G'(u)\|_\infty, \|F''(u)\|_\infty, \|F'''(u)\|_\infty, \|G''(u)\|_\infty, \|G'''(u)\|_\infty \} \leq K_1.$$

Suppose also

$$K \gg \max\{K_1, K_3\}.$$

Define  $F_K, G_K : V \rightarrow \mathbb{R}$  by

$$F_K(u) = F(u) + \frac{K}{2} \int_{\Omega} u^2 dx,$$

and

$$G_K(u) = G(u) + \frac{K}{2} \int_{\Omega} u^2 dx,$$

$\forall u \in V$ .

Define also  $G_K^*, F_K^* : V^* \rightarrow \mathbb{R}$  by

$$G_K^*(v^*) = \sup_{u \in V} \{ \langle u, v^* \rangle_V - G_K(u) \},$$

and

$$F_K^*(v^*) = \sup_{u \in V} \{ \langle u, v^* \rangle_V - F_K(u) \}.$$

Observe that since  $u_0 \in V$  is such that

$$J(u_0) = \inf_{u \in V} J(u),$$

we have

$$\delta J(u_0) = \mathbf{0}.$$

Let  $\varepsilon > 0$  be a small constant.

Define

$$v_0^* = \frac{\partial F_K(u_0)}{\partial u} \in V^*.$$

Under such hypotheses, defining  $J_1^* : V \times V^* \rightarrow \mathbb{R}$  by

$$\begin{aligned} J_1^*(u, v^*) &= F_K^*(v^*) - G_K^*(v^*) \\ &\quad + \frac{1}{2\varepsilon} \left\| \frac{\partial G_K^*(v^*)}{\partial v^*} - u \right\|_2^2 + \frac{1}{2\varepsilon} \left\| \frac{\partial F_K^*(v^*)}{\partial v^*} - u \right\|_2^2 \\ &\quad + \frac{1}{2\varepsilon} \left\| \frac{\partial G_K^*(v^*)}{\partial v^*} - \frac{\partial F_K^*(v^*)}{\partial v^*} \right\|_2^2, \end{aligned} \tag{20}$$

we have

$$\begin{aligned} J(u_0) &= \inf_{u \in V} J(u) \\ &= \inf_{(u, v^*) \in V \times V^*} J_1^*(u, v^*) \\ &= J_1^*(u_0, v_0^*). \end{aligned} \quad (21)$$

**Proof.** Observe that from the hypotheses and the results and statements of the last subsection

$$J(u_0) = \inf_{u \in V} J(u) = \inf_{v^* \in V^*} J_K^*(v^*) = J_K^*(v_0^*),$$

where

$$J_K^*(v^*) = F_K^*(v^*) - G_K^*(v^*), \forall v^* \in V^*.$$

Moreover we have

$$J_1^*(u, v^*) \geq J_K^*(v^*), \forall u \in V, v^* \in V^*.$$

Also from hypotheses and the last subsection results,

$$u_0 = \frac{\partial F_K^*(v_0^*)}{\partial v^*} = \frac{\partial G_K^*(v_0^*)}{\partial v^*},$$

so that clearly we have

$$J_1^*(u_0, v_0^*) = J_K^*(v_0^*).$$

From these last results, we may infer that

$$\begin{aligned} J(u_0) &= \inf_{u \in V} J(u) \\ &= \inf_{v^* \in V^*} J_K^*(v^*) \\ &= J_K^*(v_0^*) \\ &= \inf_{(u, v^*) \in V \times V^*} J_1^*(u, v^*) \\ &= J_1^*(u_0, v_0^*). \end{aligned} \quad (22)$$

The proof is complete.

□

**Remark 4.2.** At this point we highlight that  $J_1^*$  has a large region of convexity around the optimal point  $(u_0, v_0^*)$ , for  $K > 0$  sufficiently large and corresponding  $\varepsilon > 0$  sufficiently small.

Indeed, observe that for  $v^* \in V^*$ ,

$$G_K^*(v^*) = \sup_{u \in V} \{ \langle u, v^* \rangle_V - G_K(u) \} = \langle \hat{u}, v^* \rangle_V - G_K(\hat{u})$$

where  $\hat{u} \in V$  is such that

$$v^* = \frac{\partial G_K(\hat{u})}{\partial u} = G'(\hat{u}) + K\hat{u}.$$

Taking the variation in  $v^*$  in this last equation, we obtain

$$1 = G''(u) \frac{\partial \hat{u}}{\partial v^*} + K \frac{\partial \hat{u}}{\partial v^*},$$

so that

$$\frac{\partial \hat{u}}{\partial v^*} = \frac{1}{G''(u) + K} = \mathcal{O}\left(\frac{1}{K}\right).$$

From this we get

$$\begin{aligned}\frac{\partial^2 \hat{u}}{\partial (v^*)^2} &= -\frac{1}{(G''(u) + K)^2} G'''(u) \frac{\partial \hat{u}}{\partial v^*} \\ &= -\frac{1}{(G''(u) + K)^3} G'''(u) \\ &= \mathcal{O}\left(\frac{1}{K^3}\right).\end{aligned}\tag{23}$$

On the other hand, from the implicit function theorem

$$\frac{\partial G_K^*(v^*)}{\partial v^*} = u + [v^* - G'_K(\hat{u})] \frac{\partial \hat{u}}{\partial v^*} = u,$$

so that

$$\frac{\partial^2 G_K^*(v^*)}{\partial (v^*)^2} = \frac{\partial \hat{u}}{\partial v^*} = \mathcal{O}\left(\frac{1}{K}\right)$$

and

$$\frac{\partial^3 G_K^*(v^*)}{\partial (v^*)^3} = \frac{\partial^2 \hat{u}}{\partial (v^*)^2} = \mathcal{O}\left(\frac{1}{K^3}\right).$$

Similarly, we may obtain

$$\frac{\partial^2 F_K^*(v^*)}{\partial (v^*)^2} = \mathcal{O}\left(\frac{1}{K}\right)$$

and

$$\frac{\partial^3 F_K^*(v^*)}{\partial (v^*)^3} = \mathcal{O}\left(\frac{1}{K^3}\right).$$

Denoting

$$A = \frac{\partial^2 F_K^*(v_0^*)}{\partial (v^*)^2}$$

and

$$B = \frac{\partial^2 G_K^*(v_0^*)}{\partial (v^*)^2},$$

we have

$$\frac{\partial^2 J_1^*(u_0, v_0^*)}{\partial (v^*)^2} = A - B + \frac{1}{\varepsilon} (2A^2 + 2B^2 - 2AB),$$

$$\frac{\partial^2 J_1^*(u_0, v_0^*)}{\partial u^2} = \frac{2}{\varepsilon},$$

and

$$\frac{\partial^2 J_1^*(u_0, v_0^*)}{\partial (v^*) \partial u} = -\frac{1}{\varepsilon} (A + B).$$

From this we get

$$\begin{aligned}
\det(\delta^2 J^*(v_0^*, u_0)) &= \frac{\partial^2 J_1^*(u_0, v_0^*)}{\partial (v^*)^2} \frac{\partial^2 J_1^*(u_0, v_0^*)}{\partial u^2} - \left[ \frac{\partial^2 J_1^*(u_0, v_0^*)}{\partial (v^*) \partial u} \right]^2 \\
&= 2 \frac{A-B}{\varepsilon} + 2 \frac{(A-B)^2}{\varepsilon^2} \\
&= \mathcal{O}\left(\frac{1}{\varepsilon^2}\right) \\
&\gg 0
\end{aligned} \tag{24}$$

about the optimal point  $(u_0, v_0^*)$ .

## 5. A convex dual variational formulation

In this section, again for  $\Omega \subset \mathbb{R}^3$  an open, bounded, connected set with a regular (Lipschitzian) boundary  $\partial\Omega$ ,  $\gamma > 0$ ,  $\alpha > 0$ ,  $\beta > 0$  and  $f \in L^2(\Omega)$ , we denote  $F_1 : V \times Y \rightarrow \mathbb{R}$ ,  $F_2 : V \rightarrow \mathbb{R}$  and  $G : V \times Y \rightarrow \mathbb{R}$  by

$$\begin{aligned}
F_1(u, v_0^*) &= \frac{\gamma}{2} \int_{\Omega} \nabla u \cdot \nabla u \, dx - \frac{K}{2} \int_{\Omega} u^2 \, dx \\
&\quad + \frac{K_1}{2} \int_{\Omega} (-\gamma \nabla^2 u + 2v_0^* u - f)^2 \, dx + \frac{K_2}{2} \int_{\Omega} u^2 \, dx,
\end{aligned} \tag{25}$$

$$F_2(u) = \frac{K_2}{2} \int_{\Omega} u^2 \, dx + \langle u, f \rangle_{L^2},$$

and

$$G(u, v) = \frac{\alpha}{2} \int_{\Omega} (u^2 - \beta + v)^2 \, dx + \frac{K}{2} \int_{\Omega} u^2 \, dx.$$

We define also

$$\begin{aligned}
J_1(u, v_0^*) &= F_1(u, v_0^*) - F_2(u) + G(u, 0), \\
J(u) &= \frac{\gamma}{2} \int_{\Omega} \nabla u \cdot \nabla u \, dx + \frac{\alpha}{2} \int_{\Omega} (u^2 - \beta)^2 \, dx - \langle u, f \rangle_{L^2},
\end{aligned}$$

and  $F_1^* : [Y^*]^3 \rightarrow \mathbb{R}$ ,  $F_2^* : Y^* \rightarrow \mathbb{R}$ , and  $G^* : [Y^*]^2 \rightarrow \mathbb{R}$ , by

$$\begin{aligned}
&F_1^*(v_2^*, v_1^*, v_0^*) \\
&= \sup_{u \in V} \{ \langle u, v_1^* + v_2^* \rangle_{L^2} - F_1(u, v_0^*) \} \\
&= \frac{1}{2} \int_{\Omega} \frac{(v_1^* + v_2^* + K_1(-\gamma \nabla^2 + 2v_0^*)f)^2}{(-\gamma \nabla^2 - K + K_2 + K_1(-\gamma \nabla^2 + 2v_0^*)^2)} \, dx \\
&\quad - \frac{K_1}{2} \int_{\Omega} f^2 \, dx,
\end{aligned} \tag{26}$$

$$\begin{aligned}
F_2^*(v_2^*) &= \sup_{u \in V} \{ \langle u, v_2^* \rangle_{L^2} - F_2(u) \} \\
&= \frac{1}{2K_2} \int_{\Omega} (v_2^*)^2 \, dx,
\end{aligned} \tag{27}$$

and

$$\begin{aligned} G^*(v_1^*, v_0^*) &= \sup_{(u,v) \in V \times Y} \{ \langle u, v_1^* \rangle_{L^2} - \langle v, v_0^* \rangle_{L^2} - G(u, v) \} \\ &= \frac{1}{2} \int_{\Omega} \frac{(v_1^*)^2}{2v_0^* + K} dx + \frac{1}{2\alpha} \int_{\Omega} (v_0^*)^2 dx \\ &\quad + \beta \int_{\Omega} v_0^* dx \end{aligned} \quad (28)$$

if  $v_0^* \in B^*$  where

$$B^* = \{v_0^* \in Y^* : \|v_0^*\|_{\infty} \leq K/2 \text{ and } -\gamma \nabla^2 + 2v_0^* < -\varepsilon I_d\},$$

for some small real parameter  $\varepsilon > 0$  and where  $I_d$  denotes a concerning identity operator.

Finally, we also define  $J_1^* : [Y^*]^2 \times B^* \rightarrow \mathbb{R}$ ,

$$J_1^*(v_2^*, v_1^*, v_0^*) = -F_1^*(v_2^*, v_1^*, v_0^*) + F_2^*(v_2^*) - G^*(v_1^*, v_0^*).$$

Assuming

$$K_2 \gg K_1 \gg K \gg \max\{1/(\varepsilon^2), 1, \gamma, \alpha\}$$

by directly computing  $\delta^2 J_1^*(v_2^*, v_1^*, v_0^*)$  we may obtain that for such specified real constants,  $J_1^*$  is convex in  $v_2^*$  and it is concave in  $(v_1^*, v_0^*)$  on  $Y^* \times Y^* \times B^*$ .

Considering such statements and definitions, we may prove the following theorem.

**Theorem 5.1.** *Let  $(\hat{v}_2^*, \hat{v}_1^*, \hat{v}_0^*) \in Y^* \times Y^* \times B^*$  be such that*

$$\delta J_1^*(\hat{v}_2^*, \hat{v}_1^*, \hat{v}_0^*) = \mathbf{0}$$

and  $u_0 \in V$  be such that

$$u_0 = \frac{\hat{v}_1^* + \hat{v}_2^* + K_1(-\gamma \nabla^2 + 2v_0^*)f}{K_2 - K - \gamma \nabla^2 + K_1(-\gamma \nabla^2 + 2\hat{v}_0^*)^2}.$$

Under such hypotheses, we have

$$\delta J(u_0) = \mathbf{0},$$

so that

$$\begin{aligned} J(u_0) &= \inf_{u \in V} \left\{ J(u) + \frac{K_1}{2} \int_{\Omega} (-\gamma \nabla^2 u + 2\hat{v}_0^* u - f)^2 dx \right\} \\ &= \inf_{v_2^* \in Y^*} \left\{ \sup_{(v_1^*, v_0^*) \in Y^* \times B^*} J_1^*(v_2^*, v_1^*, v_0^*) \right\} \\ &= J_1^*(\hat{v}_2^*, \hat{v}_1^*, \hat{v}_0^*). \end{aligned} \quad (29)$$

**Proof.** Observe that  $\delta J_1^*(\hat{v}_2^*, \hat{v}_1^*, \hat{v}_0^*) = \mathbf{0}$  so that, since  $J_1^*$  is convex in  $v_2^*$  and concave in  $(v_1^*, v_0^*)$  on  $Y^* \times Y^* \times B^*$ , we obtain

$$J_1^*(\hat{v}_2^*, \hat{v}_1^*, \hat{v}_0^*) = \inf_{v_2^* \in Y^*} \left\{ \sup_{(v_1^*, v_0^*) \in Y^* \times B^*} J_1^*(v_2^*, v_1^*, v_0^*) \right\}.$$

Now we are going to show that

$$\delta J(u_0) = \mathbf{0}.$$



From

$$\frac{\partial J_1^*(\vartheta_2^*, \vartheta_1^*, \vartheta_0^*)}{\partial v_2^*} = 0,$$

we have

$$-u_0 + \frac{\vartheta_2^*}{K_2} = 0,$$

and thus

$$\vartheta_2^* = K_2 u_0.$$

From

$$\frac{\partial J_1^*(\vartheta_2^*, \vartheta_1^*, \vartheta_0^*)}{\partial v_1^*} = 0,$$

we obtain

$$-u_0 - \frac{\vartheta_1^* - f}{2\vartheta_0^* + K} = 0,$$

and thus

$$\vartheta_1^* = -2\vartheta_0^* u_0 - K u_0 + f.$$

Finally, denoting

$$D = -\gamma \nabla^2 u_0 + 2\vartheta_0^* u_0 - f,$$

from

$$\frac{\partial J_1^*(\vartheta_2^*, \vartheta_1^*, \vartheta_0^*)}{\partial v_0^*} = 0,$$

we have

$$-2D u_0 + u_0^2 - \frac{\vartheta_0^*}{\alpha} - \beta = 0,$$

so that

$$\vartheta_0^* = \alpha(u_0^2 - \beta - 2D u_0). \quad (30)$$

Observe now that

$$\vartheta_1^* + \vartheta_2^* + K_1(-\gamma \nabla^2 + 2\vartheta_0^*)f = (K_2 - K - \gamma \nabla^2 + K_1(-\gamma \nabla^2 + 2\vartheta_0^*))u_0$$

so that

$$\begin{aligned} & K_2 u_0 - 2\vartheta_0^* u_0 - K u_0 + f \\ = & K_2 u_0 - K u_0 - \gamma \nabla^2 u_0 + K_1(-\gamma \nabla^2 + 2\vartheta_0^*)(-\gamma \nabla^2 u_0 + 2\vartheta_0^* u_0 - f). \end{aligned} \quad (31)$$

The solution for this last system of equations (30) and (31) is obtained through the relations

$$\vartheta_0^* = \alpha(u_0^2 - \beta)$$

and

$$-\gamma \nabla^2 u_0 + 2\vartheta_0^* u_0 - f = D = 0,$$

so that

$$\delta J(u_0) = -\gamma \nabla^2 u_0 + 2\alpha(u_0^2 - \beta)u_0 - f = 0$$

and

$$\delta \left\{ J(u_0) + \frac{K_1}{2} \int_{\Omega} (-\gamma \nabla^2 u_0 + 2\vartheta_0^* u_0 - f)^2 dx \right\} = 0,$$

and hence, from the concerning convexity in  $u$  on  $V$ ,

$$J(u_0) = \min_{u \in V} \left\{ J(u) + \frac{K_1}{2} \int_{\Omega} (-\gamma \nabla^2 u + 2\hat{v}_0^* u - f)^2 dx \right\}.$$

Moreover, from the Legendre transform properties

$$F_1^*(\hat{v}_2^*, \hat{v}_1^*, \hat{v}_0^*) = \langle u_0, \hat{v}_2^* + \hat{v}_1^* \rangle_{L^2} - F_1(u_0, \hat{v}_0^*),$$

$$F_2^*(\hat{v}_2^*) = \langle u_0, \hat{v}_2^* \rangle_{L^2} - F_2(u_0),$$

$$G^*(\hat{v}_1^*, \hat{v}_0^*) = -\langle u_0, \hat{v}_1^* \rangle_{L^2} - \langle 0, \hat{v}_0^* \rangle_{L^2} - G(u_0, 0),$$

so that

$$\begin{aligned} J_1^*(\hat{v}_2^*, \hat{v}_1^*, \hat{v}_0^*) &= -F_1^*(\hat{v}_2^*, \hat{v}_1^*, \hat{v}_0^*) + F_2^*(\hat{v}_2^*) - G^*(\hat{v}_1^*, \hat{v}_0^*) \\ &= F_1(u_0, \hat{v}_0^*) - F_2(u_0) + G(u_0, 0) \\ &= J(u_0). \end{aligned} \quad (32)$$

Joining the pieces, we have got

$$\begin{aligned} J(u_0) &= \inf_{u \in V} \left\{ J(u) + \frac{K_1}{2} \int_{\Omega} (-\gamma \nabla^2 u + 2\hat{v}_0^* u - f)^2 dx \right\} \\ &= \inf_{v_2^* \in Y^*} \left\{ \sup_{(v_1^*, v_0^*) \in Y^* \times B^*} J_1^*(v_2^*, v_1^*, v_0^*) \right\} \\ &= J_1^*(\hat{v}_2^*, \hat{v}_1^*, \hat{v}_0^*). \end{aligned} \quad (33)$$

The proof is complete.

□

**Remark 5.2.** We could have also defined

$$B^* = \{v_0^* \in Y^* : \|v_0^*\|_{\infty} \leq K/2 \text{ and } -\gamma \nabla^2 + 2v_0^* > \varepsilon I_d\},$$

for some small real parameter  $\varepsilon > 0$ . In this case,  $-\gamma \nabla^2 + 2v_0^*$  is positive definite, whereas in the previous case,  $-\gamma \nabla^2 + 2v_0^*$  is negative definite.

## 6. Another convex dual variational formulation

In this section, again for  $\Omega \subset \mathbb{R}^3$  an open, bounded, connected set with a regular (Lipschitzian) boundary  $\partial\Omega$ ,  $\gamma > 0$ ,  $\alpha > 0$ ,  $\beta > 0$  and  $f \in L^2(\Omega)$ , we denote  $F_1 : V \times Y \rightarrow \mathbb{R}$ ,  $F_2 : V \rightarrow \mathbb{R}$  and  $G : Y \rightarrow \mathbb{R}$  by

$$\begin{aligned} F_1(u, v_0^*) &= \frac{\gamma}{2} \int_{\Omega} \nabla u \cdot \nabla u dx + \langle u^2, v_0^* \rangle_{L^2} \\ &\quad + \frac{K_1}{2} \int_{\Omega} (-\gamma \nabla^2 u + 2v_0^* u - f)^2 dx + \frac{K_2}{2} \int_{\Omega} u^2 dx, \end{aligned} \quad (34)$$

$$F_2(u) = \frac{K_2}{2} \int_{\Omega} u^2 dx + \langle u, f \rangle_{L^2},$$

and

$$G(u^2) = \frac{\alpha}{2} \int_{\Omega} (u^2 - \beta)^2 dx.$$

We define also

$$\begin{aligned} J_1(u, v_0^*) &= F_1(u, v_0^*) - F_2(u) - \langle u^2, v_0^* \rangle_{L^2} + G(u^2), \\ J(u) &= \frac{\gamma}{2} \int_{\Omega} \nabla u \cdot \nabla u \, dx + \frac{\alpha}{2} \int_{\Omega} (u^2 - \beta)^2 \, dx - \langle u, f \rangle_{L^2}, \\ A^+ &= \{u \in V : u f > 0, \text{ a.e. in } \Omega\}, \\ V_2 &= \{u \in V : \|u\|_{\infty} \leq K_3\}, \\ V_1 &= A^+ \cap V_1, \end{aligned}$$

and  $F_1^* : [Y^*]^2 \rightarrow \mathbb{R}$ ,  $F_2^* : Y^* \rightarrow \mathbb{R}$ , and  $G^* : Y^* \rightarrow \mathbb{R}$ , by

$$\begin{aligned} &F_1^*(v_2^*, v_0^*) \\ &= \sup_{u \in V} \{ \langle u, v_2^* \rangle_{L^2} - F_1(u, v_0^*) \} \\ &= \frac{1}{2} \int_{\Omega} \frac{(v_2^* + K_1(-\gamma \nabla^2 + 2v_0^*)f)^2}{(-\gamma \nabla^2 + 2v_0^* + K_2 + K_1(-\gamma \nabla^2 + 2v_0^*)^2)} \, dx \\ &\quad - \frac{K_1}{2} \int_{\Omega} f^2 \, dx, \end{aligned} \tag{35}$$

$$\begin{aligned} F_2^*(v_2^*) &= \sup_{u \in V} \{ \langle u, v_2^* \rangle_{L^2} - F_2(u) \} \\ &= \frac{1}{2K_2} \int_{\Omega} (v_2^* + f)^2 \, dx, \end{aligned} \tag{36}$$

and

$$\begin{aligned} G^*(v_0^*) &= \sup_{v \in Y} \{ \langle v, v_0^* \rangle_{L^2} - G(v) \} \\ &= \frac{1}{2\alpha} \int_{\Omega} (v_0^*)^2 \, dx + \beta \int_{\Omega} v_0^* \, dx \end{aligned} \tag{37}$$

At this point we define

$$B_1^* = \{v_0^* \in Y^* : \|v_0^*\|_{\infty} \leq K/2\},$$

$$B_2^* = \{v_0^* \in Y^* : -\gamma \nabla^2 + 2v_0^* + K_1(-\gamma \nabla^2 + 2v_0^*)^2 > \mathbf{0}\},$$

$$B_3^* = \{v_0^* \in Y^* : -1/\alpha + 4K_1[u(v_2^*, v_0^*)^2] + 100/K_2 \leq \mathbf{0}, \forall v_2^* \in E_1^*\},$$

where

$$u(v_2^*, v_0^*) = \frac{\varphi_1}{\varphi},$$

$$\varphi_1 = (v_2^* + K_1(-\gamma \nabla^2 + 2v_0^*)f)$$

and

$$\varphi = (-\gamma \nabla^2 + 2v_0^* + K_1(-\gamma \nabla^2 + 2v_0^*)^2 + K_2),$$

Finally, we also define

$$E_1^* = \{v_2^* \in Y^* : \|v_2^*\|_{\infty} \leq (5/4)K_2\}.$$

$$E_2^* = \{v_2^* \in Y^* : f v_2^* > 0, \text{ a.e. in } \Omega\},$$

$$E^* = E_1^* \cap E_2^*,$$

$$B^* = B_1^* \cap B_3^*,$$

and  $J_1^* : E^* \times B^* \rightarrow \mathbb{R}$ , by

$$J_1^*(v_2^*, v_0^*) = -F_1^*(v_2^*, v_0^*) + F_2^*(v_2^*) - G^*(v_0^*).$$

Moreover, assume

$$K_2 \gg K_1 \gg K \gg K_3 \gg \max\{1, \gamma, \alpha\}.$$

By directly computing  $\delta^2 J_1^*(v_2^*, v_0^*)$  we may obtain that for such specified real constants,  $J_1^*$  is concave in  $v_0^*$  on  $E^* \times B^*$ .

Indeed, recalling that

$$\varphi = (-\gamma \nabla^2 + 2v_0^* + K_1(-\gamma \nabla^2 + 2v_0^*)^2 + K_2),$$

$$\varphi_1 = (v_2^* + K_1(-\gamma \nabla^2 + 2v_0^*)f),$$

and

$$u = \frac{\varphi_1}{\varphi},$$

we obtain

$$\frac{\partial^2 J_1^*(v_2^*, v_0^*)}{\partial (v_2^*)^2} = 1/K_2 - 1/\varphi > 0,$$

in  $E^* \times B_3^*$  and

$$\frac{\partial^2 J_1^*(v_2^*, v_0^*)}{\partial (v_0^*)^2} = 4u^2 K_1 - 1/\alpha + \mathcal{O}(1/K_2) < 0,$$

in  $E^* \times B^*$ .

Considering such statements and definitions, we may prove the following theorem.

**Theorem 6.1.** Let  $(\hat{v}_2^*, \hat{v}_0^*) \in E^* \times (B^* \cap B_2^*)$  be such that

$$\delta J_1^*(\hat{v}_2^*, \hat{v}_0^*) = 0$$

and  $u_0 \in V_1$  be such that

$$u_0 = \frac{\hat{v}_2^* + K_1(-\gamma \nabla^2 + 2\hat{v}_0^*)f}{K_2 + 2\hat{v}_0^* - \gamma \nabla^2 + K_1(-\gamma \nabla^2 + 2\hat{v}_0^*)^2}.$$

Under such hypotheses, we have

$$\delta J(u_0) = 0,$$

so that

$$\begin{aligned} J(u_0) &= \inf_{u \in V_1} \left\{ J(u) + \frac{K_1}{2} \int_{\Omega} (-\gamma \nabla^2 u + 2\hat{v}_0^* u - f)^2 dx \right\} \\ &= \inf_{v_2^* \in E^*} \left\{ \sup_{v_0^* \in B^*} J_1^*(v_2^*, v_0^*) \right\} \\ &= J_1^*(\hat{v}_2^*, \hat{v}_0^*). \end{aligned} \quad (38)$$

**Proof.** Observe that  $\delta J_1^*(\hat{v}_2^*, \hat{v}_0^*) = 0$  so that, since  $J_1^*$  concave in  $v_0^*$  on  $E^* \times B^*$ ,  $v_0^* \in B_2^*$  and  $J_1^*$  is quadratic in  $v_2^*$ , we get

$$\sup_{v_0^* \in B^*} J_1^*(\hat{v}_2^*, v_0^*) = J_1^*(\hat{v}_2^*, \hat{v}_0^*) = \inf_{v_2^* \in E^*} J_1^*(v_2^*, \hat{v}_0^*).$$

Consequently, from this and the Min-Max Theorem, we obtain

$$J_1^*(\hat{v}_2^*, \hat{v}_0^*) = \inf_{v_2^* \in E^*} \left\{ \sup_{v_0^* \in B^*} J_1^*(v_2^*, v_0^*) \right\} = \sup_{v_0^* \in B^*} \left\{ \inf_{v_2^* \in E^*} J_1^*(v_2^*, v_0^*) \right\}.$$

Now we are going to show that

$$\delta J(u_0) = 0.$$

From

$$\frac{\partial J_1^*(\hat{v}_2^*, \hat{v}_0^*)}{\partial v_2^*} = 0,$$

we have

$$-u_0 + \frac{\hat{v}_2^*}{K_2} = 0,$$

and thus

$$\hat{v}_2^* = K_2 u_0.$$

Finally, denoting

$$D = -\gamma \nabla^2 u_0 + 2\hat{v}_0^* u_0 - f,$$

from

$$\frac{\partial J_1^*(\hat{v}_2^*, \hat{v}_0^*)}{\partial v_0^*} = 0,$$

we have

$$-2Du_0 + u_0^2 - \frac{\hat{v}_0^*}{\alpha} - \beta = 0,$$

so that

$$\hat{v}_0^* = \alpha(u_0^2 - \beta - 2Du_0). \quad (39)$$

Observe now that

$$\hat{v}_2^* + K_1(-\gamma \nabla^2 + 2\hat{v}_0^*)f = (K_2 - \gamma \nabla^2 + 2\hat{v}_0^* + K_1(-\gamma \nabla^2 + 2\hat{v}_0^*)^2)u_0$$

so that

$$\begin{aligned} & K_2 u_0 - 2\hat{v}_0^* u_0 - K u_0 + f \\ = & K_2 u_0 - K u_0 - \gamma \nabla^2 u_0 + K_1(-\gamma \nabla^2 + 2\hat{v}_0^*)(-\gamma \nabla^2 u_0 + 2\hat{v}_0^* u_0 - f). \end{aligned} \quad (40)$$

The solution for this last equation is obtained through the relation

$$-\gamma \nabla^2 u_0 + 2\hat{v}_0^* u_0 - f = D = 0,$$

so that from this and (49), we get

$$\hat{v}_0^* = \alpha(u_0^2 - \beta).$$

Thus,

$$\delta J(u_0) = -\gamma \nabla^2 u_0 + 2\alpha(u_0^2 - \beta)u_0 - f = 0$$

and

$$\delta \left\{ J(u_0) + \frac{K_1}{2} \int_{\Omega} (-\gamma \nabla^2 u_0 + 2\hat{v}_0^* u_0 - f)^2 dx \right\} = 0,$$

and hence, from the concerning convexity in  $u$  on  $V$ ,

$$J(u_0) = \min_{u \in V} \left\{ J(u) + \frac{K_1}{2} \int_{\Omega} (-\gamma \nabla^2 u + 2\hat{v}_0^* u - f)^2 dx \right\}.$$

Moreover, from the Legendre transform properties

$$\begin{aligned} F_1^*(\vartheta_2^*, \vartheta_0^*) &= \langle u_0, \vartheta_2^* \rangle_{L^2} - F_1(u_0, \vartheta_0^*), \\ F_2^*(\vartheta_2^*) &= \langle u_0, \vartheta_2^* \rangle_{L^2} - F_2(u_0), \\ G^*(\vartheta_0^*) &= \langle u_0^2, \vartheta_0^* \rangle_{L^2} - G(u_0^2), \end{aligned}$$

so that

$$\begin{aligned} J_1^*(\vartheta_2^*, \vartheta_0^*) &= -F_1^*(\vartheta_2^*, \vartheta_0^*) + F_2^*(\vartheta_2^*) - G^*(\vartheta_0^*) \\ &= F_1(u_0, \vartheta_0^*) - F_2(u_0) - \langle u_0^2, \vartheta_0^* \rangle_{L^2} + G(u_0^2) \\ &= J(u_0). \end{aligned} \quad (41)$$

Joining the pieces, we have got

$$\begin{aligned} J(u_0) &= \inf_{u \in V_1} \left\{ J(u) + \frac{K_1}{2} \int_{\Omega} (-\gamma \nabla^2 u + 2\vartheta_0^* u - f)^2 dx \right\} \\ &= \inf_{v_2^* \in E^*} \left\{ \sup_{v_0^* \in B^*} J_1^*(v_2^*, v_0^*) \right\} \\ &= J_1^*(\vartheta_2^*, \vartheta_0^*). \end{aligned} \quad (42)$$

The proof is complete.

□

## 7. A third duality principle and related convex dual variational formulation

In this section, we assume a finite dimensional version for the model in question, in a finite differences or finite elements context, although the concerning spaces and operators have not been relabeled.

Again, for  $\Omega \subset \mathbb{R}^3$  an open, bounded, connected set with a regular (Lipschitzian) boundary  $\partial\Omega$ ,  $\gamma < 0$ ,  $\alpha < 0$ ,  $\beta > 0$ ,  $K_2 < 0$  and  $f \in L^2(\Omega)$ , we denote  $F_1 : V \times Y \rightarrow \mathbb{R}$ ,  $F_2 : V \rightarrow \mathbb{R}$  and  $G : Y \rightarrow \mathbb{R}$  by

$$\begin{aligned} F_1(u, v_0^*) &= \frac{\gamma}{2} \int_{\Omega} \nabla u \cdot \nabla u dx + \langle u^2, v_0^* \rangle_{L^2} \\ &\quad + \frac{K_1}{2} \int_{\Omega} (-\gamma \nabla^2 u + 2v_0^* u + f)^2 dx + \frac{K_2}{2} \int_{\Omega} u^2 dx, \end{aligned} \quad (43)$$

$$F_2(u) = \frac{K_2}{2} \int_{\Omega} u^2 dx - \langle u, f \rangle_{L^2},$$

and

$$G(u^2) = \frac{\alpha}{2} \int_{\Omega} (u^2 - \beta)^2 dx.$$

We define also

$$\begin{aligned} J_1(u, v_0^*) &= F_1(u, v_0^*) - F_2(u) - \langle u^2, v_0^* \rangle_{L^2} + G(u^2), \\ J(u) &= \frac{\gamma}{2} \int_{\Omega} \nabla u \cdot \nabla u dx + \frac{\alpha}{2} \int_{\Omega} (u^2 - \beta)^2 dx + \langle u, f \rangle_{L^2}, \\ A^- &= \{u \in V : u f < 0, \text{ a.e. in } \Omega\}, \\ V_2 &= \{u \in V : \|u\|_{\infty} \leq K_3\}, \\ V_1 &= A^- \cap V_2, \end{aligned}$$

and  $F_1^* : [Y^*]^2 \rightarrow \mathbb{R}$ ,  $F_2^* : Y^* \rightarrow \mathbb{R}$ , and  $G^* : Y^* \rightarrow \mathbb{R}$ , by

$$\begin{aligned} & F_1^*(v_2^*, v_0^*) \\ &= \inf_{u \in V} \{ \langle u, v_2^* \rangle_{L^2} - F_1(u, v_0^*) \} \\ &= \frac{1}{2} \int_{\Omega} \frac{(v_2^* - K_1(-\gamma \nabla^2 + 2v_0^*)f)^2}{(-\gamma \nabla^2 + 2v_0^* + K_2 + K_1(-\gamma \nabla^2 + 2v_0^*)^2)} dx \\ &\quad - \frac{K_1}{2} \int_{\Omega} f^2 dx, \end{aligned} \quad (44)$$

$$\begin{aligned} F_2^*(v_2^*) &= \inf_{u \in V} \{ \langle u, v_2^* \rangle_{L^2} - F_2(u) \} \\ &= \frac{1}{2K_2} \int_{\Omega} (v_2^* - f)^2 dx, \end{aligned} \quad (45)$$

and

$$\begin{aligned} G^*(v_0^*) &= \inf_{v \in Y} \{ \langle v, v_0^* \rangle_{L^2} - G(v) \} \\ &= \frac{1}{2\alpha} \int_{\Omega} (v_0^*)^2 dx + \beta \int_{\Omega} v_0^* dx \end{aligned} \quad (46)$$

At this point we define

$$B_1^* = \{v_0^* \in Y^* : \|v_0^*\|_{\infty} \leq K/2\},$$

$$B_2^* = \{v_0^* \in Y^* : -\gamma \nabla^2 + 2v_0^* + K_1(-\gamma \nabla^2 + 2v_0^*)^2 > 0\},$$

$$B_3^* = \{v_0^* \in Y^* : -1/\alpha + 4K_1[u(v_2^*, v_0^*)^2] + 100/|K_2| > 0, \forall v_2^* \in E_1^*\},$$

where

$$u(v_2^*, v_0^*) = \frac{\varphi_1}{\varphi},$$

$$\varphi_1 = (v_2^* + K_1(-\gamma \nabla^2 + 2v_0^*)f)$$

and

$$\varphi = (-\gamma \nabla^2 + 2v_0^* + K_1(-\gamma \nabla^2 + 2v_0^*)^2 + K_2),$$

By direct computation we may obtain

$$\frac{\partial^2 [u(v_2^*, v_0^*)^2]}{\partial (v_0^*)^2} \geq 0, \forall v_0^* \in B^*, \forall v_2^* \in E_1^*$$

so that  $B_3^*$  is convex.

Finally, we also define

$$B_4^* = \{v_0^* \in Y^* : -[-\gamma \nabla^2 + 2v_0^*] \leq -\varepsilon I_d\},$$

$$E_1^* = \{v_2^* \in Y^* : \|v_2^*\|_{\infty} \leq (5/4)|K_2|\},$$

$$E_2^* = \{v_2^* \in Y^* : f v_2^* > 0, \text{ a.e. in } \Omega\},$$

$$E^* = E_1^* \cap E_2^*,$$

And  $J_1^*$  by

$$J_1^*(v_2^*, v_0^*) = -F_1^*(v_2^*, v_0^*) + F_2^*(v_2^*) - G^*(v_0^*).$$

We assume  $K_2 < 0$ , and

$$|K_2| \gg K_1 \gg K \gg K_3 \gg \max\{|\alpha|, |\gamma|, \beta, 1/\varepsilon^2\}.$$

Recalling that

$$\begin{aligned}\varphi &= (-\gamma \nabla^2 + 2v_0^* + K_1(-\gamma \nabla^2 + 2v_0^*)^2 + K_2), \\ \varphi_1 &= (v_2^* + K_1(-\gamma \nabla^2 + 2v_0^*)f),\end{aligned}$$

and

$$u = \frac{\varphi_1}{\varphi},$$

we obtain

$$\frac{\partial^2 J_1^*(v_2^*, v_0^*)}{\partial (v_2^*)^2} = 1/K_2 - 1/\varphi > 0,$$

in  $E^* \times B_3^*$  and

$$\frac{\partial^2 J_1^*(v_2^*, v_0^*)}{\partial (v_0^*)^2} = 4u^2 K_1 - 1/\alpha + \mathcal{O}(1/|K_2|).$$

Also,

$$\begin{aligned}& \frac{\partial^2 J_1^*(v_2^*, v_0^*)}{\partial (v_2^*)^2} \frac{\partial^2 J_1^*(v_2^*, v_0^*)}{\partial (v_0^*)^2} - \frac{\partial^2 J_1^*(v_2^*, v_0^*)}{\partial v_2^* \partial v_0^*} \\ &= \mathcal{O}\left(\frac{K_1^2 A_3 + K_1 A_4}{-\alpha K_2 \varphi}\right),\end{aligned}\tag{47}$$

where

$$A_3 = 8\alpha(f^2 + 4f(-\gamma \nabla^2 + 2v_0^*)u + 3[(-\gamma \nabla^2 + 2v_0^*)u]^2$$

and

$$A_4 = (-\gamma \nabla^2 + 2v_0^*)^2 - 12\alpha[(-\gamma \nabla^2 + 2v_0^*)u]u.$$

Observe that at a critical point  $A_3 = 0$  and  $A_4 > 0$  so that, for the dual formulation, we set the restrictions  $A_3 \geq 0$  and  $A_4 \geq \varepsilon I_d$ .

Thus, we define

$$B_5^* = \{v_0^* \in Y^* : A_3 \geq 0 \text{ and } A_4 \geq \varepsilon I_d\},$$

and

$$B^* = B_1^* \cap B_2^* \cap B_3^* \cap B_4^* \cap B_5^*.$$

Observe also that

$$\frac{\partial^2 J_1^*(v_2^*, v_0^*)}{\partial (v_2^*)^2} \frac{\partial^2 J_1^*(v_2^*, v_0^*)}{\partial (v_0^*)^2} - \frac{\partial^2 J_1^*(v_2^*, v_0^*)}{\partial v_2^* \partial v_0^*} > 0,$$

on  $B^* \times E^*$ , so that  $J_1^*$  is convex on  $E^* \times B^*$

Considering such statements and definitions, we may prove the following theorem.

**Theorem 7.1.** Let  $(\hat{v}_2^*, \hat{v}_0^*) \in E^* \times B^*$  be such that

$$\delta J_1^*(\hat{v}_2^*, \hat{v}_0^*) = 0$$



and  $u_0 \in V_1$  be such that

$$u_0 = \frac{\hat{v}_2^* - K_1(-\gamma \nabla^2 + 2\hat{v}_0^*)f}{K_2 + 2\hat{v}_0^* - \gamma \nabla^2 + K_1(-\gamma \nabla^2 + 2\hat{v}_0^*)^2}.$$

Under such hypotheses, we have

$$\delta J(u_0) = \mathbf{0},$$

so that

$$\begin{aligned} J(u_0) &= \sup_{u \in V_1} \left\{ J(u) + \frac{K_2}{2} \int_{\Omega} (u - u_0)^2 dx \right\} \\ &= \inf_{(v_2^*, v_0^*) \in E^* \times B^*} J_1^*(v_2^*, v_0^*) \\ &= J_1^*(\hat{v}_2^*, \hat{v}_0^*). \end{aligned} \quad (48)$$

**Proof.** Observe that  $\delta J_1^*(\hat{v}_2^*, \hat{v}_0^*) = \mathbf{0}$  so that, since  $J_1^*$  convex on the convex set  $E^* \times B^*$ , we have that

$$J_1^*(\hat{v}_2^*, \hat{v}_0^*) = \inf_{(v_2^*, v_0^*) \in E^* \times B^*} J_1^*(v_2^*, v_0^*).$$

Now we are going to show that

$$\delta J(u_0) = \mathbf{0}.$$

From

$$\frac{\partial J_1^*(\hat{v}_2^*, \hat{v}_0^*)}{\partial v_2^*} = \mathbf{0},$$

we have

$$-u_0 + \frac{\hat{v}_2^*}{K_2} = 0,$$

and thus

$$\hat{v}_2^* = K_2 u_0.$$

Finally, denoting

$$D = -\gamma \nabla^2 u_0 + 2\hat{v}_0^* u_0 - f,$$

from

$$\frac{\partial J_1^*(\hat{v}_2^*, \hat{v}_0^*)}{\partial v_0^*} = \mathbf{0},$$

we have

$$-2D u_0 + u_0^2 - \frac{\hat{v}_0^*}{\alpha} - \beta = 0,$$

so that

$$\hat{v}_0^* = \alpha(u_0^2 - \beta - 2D u_0). \quad (49)$$

Observe now that

$$\hat{v}_2^* + K_1(-\gamma \nabla^2 + 2\hat{v}_0^*)f = (K_2 - \gamma \nabla^2 + 2\hat{v}_0^* + K_1(-\gamma \nabla^2 + 2\hat{v}_0^*)^2)u_0$$

so that

$$\begin{aligned} &K_2 u_0 - 2\hat{v}_0^* u_0 - K u_0 + f \\ &= K_2 u_0 - K u_0 - \gamma \nabla^2 u_0 + K_1(-\gamma \nabla^2 + 2\hat{v}_0^*)(-\gamma \nabla^2 u_0 + 2\hat{v}_0^* u_0 - f). \end{aligned} \quad (50)$$

The solution for this last equation is obtained through the relation

$$-\gamma \nabla^2 u_0 + 2\hat{\vartheta}_0^* u_0 - f = D = 0,$$

so that from this and (49), we get

$$\hat{\vartheta}_0^* = \alpha(u_0^2 - \beta).$$

Thus,

$$\delta J(u_0) = -\gamma \nabla^2 u_0 + 2\alpha(u_0^2 - \beta)u_0 - f = 0$$

and

$$\delta \left\{ J(u_0) + \frac{K_2}{2} \int_{\Omega} (u - u_0)^2 dx \right\} = 0,$$

and hence, from the concerning concavity in  $u$  on  $V$ ,

$$J(u_0) = \min_{u \in V_1} \left\{ J(u) + \frac{K_2}{2} \int_{\Omega} (u - u_0)^2 dx \right\}.$$

Moreover, from the Legendre transform properties

$$F_1^*(\hat{\vartheta}_2^*, \hat{\vartheta}_0^*) = \langle u_0, \hat{\vartheta}_2^* \rangle_{L^2} - F_1(u_0, \hat{\vartheta}_0^*),$$

$$F_2^*(\hat{\vartheta}_2^*) = \langle u_0, \hat{\vartheta}_2^* \rangle_{L^2} - F_2(u_0),$$

$$G^*(\hat{\vartheta}_0^*) = \langle u_0^2, \hat{\vartheta}_0^* \rangle_{L^2} - G(u_0^2),$$

so that

$$\begin{aligned} J_1^*(\hat{\vartheta}_2^*, \hat{\vartheta}_0^*) &= -F_1^*(\hat{\vartheta}_2^*, \hat{\vartheta}_0^*) + F_2^*(\hat{\vartheta}_2^*) - G^*(\hat{\vartheta}_0^*) \\ &= F_1(u_0, \hat{\vartheta}_0^*) - F_2(u_0) - \langle u_0^2, \hat{\vartheta}_0^* \rangle_{L^2} + G(u_0^2) \\ &= J(u_0). \end{aligned} \tag{51}$$

Finally, observe that

$$\begin{aligned} J_1^*(\hat{\vartheta}_2^*, \hat{\vartheta}_0^*) &\geq F_1(u, \hat{\vartheta}_0^*) - \langle u, \hat{\vartheta}_2^* \rangle_{L^2} + F_2^*(\hat{\vartheta}_2^*) - G^*(\hat{\vartheta}_0^*) \\ &\geq \inf_{v_0^* \in Y^*} \left\{ \frac{\gamma}{2} \int_{\Omega} \nabla u \cdot \nabla u dx + \frac{K_2}{2} \int_{\Omega} u^2 dx \right. \\ &\quad \left. - \langle u, \hat{\vartheta}_2^* \rangle_{L^2} + F_2^*(\hat{\vartheta}_2^*) + \langle u^2, v_0^* \rangle_{L^2} - \frac{\alpha}{2} \int_{\Omega} (v_0^*)^2 dx \right. \\ &\quad \left. - \beta \int_{\Omega} v_0^* dx \right\} \\ &= \frac{\gamma}{2} \int_{\Omega} \nabla u \cdot \nabla u dx + \frac{\alpha}{2} \int_{\Omega} (u^2 - \beta)^2 dx \\ &\quad + \langle u, f \rangle_{L^2} + \frac{K_2}{2} \int_{\Omega} u^2 dx \\ &\quad - \langle u, K_2 u_0 \rangle_{L^2} + \frac{K_2}{2} \int_{\Omega} u_0^2 dx \\ &= J(u) + \frac{K_2}{2} \int_{\Omega} (u - u_0)^2 dx, \end{aligned} \tag{52}$$

$\forall u \in V_1$  where we recall that  $K_2 < 0$ .

Joining the pieces, we have got

$$\begin{aligned}
 J(u_0) &= \sup_{u \in V_1} \left\{ J(u) + \frac{K_2}{2} \int_{\Omega} (u - u_0)^2 dx \right\} \\
 &= \inf_{(v_2^*, v_0^*) \in E^* \times B^*} J_1^*(v_2^*, v_0^*) \\
 &= J_1^*(\vartheta_2^*, \vartheta_0^*).
 \end{aligned} \tag{53}$$

The proof is complete.

□

## 8. Closely related primal-dual variational formulations

Consider again the functional  $J : V \rightarrow \mathbb{R}$  where

$$J(u) = \frac{\gamma}{2} \int_{\Omega} \nabla u \cdot \nabla u dx + \frac{\alpha}{2} \int_{\Omega} (u^2 - \beta)^2 dx - \langle u, f \rangle_{L^2},$$

where  $\alpha > 0, \gamma > 0, \beta > 0, f \in L^2(\Omega)$  and  $V = W_0^{1,2}(\Omega)$ .

Observe that

$$\begin{aligned}
 J(u) &= J(u) + \langle u^2, v_0^* \rangle_{L^2} - \langle u^2, v_0^* \rangle_{L^2} \\
 &= \frac{\gamma}{2} \int_{\Omega} \nabla u \cdot \nabla u dx + \langle u^2, v_0^* \rangle_{L^2} - \langle u, f \rangle_{L^2} \\
 &\quad - \langle u^2, v_0^* \rangle_{L^2} + \frac{\alpha}{2} \int_{\Omega} (u^2 - \beta)^2 dx \\
 &\geq \frac{\gamma}{2} \int_{\Omega} \nabla u \cdot \nabla u dx + \langle u^2, v_0^* \rangle_{L^2} - \langle u, f \rangle_{L^2} \\
 &\quad + \inf_{v \in Y} \left\{ -\langle v, v_0^* \rangle_{L^2} + \frac{\alpha}{2} \int_{\Omega} (v - \beta)^2 dx \right\} \\
 &= \frac{\gamma}{2} \int_{\Omega} \nabla u \cdot \nabla u dx + \langle u^2, v_0^* \rangle_{L^2} - \langle u, f \rangle_{L^2} \\
 &\quad - \frac{1}{2\alpha} \int_{\Omega} (v_0^*)^2 dx - \beta \int_{\Omega} v_0^* dx \\
 &= J_1(u, v_0^*).
 \end{aligned} \tag{54}$$

Having obtained  $J_1^*(u, v_0^*)$ , we propose the following exactly penalized primal-dual formulation  $J_2^*(u, v_0^*)$ , where

$$J_2^*(u, v_0^*) = J_1^*(u, v_0^*) + \frac{K_1}{2} \int_{\Omega} (-\gamma \nabla^2 u + 2v_0^* u - f)^2 dx,$$

so that

$$\begin{aligned}
 J_2^*(u, v_0^*) &= \frac{\gamma}{2} \int_{\Omega} \nabla u \cdot \nabla u dx + \langle u^2, v_0^* \rangle_{L^2} - \langle u, f \rangle_{L^2} \\
 &\quad - \frac{1}{2\alpha} \int_{\Omega} (v_0^*)^2 dx - \beta \int_{\Omega} v_0^* dx \\
 &\quad + \frac{K_1}{2} \int_{\Omega} (-\gamma \nabla^2 u + 2v_0^* u - f)^2 dx,
 \end{aligned} \tag{55}$$

In particular, if we set

$$V_1 = \{u \in V : \|u\|_{\infty} \leq K_3\},$$

and

$$K_1 = 1/(8K_3^2\alpha),$$

we may also define

$$J_3(u) = \sup_{v_0^* \in B^*} J_2^*(u, v_0^*),$$

where

$$B^* = \{v_0^* \in Y^* : \|v_0^*\|_\infty \leq K/8\},$$

for appropriate  $K, K_3 > 0$ .

Here we highlight that  $J_2^*$  is concave in  $v_0^*$  on  $B^*$  (indeed it is concave on  $Y^*$ ) and the parameter  $K_1 > 0$  multiplying a positive definite quadratic functional in  $u$  improves the convexity conditions of  $J_3$ .

### 9. One more duality principle suitable for the primal formulation global optimization

In this section we establish one more duality principle and related convex dual formulation suitable for a global optimization of the primal variational formulation.

Let  $\Omega \subset \mathbb{R}^3$  be an open, bounded, connected set with a regular (Lipschitzian) boundary denoted by  $\partial\Omega$ .

For the primal formulation, we define  $V = W_0^{1,2}(\Omega)$  and consider a functional  $J : V \rightarrow \mathbb{R}$  where

$$J(u) = \frac{\gamma}{2} \int_{\Omega} \nabla u \cdot \nabla u \, dx + \frac{\alpha}{2} \int_{\Omega} (u^2 - \beta)^2 \, dx - \langle u, f \rangle_{L^2}. \quad (56)$$

Here we assume  $f \in L^2(\Omega)$ , and define  $Y = Y^* = L^2(\Omega)$

$$V_2 = \{u \in V : \|u\|_\infty \leq K_3\},$$

$$A^+ = \{u \in V : u f > 0, \text{ a.e. in } \Omega\},$$

and

$$V_1^* = A^+ \cap V_1,$$

for an appropriate constant  $K_3 > 0$  to be specified.

Define also the functionals  $F_1 : V \rightarrow \mathbb{R}$ ,  $F_2 : V \times Y \rightarrow \mathbb{R}$  and  $G : Y \rightarrow \mathbb{R}$  by

$$F_1(u) = \frac{K_2}{2} \int_{\Omega} (\nabla^2 u)^2 \, dx - \langle u, f \rangle_{L^2},$$

$$\begin{aligned} F_2(u, v_3^*, v_0^*) &= -\frac{\gamma}{2} \int_{\Omega} \nabla u \cdot \nabla u \, dx - \langle u^2, v_0^* \rangle_{L^2} + \frac{K_2}{2} \int_{\Omega} (\nabla^2 u)^2 \, dx \\ &\quad - \frac{K_1}{2} \int_{\Omega} (-\gamma_1 \nabla^2 u + 2v_3^* u - h_1)^2 \, dx, \end{aligned} \quad (57)$$

and

$$G(u^2) = \frac{\alpha}{2} \int_{\Omega} (u^2 - \beta)^2 \, dx,$$

for appropriate positive constants  $K_1, K_2, K_3$  to be specified.

Moreover, define  $F_1^* : Y^* \rightarrow \mathbb{R}$ , and  $F_2^* : [Y^*]^2 \rightarrow \mathbb{R}$  and  $G^* : Y^* \rightarrow \mathbb{R}$ , by

$$\begin{aligned} F_1^*(v_2^*) &= \sup_{u \in V} \{\langle u, v_2^* \rangle_{L^2} - F_1(u)\} \\ &= \frac{1}{2K_2} \int_{\Omega} \frac{(v_2^* + f)^2}{\nabla^4} \, dx, \end{aligned} \quad (58)$$

and

$$\begin{aligned} F_2^*(v_2^*, v_3^*, v_0^*) &= \sup_{u \in V} \{ \langle u, v_2^* \rangle_{L^2} - F_2(u, v_3^*, v_0^*) \} \\ &= \frac{1}{2} \int_{\Omega} \frac{(v_2^* + K_1(-\gamma_1 \nabla^2 + 2v_3^*)h_1)^2}{K_2 \nabla^4 + \gamma \nabla^2 - 2v_0^* - K_1(-\gamma_1 \nabla^2 + 2v_3^*)^2} \\ &\quad - \frac{K_1}{2} \int_{\Omega} h_1^2 dx \end{aligned}$$

for appropriate  $\gamma_1 > 0$  and  $H_1 \in L^2(\Omega)$ , and

$$\begin{aligned} G^*(v_0^*) &= \sup_{v \in Y} \{ \langle v, v_0^* \rangle_{L^2} - G(v) \} \\ &= \frac{1}{2\alpha} \int_{\Omega} (v_0^*)^2 dx + \beta \int_{\Omega} v_0^* dx. \end{aligned} \quad (59)$$

Furthermore, we define

$$D^* = \{v_2^* \in Y^* : \|v_2^*\|_{\infty} \leq (3/2)K_2\},$$

$$B^* = \{v_3^* \in Y^* : \|v_3^*\|_{\infty} \leq K_4\},$$

for an appropriate constant  $K_4 > 0$  to be specified.

Define also

$$C_1^* = \{v_0^* \in Y^* : \|v_0^*\|_{\infty} \leq K_4\}.$$

and  $J_1^* : D^* \times C_1^* \rightarrow \mathbb{R}$  by

$$J_1^*(v_2^*, v_3^*, v_0^*) = -F_1^*(v_2^*) + F_2^*(v_2^*, v_3^*, v_0^*) - G^*(v_0^*).$$

Moreover, assuming  $K_2 \gg K_1 \gg K_4 \gg \max\{1, K_3, \alpha, \beta, \gamma, \gamma_1, \|f\|_{\infty}, \|h_1\|_{\infty}\}$ .

By directly computing  $\delta^2 J_1^*(v_2^*, v_3^*, v_0^*)$  denoting

$$A = -2K_1 h_1,$$

$$B = 4K_1(-\gamma_1 \nabla^2 + 2v_3^*),$$

$$\varphi = -K_2 \nabla^4 - \gamma \nabla^2 + 2v_0^* + K_1(-\gamma_1 \nabla^2 + 2v_3^*)^2,$$

$$\varphi_1 = v_2^* - K_1(-\gamma_1 \nabla^2 + 2v_3^*)h_1,$$

$$u = -\frac{\varphi_1}{\varphi},$$

we may obtain, considering that  $\varphi < 0$

$$\frac{\partial^2 J_1^*(v_2^*, v_3^*, v_0^*)}{\partial (v_3^*)^2} = 4K_1 u^2 - \frac{(A - uB)^2}{\varphi} > 0$$

on  $D^* \times B^*$ .

Moreover,

$$\begin{aligned} &\frac{\partial^2 J_1^*(v_2^*, v_3^*, v_0^*)}{\partial (v_2^*)^2} \frac{\partial^2 J_1^*(v_2^*, v_3^*, v_0^*)}{\partial (v_3^*)^2} - \left( \frac{\partial^2 J_1^*(v_2^*, v_3^*, v_0^*)}{\partial v_2^* \partial v_3^*} \right)^2 \\ &= \mathcal{O} \left( \frac{K_1^2 H_1 + K_1 H_2}{-K_2 \varphi} \right), \end{aligned} \quad (60)$$

where

$$H_1 = (8(-h_1^2 + 4h_1(-\gamma_1 \nabla^2 + 2v_3^*)u - 3[(-\gamma_1 \nabla^2 + 2v_3^*)^2 u]u),$$

and

$$H_2 = [(-\gamma \nabla^2 + 2v_0^*)u]u.$$

At a critical point we have  $H_1 = \mathbf{0}$  and

$$H_2 = fu_0 > 0, \text{ a.e in } \Omega.$$

With such results, we may define the restrictions

$$C_2^* = \{v_0^* \in Y^* : H_1(v_2^*, v_3^*, v_0^*) \geq 0, \forall v_2^* \in D^*, v_3^* \in B^*\}.$$

$$C_3^* = \{v_0^* \in Y^* : H_2(v_2^*, v_3^*, v_0^*) \geq 0, \forall v_2^* \in D^*, v_3^* \in B^*\}.$$

Here, we define  $C^* = C_1^* \cap C_2^* \cap C_3^*$ .

On the other hand, clearly we have

$$\frac{\partial^2 J_1^*(v_2^*, v_3^*, v_0^*)}{\partial (v_0^*)^2} < 0$$

From such results, we may obtain that  $J_1^*$  is convex in  $(v_2^*, v_3^*)$  and it is concave in  $v_0^*$  on  $D^* \times B^* \times C^*$ .

### 9.1. The main duality principle and a related convex dual formulation

Considering the statements and definitions presented in the previous section, we may prove the following theorem.

**Theorem 9.1.** Let  $(\hat{v}_2^*, \hat{v}_3^*, \hat{v}_0^*) \in D^* \times B^* \times C^*$  be such that

$$\delta J_1^*(\hat{v}_2^*, \hat{v}_3^*, \hat{v}_0^*) = \mathbf{0}$$

and  $u_0 \in V_1$  be such that

$$u_0 = \frac{\partial F_1^*(\hat{v}_2^*)}{\partial v_2^*}.$$

Assume also

$$u_0 \neq 0, \text{ a.e. in } \Omega.$$

Under such hypotheses, we have

$$\delta J(u_0) = \mathbf{0},$$

$$-\gamma_1 \nabla^2 u_0 + 2\hat{v}_3^* u_0 - h_1 = \mathbf{0},$$

and

$$\begin{aligned} J(u_0) &= \inf_{u \in V_1} J(u) \\ &= \inf_{(v_2^*, v_3^*) \in D^* \times B^*} \left\{ \sup_{v_0^* \in C^*} J_1^*(v_2^*, v_3^*, v_0^*) \right\} \\ &= J_1^*(\hat{v}_2^*, \hat{v}_3^*, \hat{v}_0^*). \end{aligned} \tag{61}$$

**Proof.** Observe that  $\delta J_1^*(\hat{v}_2^*, \hat{v}_3^*, \hat{v}_0^*) = \mathbf{0}$  so that, since  $J_1^*$  is convex in  $(v_2^*, v_3^*) \in D^* \times B^* \times C^*$  and

$$\frac{\partial^2 J_1^*(\hat{v}_2^*, \hat{v}_3^*, v_0^*)}{\partial (v_0^*)^2} > 0, \forall v_0^* \in C_1^*,$$

we obtain

$$J_1^*(\hat{v}_2^*, \hat{v}_3^*, \hat{v}_0^*) = \inf_{(v_2^*, v_3^*) \in D^* \times B^*} J_1^*(v_2^*, v_3^*, \hat{v}_0^*) = \sup_{v_0^* \in C^*} J_1^*(\hat{v}_2^*, \hat{v}_3^*, v_0^*).$$

Consequently, from this and the Saddle Point Theorem, we obtain

$$J_1^*(\hat{v}_2^*, \hat{v}_3^*, \hat{v}_0^*) = \inf_{(v_2^*, v_3^*) \in D^* \times B^*} \left\{ \sup_{v_0^* \in C^*} J_1^*(v_2^*, v_3^*, v_0^*) \right\}.$$

Now we are going to show that

$$\delta J(u_0) = \mathbf{0}.$$

From

$$\frac{\partial J_1^*(\hat{v}_2^*, \hat{v}_3^*, \hat{v}_0^*)}{\partial v_2^*} = \mathbf{0},$$

and

$$\frac{\partial F_1^*(\hat{v}_2^*)}{\partial v_2^*} = u_0$$

we have

$$-\frac{\partial F_2^*(\hat{v}_2^*, \hat{v}_3^*, \hat{v}_0^*)}{\partial v_2^*} - u_0 = \mathbf{0}$$

and

$$\hat{v}_2^* = K_2 \nabla^4 u_0 - f.$$

Observe now that

$$F_2^*(\hat{v}_2^*, \hat{v}_3^*, v_0^*) = \sup_{u \in V} \{ -\langle u, v_2^* \rangle_{L^2} - F_2(u, v_3^*, v_0^*) \}.$$

Denoting

$$H(v_2^*, v_3^*, v_0^*, u) = \langle u, v_2^* \rangle_{L^2} - F_2(u, v_3^*, v_0^*),$$

there exists  $\hat{u} \in V$  such that

$$\frac{\partial H(\hat{v}_2^*, \hat{v}_3^*, \hat{v}_0^*, \hat{u})}{\partial u} = \mathbf{0},$$

and

$$F_2^*(\hat{v}_2^*, \hat{v}_3^*, \hat{v}_0^*) = H(\hat{v}_2^*, \hat{v}_3^*, \hat{v}_0^*, \hat{u}),$$

so that

$$\begin{aligned} \frac{\partial F_2^*(\hat{v}_2^*, \hat{v}_3^*, \hat{v}_0^*)}{\partial v_2^*} &= \frac{\partial H(\hat{v}_2^*, \hat{v}_3^*, \hat{v}_0^*, \hat{u})}{\partial v_2^*} \\ &\quad + \frac{\partial H(\hat{v}_2^*, \hat{v}_3^*, \hat{v}_0^*, \hat{u})}{\partial u} \frac{\partial \hat{u}}{\partial v_2^*} \\ &= \hat{u}. \end{aligned} \tag{62}$$

Summarizing, we have got

$$u_0 = \frac{\partial F_2^*(\hat{v}_2^*, \hat{v}_3^*, \hat{v}_0^*)}{\partial v_2^*} = \hat{u}.$$

From such results and the Legendre transform proprieties we get

$$v_2^* = \frac{\partial F_1(u_0)}{\partial u}$$

and

$$v_2^* = \frac{\partial F_2(u_0, \hat{v}_3^*, \hat{v}_0^*)}{\partial u}.$$

On the other hand, from the variation of  $J_1^*$  in  $v_3^*$ , we have

$$\begin{aligned} & \frac{\partial F_2^*(\hat{v}_2^*, \hat{v}_3^*, \hat{v}_0^*)}{\partial v_3^*} \\ &= -K_1(-\gamma_1 \nabla^2 u_0 + 2\hat{v}_3^* u_0 - h_1)2u_0 + \frac{\partial H(\hat{v}_2^*, \hat{v}_3^*, \hat{v}_0^*, \hat{u})}{\partial u} \frac{\partial \hat{u}}{\partial v_3^*} \\ &= -K_1(-\gamma_1 \nabla^2 u_0 + 2\hat{v}_3^* u_0 - h_1)2u_0 \\ &= \mathbf{0}. \end{aligned} \tag{63}$$

From such results, since

$$u_0 \neq 0, \text{ a.e. in } \Omega,$$

we get

$$-\gamma_1 \nabla^2 u_0 + 2\hat{v}_3^* u_0 - h_1 = 0, \text{ a.e. in } \Omega.$$

Finally, from the variation of  $J_1^*$  in  $v_0^*$  we obtain

$$\frac{\partial F_2^*(\hat{v}_2^*, \hat{v}_3^*, \hat{v}_0^*)}{\partial v_0^*} - \frac{\partial G^*(v_0^*)}{\partial v_0^*} = 0,$$

so that

$$u_0^2 + \frac{\partial H(\hat{v}_2^*, \hat{v}_3^*, \hat{v}_0^*, \hat{u})}{\partial u} \frac{\partial \hat{u}}{\partial v_0^*} - \frac{v_0^*}{\alpha} - \beta = \mathbf{0}.$$

Thus,

$$v_0^* = \alpha(u_0^2 - \beta).$$

Consequently, from such last results, we have

$$\begin{aligned} \mathbf{0} &= \hat{v}_2^* - \hat{v}_2^* \\ &= \frac{\partial F_1(u_0)}{\partial u} - \frac{\partial F_2(u_0, \hat{v}_3^*, \hat{v}_0^*)}{\partial u} \\ &= K_2 \nabla^4 u_0 - f - K_2 \nabla^4 u_0 - \gamma \nabla^2 u_0 + 2v_0^* u_0 \\ &= -\gamma \nabla^2 u_0 + 2\alpha(u_0^2 - \beta)u_0 - f \\ &= \delta J(u_0). \end{aligned} \tag{64}$$

Summarizing,

$$\delta J(u_0) = \mathbf{0}.$$

Furthermore, also from such last results and the Legendre transform properties, we have

$$\begin{aligned} F_1^*(\hat{v}_2^*) &= \langle u_0, \hat{v}_2^* \rangle_{L^2} - F_1(u_0), \\ F_2^*(\hat{v}_2^*, \hat{v}_3^*, \hat{v}_0^*) &= \langle u_0, \hat{v}_2^* \rangle_{L^2} - F_2(u_0, \hat{v}_3^*, \hat{v}_0^*), \\ G^*(\hat{v}_0^*) &= \langle u_0^2, v_0^* \rangle_{L^2} - G(u_0^2), \end{aligned}$$



so that

$$\begin{aligned} & J_1^*(\hat{v}_2^*, \hat{v}_3^*, \hat{v}_0^*) \\ &= -F_1^*(\hat{v}_2^*) + F_2^*(\hat{v}_2^*, \hat{v}_3^*, \hat{v}_0^*) - G^*(\hat{v}_0^*) \\ &= J(u_0). \end{aligned} \quad (65)$$

Finally, observe that

$$J_1^*(v_2^*, v_3^*, v_0^*) \leq F_1(u) - \langle u, v_2^* \rangle_{L^2} + F_2^*(v_2^*, v_3^*, v_0^*) - G^*(v_0^*),$$

$$\forall u \in V_1, v_2^* \in D^*, v_3^* \in B^*, v_0^* \in C^*.$$

Therefore,

$$\sup_{v_0^* \in C^*} J_1^*(v_2^*, v_3^*, v_0^*) \leq \sup_{v_0^* \in C_1^*} \{-\langle u, v_2^* \rangle_{L^2} + F_1(u) + F_2^*(v_2^*, v_3^*, v_0^*) - G^*(v_0^*)\},$$

so that

$$\begin{aligned} & \inf_{(v_2^*, v_3^*) \in D^* \times B^*} \left\{ \sup_{v_0^* \in C^*} J_1^*(v_2^*, v_3^*, v_0^*) \right\} \\ & \leq \inf_{(v_2^*, v_3^*) \in D^* \times B^*} \left\{ \sup_{v_0^* \in C_1^*} \{-\langle u, v_2^* \rangle_{L^2} + F_1(u) + F_2^*(v_2^*, v_3^*, v_0^*) - G^*(v_0^*)\} \right\} \\ & = J(u), \forall u \in V_1. \end{aligned} \quad (66)$$

Summarizing, we have got

$$\begin{aligned} J_1^*(\hat{v}_2^*, \hat{v}_3^*, \hat{v}_0^*) &= \inf_{(v_2^*, v_3^*) \in D^* \times B^*} \left\{ \sup_{v_0^* \in C^*} J_1^*(v_2^*, v_3^*, v_0^*) \right\} \\ &\leq \inf_{u \in V_1} J(u). \end{aligned} \quad (67)$$

Joining the pieces, we have got

$$\begin{aligned} J(u_0) &= \inf_{u \in V_1} J(u) \\ &= \inf_{(v_2^*, v_3^*) \in D^* \times B^*} \left\{ \sup_{v_0^* \in C^*} J_1^*(v_2^*, v_3^*, v_0^*) \right\} \\ &= J_1^*(\hat{v}_2^*, \hat{v}_3^*, \hat{v}_0^*). \end{aligned} \quad (68)$$

The proof is complete.

□

## 10. A duality principle for a related model in phase transition

In this section we present a duality principle for a related model in phase transition.

This case corresponds to the vectorial one in the calculus of variations.

Let  $\Omega \subset \mathbb{R}^n$  be an open, bounded, connected set with a regular (Lipschitzian) boundary denoted by  $\partial\Omega$ .

Consider a functional  $J : V \rightarrow \mathbb{R}$  where

$$J(u) = F(\nabla u_1, \dots, \nabla u_N) + G(u_1, \dots, u_N) - \langle u_i, f_i \rangle_{L^2},$$

and where

$$V = \{u = (u_1, \dots, u_N) \in W^{1,p}(\Omega; \mathbb{R}^N) : u = u_0 \text{ on } \partial\Omega\},$$

$f \in L^2(\Omega; \mathbb{R}^N)$ , and  $1 < p < +\infty$ .

We assume there exists  $\alpha \in \mathbb{R}$  such that

$$\alpha = \inf_{u \in V} J(u).$$

Moreover, suppose  $F$  and  $G$  are Fréchet differentiable but not necessarily convex. A global optimum point may not be attained for  $J$  so that the problem of finding a global minimum for  $J$  may not be a solution.

Anyway, one question remains, how the minimizing sequences behave close the infimum of  $J$ .

We intend to use duality theory to approximately solve such a global optimization problem.

Denoting  $V_0 = W_0^{1,p}(\Omega; \mathbb{R}^N)$ ,  $Y_1 = Y_1^* = L^2(\Omega; \mathbb{R}^{N \times n})$ ,  $Y_2 = Y_2^* = L^2(\Omega; \mathbb{R}^{N \times n})$ ,  $Y_3 = Y_3^* = L^2(\Omega; \mathbb{R}^N)$ , at this point we define,  $F_1 : V \times V_0 \rightarrow \mathbb{R}$ ,  $G_1 : V \rightarrow \mathbb{R}$ ,  $G_2 : V \rightarrow \mathbb{R}$ ,  $G_3 : V_0 \rightarrow \mathbb{R}$  and  $G_4 : V \rightarrow \mathbb{R}$ , by

$$F_1(\nabla u, \nabla \phi) = F(\nabla u_1 + \nabla \phi_1, \dots, \nabla u_N + \nabla \phi_N) + \frac{K}{2} \int_{\Omega} \nabla u_j \cdot \nabla u_j \, dx + \frac{K_2}{2} \int_{\Omega} \nabla \phi_j \cdot \nabla \phi_j \, dx,$$

and

$$G_1(u_1, \dots, u_n) = G(u_1, \dots, u_N) + \frac{K_1}{2} \int_{\Omega} u_j \, u_j \, dx - \langle u_i, f_i \rangle_{L^2},$$

$$G_2(\nabla u_1, \dots, \nabla u_N) = \frac{K_1}{2} \int_{\Omega} \nabla u_j \cdot \nabla u_j \, dx,$$

$$G_3(\nabla \phi_1, \dots, \nabla \phi_N) = \frac{K_2}{2} \int_{\Omega} \nabla \phi_j \cdot \nabla \phi_j \, dx,$$

and

$$G_4(u_1, \dots, u_N) = \frac{K_1}{2} \int_{\Omega} u_j \, u_j \, dx.$$

Define now  $J_1 : V \times V_0 \rightarrow \mathbb{R}$ ,

$$J_1(u, \phi) = F(\nabla u + \nabla \phi) + G(u) - \langle u_i, f_i \rangle_{L^2}.$$

Observe that

$$\begin{aligned} J_1(u, \phi) &= F_1(\nabla u, \nabla \phi) + G_1(u) - G_2(\nabla u) - G_3(\nabla \phi) - G_4(u) \\ &\leq F_1(\nabla u, \nabla \phi) + G_1(u) - \langle \nabla u, z_1^* \rangle_{L^2} - \langle \nabla \phi, z_2^* \rangle_{L^2} - \langle u, z_3^* \rangle_{L^2} \\ &\quad + \sup_{v_1 \in Y_1} \{ \langle v_1, z_1^* \rangle_{L^2} - G_2(v_1) \} \\ &\quad + \sup_{v_2 \in Y_2} \{ \langle v_2, z_2^* \rangle_{L^2} - G_3(v_2) \} \\ &\quad + \sup_{u \in V} \{ \langle u, z_3^* \rangle_{L^2} - G_4(u) \} \\ &= F_1(\nabla u, \nabla \phi) + G_1(u) - \langle \nabla u, z_1^* \rangle_{L^2} - \langle \nabla \phi, z_2^* \rangle_{L^2} - \langle u, z_3^* \rangle_{L^2} \\ &\quad + G_2^*(z_1^*) + G_3^*(z_2^*) + G_4^*(z_3^*) \\ &= J_1^*(u, \phi, z^*), \end{aligned} \tag{69}$$

$\forall u \in V, \phi \in V_0, z^* = (z_1^*, z_2^*, z_3^*) \in Y^* = Y_1^* \times Y_2^* \times Y_3^*$ .

Here we assume  $K, K_1, K_2$  are large enough so that  $F_1$  and  $G_1$  are convex.

Hence, from the general results in [15], we may infer that

$$\inf_{(u,\phi) \in V \times V_0} J(u, \phi) = \inf_{(u,\phi,z^*) \in V \times V_0 \times Y^*} J_1^*(u, \phi, z^*). \quad (70)$$

On the other hand

$$\inf_{u \in V} J(u) \geq \inf_{(u,\phi) \in V \times V_0} J_1(u, \phi) \geq \inf_{u \in V} Q_J(u) = \inf_{u \in V} J(u),$$

where  $Q_J(u)$  refers to a standard quasi-convex regularization of  $J$ .

From these last two results we may obtain

$$\inf_{u \in V} J(u) = \inf_{(u,\phi,z^*) \in V \times V_0 \times Y^*} J_1^*(u, \phi, z^*).$$

Moreover, from standards results on convex analysis, we may have

$$\begin{aligned} \inf_{u \in V} J_1^*(u, \phi, z^*) &= \inf_{u \in V} \{F_1(\nabla u, \nabla \phi) + G_1(u) \\ &\quad - \langle \nabla u, z_1^* \rangle_{L^2} - \langle \nabla \phi, z_2^* \rangle_{L^2} - \langle u, z_3^* \rangle_{L^2} \\ &\quad + G_2^*(z_1^*) + G_3^*(z_2^*) + G_4^*(z_3^*)\} \\ &= \sup_{(v_1^*, v_2^*) \in C^*} \{-F_1^*(v_1^* + z_1^*, \nabla \phi) - G_1^*(v_2^* + z_3^*) - \langle \nabla \phi, z_2^* \rangle_{L^2} \\ &\quad + G_2^*(z_1^*) + G_3^*(z_2^*) + G_4^*(z_3^*)\}, \end{aligned} \quad (71)$$

where

$$\begin{aligned} C^* &= \{v^* = (v_1^*, v_2^*) \in Y_1^* \times Y_3^* : -\operatorname{div}(v_1^*)_i + (v_2^*)_i = 0, \forall i \in \{1, \dots, N\}\}, \\ F_1^*(v_1^* + z_1^*, \nabla \phi) &= \sup_{v_1 \in Y_1} \{\langle v_1, z_1^* + v_1^* \rangle_{L^2} - F_1(v_1, \nabla \phi)\}, \end{aligned}$$

and

$$G_1^*(v_2^* + z_2^*) = \sup_{u \in V} \{\langle u, v_2^* + z_2^* \rangle_{L^2} - G_1(u)\}.$$

Thus, defining

$$J_2^*(\phi, z^*, v^*) = F_1^*(v_1^* + z_1^*, \nabla \phi) - G_1^*(v_2^* + z_3^*) - \langle \nabla \phi, z_2^* \rangle_{L^2} + G_2^*(z_1^*) + G_3^*(z_2^*) + G_4^*(z_3^*),$$

we have got

$$\begin{aligned} \inf_{u \in V} J(u) &= \inf_{(u,\phi) \in V \times V_0} J_1(u, \phi) \\ &= \inf_{(u,\phi,z^*) \in V \times V_0 \times Y^*} J_1^*(u, \phi, z^*) \\ &= \inf_{z^* \in Y^*} \left\{ \inf_{\phi \in V_0} \left\{ \sup_{v^* \in C^*} J_2^*(\phi, z^*, v^*) \right\} \right\}. \end{aligned} \quad (72)$$

Finally, observe that

$$\begin{aligned} & \inf_{u \in V} J(u) \\ &= \inf_{z^* \in Y^*} \left\{ \inf_{\phi \in V_0} \left\{ \sup_{v^* \in C^*} J_2^*(\phi, z^*, v^*) \right\} \right\} \\ &\geq \sup_{v^* \in C^*} \left\{ \inf_{(z^*, \phi) \in Y^* \times V_0} J_2^*(\phi, z^*, v^*) \right\}. \end{aligned} \quad (73)$$

This last variational formulation corresponds to a concave relaxed formulation in  $v^*$  concerning the original primal formulation.

### 11. Another duality principle for a simpler related model in phase transition with a respective numerical example

In this section we present another duality principle for a related model in phase transition.

Let  $\Omega = [0, 1] \subset \mathbb{R}$  and consider a functional  $J : V \rightarrow \mathbb{R}$  where

$$J(u) = \frac{1}{2} \int_{\Omega} ((u')^2 - 1)^2 dx + \frac{1}{2} \int_{\Omega} u^2 dx - \langle u, f \rangle_{L^2},$$

and where

$$V = \{u \in W^{1,4}(\Omega) : u(0) = 0 \text{ and } u(1) = 1/2\}$$

and  $f \in L^2(\Omega)$ .

A global optimum point is not attained for  $J$  so that the problem of finding a global minimum for  $J$  has no solution.

Anyway, one question remains, how the minimizing sequences behave close the infimum of  $J$ .

We intend to use duality theory to approximately solve such a global optimization problem.

Denoting  $V_0 = W_0^{1,4}(\Omega)$ , at this point we define,  $F : V \rightarrow \mathbb{R}$  and  $F_1 : V \times V_0 \rightarrow \mathbb{R}$  by

$$F(u) = \frac{1}{2} \int_{\Omega} ((u')^2 - 1)^2 dx,$$

and

$$F_1(u, \phi) = \frac{1}{2} \int_{\Omega} ((u' + \phi')^2 - 1)^2 dx.$$

Observe

$$F(u) \geq \inf_{\phi \in V_0} F_1(u, \phi) \geq Q_F(u), \quad \forall u \in V,$$

where  $Q_F(u)$  refers to a quasi-convex regularization of  $F$ .

We define also

$$F_2 : V \times V_0 \rightarrow \mathbb{R},$$

$$F_3 : V \times V_0 \rightarrow \mathbb{R}$$

and

$$G : V \times V_0 \rightarrow \mathbb{R}$$

by

$$F_2(u, \phi) = \frac{1}{2} \int_{\Omega} ((u' + \phi')^2 - 1)^2 dx + \frac{1}{2} \int_{\Omega} u^2 dx - \langle u, f \rangle_{L^2},$$

$$F_3(u, \phi) = F_2(u, \phi) + \frac{K}{2} \int_{\Omega} (u')^2 dx + \frac{K_1}{2} \int_{\Omega} (\phi')^2 dx \quad (74)$$

and

$$G(u, \phi) = \frac{K}{2} \int_{\Omega} (u')^2 dx + \frac{K_1}{2} \int_{\Omega} (\phi')^2 dx \quad (75)$$

Observe that if  $K > 0, K_1 > 0$  is large enough, both  $F_3$  and  $G$  are convex.

Denoting  $Y = Y^* = L^2(\Omega)$  we also define the polar functional  $G^* : Y^* \times Y^* \rightarrow \mathbb{R}$  by

$$G^*(v^*, v_0^*) = \sup_{(u, \phi) \in V \times V_0} \{ \langle u, v^* \rangle_{L^2} + \langle \phi, v_0^* \rangle_{L^2} - G(u, \phi) \}.$$

Observe that

$$\inf_{u \in U} J(u) \geq \inf_{((u, \phi), (v^*, v_0^*)) \in V \times V_0 \times [Y^*]^2} \{ G^*(v^*, v_0^*) - \langle u, v^* \rangle_{L^2} - \langle \phi, v_0^* \rangle_{L^2} + F_3(u, \phi) \}.$$

With such results in mind, we define a relaxed primal dual variational formulation for the primal problem, represented by  $J_1^* : V \times V_0 \times [Y^*]^2 \rightarrow \mathbb{R}$ , where

$$J_1^*(u, \phi, v^*, v_0^*) = G^*(v^*, v_0^*) - \langle u, v^* \rangle_{L^2} - \langle \phi, v_0^* \rangle_{L^2} + F_3(u, \phi).$$

Having defined such a functional, we may obtain numerical results by solving a sequence of convex auxiliary sub-problems, through the following algorithm.

1. Set  $K \approx 150$  and  $K_1 = K/20$  and  $0 < \varepsilon \ll 1$ .
2. Choose  $(u_1, \phi_1) \in V \times V_0$ , such that  $\|u_1\|_{1,\infty} \ll K/4$  and  $\|\phi_1\|_{1,\infty} \ll K/4$ .
3. Set  $n = 1$ .
4. Calculate  $(v_n^*, (v_0^*)_n)$  solution of the system of equations:

$$\frac{\partial J_1^*(u_n, \phi_n, v_n^*, (v_0^*)_n)}{\partial v^*} = 0$$

and

$$\frac{\partial J_1^*(u_n, \phi_n, v_n^*, (v_0^*)_n)}{\partial v_0^*} = 0,$$

that is

$$\frac{\partial G^*(v_n^*, (v_0^*)_n)}{\partial v^*} - u_n = 0$$

and

$$\frac{\partial G^*(v_n^*, (v_0^*)_n)}{\partial v_0^*} - \phi_n = 0$$

so that

$$v_n^* = \frac{\partial G(u_n, \phi_n)}{\partial u}$$

and

$$(v_0^*)_n = \frac{\partial G(u_n, \phi_n)}{\partial \phi}$$

5. Calculate  $(u_{n+1}, \phi_{n+1})$  by solving the system of equations:

$$\frac{\partial J_1^*(u_{n+1}, \phi_{n+1}, v_n^*, (v_0^*)_n)}{\partial u} = 0$$

and

$$\frac{\partial J_1^*(u_{n+1}, \phi_{n+1}, v_n^*, (v_0^*)_n)}{\partial \phi} = 0$$

that is

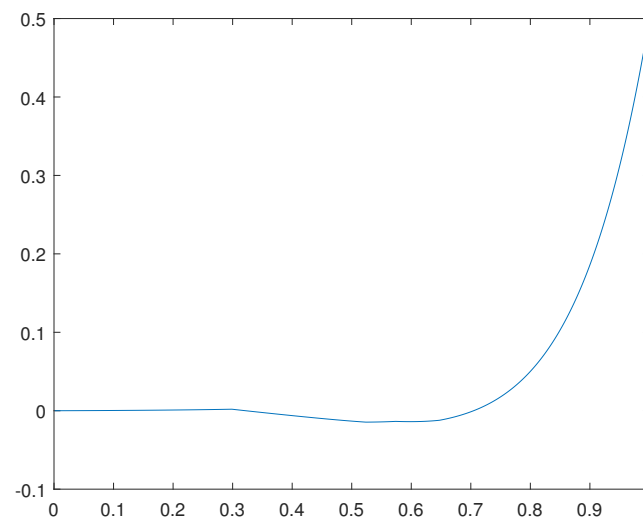
$$-v_n^* + \frac{\partial F_3(u_{n+1}, \phi_{n+1})}{\partial u} = 0$$

and

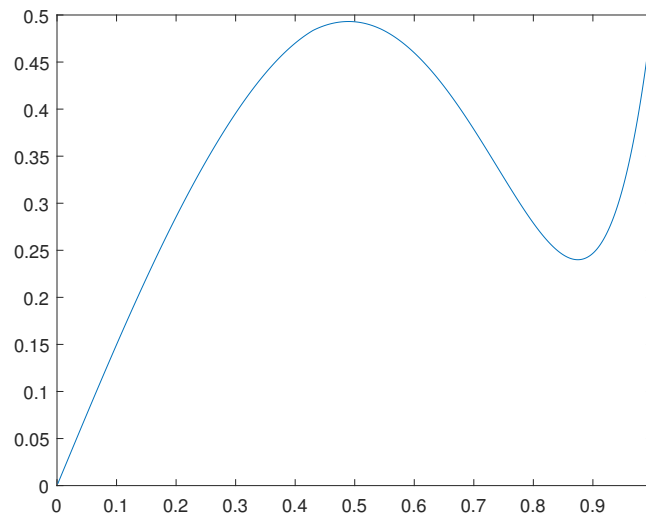
$$-(v_0^*)_n + \frac{\partial F_3(u_{n+1}, \phi_{n+1})}{\partial \phi} = 0$$

6. If  $\max\{\|u_n - u_{n+1}\|, \|\phi_{n+1} - \phi_n\|_\infty\} \leq \varepsilon$ , then stop, else set  $n := n + 1$  and go to item 4.

For the case in which  $f(x) = 0$ , we have obtained numerical results for  $K = 1500$  and  $K_1 = K/20$ . For such a concerning solution  $u_0$  obtained, please see Figure 1. For the case in which  $f(x) = \sin(\pi x)/2$ , we have obtained numerical results for  $K = 100$  and  $K_1 = K/20$ . For such a concerning solution  $u_0$  obtained, please see Figure 2.



**Figure 1.** solution  $u_0(x)$  for the case  $f(x) = 0$ .



**Figure 2.** solution  $u_0(x)$  for the case  $f(x) = \sin(\pi x)/2$ .

**Remark 11.1.** Observe that the solutions obtained are approximate critical points. They are not, in a classical sense, the global solutions for the related optimization problems. Indeed, such solutions reflect the average behavior of weak cluster points for concerning minimizing sequences.

## 12. A convex dual variational formulation for a third similar model

In this section we present another duality principle for a third related model in phase transition.

Let  $\Omega = [0, 1] \subset \mathbb{R}$  and consider a functional  $J : V \rightarrow \mathbb{R}$  where

$$J(u) = \frac{1}{2} \int_{\Omega} \min\{(u' - 1)^2, (u' + 1)^2\} dx + \frac{1}{2} \int_{\Omega} u^2 dx - \langle u, f \rangle_{L^2},$$

and where

$$V = \{u \in W^{1,2}(\Omega) : u(0) = 0 \text{ and } u(1) = 1/2\}$$

and  $f \in L^2(\Omega)$ .

A global optimum point is not attained for  $J$  so that the problem of finding a global minimum for  $J$  has no solution.

Anyway, one question remains, how the minimizing sequences behave close to the infimum of  $J$ .

We intend to use the duality theory to solve such a global optimization problem in an appropriate sense to be specified.

At this point we define,  $F : V \rightarrow \mathbb{R}$  and  $G : V \rightarrow \mathbb{R}$  by

$$\begin{aligned} F(u) &= \frac{1}{2} \int_{\Omega} \min\{(u' - 1)^2, (u' + 1)^2\} dx \\ &= \frac{1}{2} \int_{\Omega} (u')^2 dx - \int_{\Omega} |u'| dx + 1/2 \\ &\equiv F_1(u'), \end{aligned} \tag{76}$$

and

$$G(u) = \frac{1}{2} \int_{\Omega} u^2 dx - \langle u, f \rangle_{L^2}.$$

Denoting  $Y = Y^* = L^2(\Omega)$  we also define the polar functional  $F_1^* : Y^* \rightarrow \mathbb{R}$  and  $G^* : Y^* \rightarrow \mathbb{R}$  by

$$\begin{aligned}
 F_1^*(v^*) &= \sup_{v \in Y} \{ \langle v, v^* \rangle_{L^2} - F_1(v) \} \\
 &= \frac{1}{2} \int_{\Omega} (v^*)^2 dx + \int_{\Omega} |v^*| dx,
 \end{aligned} \tag{77}$$

and

$$\begin{aligned}
 G^*(-(v^*)') &= \sup_{u \in V} \{ \langle u', v^* \rangle_{L^2} - G(u) \} \\
 &= \frac{1}{2} \int_{\Omega} ((v^*)' + f)^2 dx - \frac{1}{2} v^*(1).
 \end{aligned} \tag{78}$$

Observe this is the scalar case of the calculus of variations, so that from the standard results on convex analysis, we have

$$\inf_{u \in V} J(u) = \max_{v^* \in Y^*} \{ -F_1^*(v^*) - G^*(-(v^*)') \}.$$

Indeed, from the direct method of the calculus of variations, the maximum for the dual formulation is attained at some  $\hat{v}^* \in Y^*$ .

Moreover, the corresponding solution  $u_0 \in V$  is obtained from the equation

$$u_0 = \frac{\partial G(-(\hat{v}^*))}{\partial (v^*)'} = (\hat{v}^*)' + f.$$

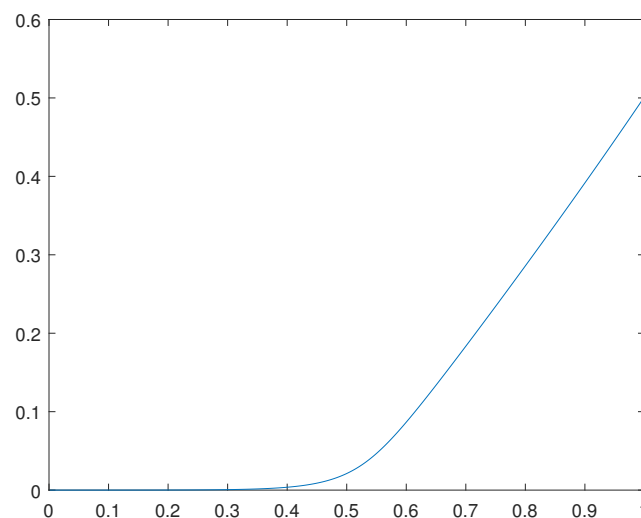
Finally, the Euler-Lagrange equations for the dual problem stands for

$$\begin{cases} (v^*)'' + f' - v^* - \text{sign}(v^*) = 0, & \text{in } \Omega, \\ (v^*)'(0) = 0, (v^*)'(1) = 1/2. \end{cases} \tag{79}$$

We have computed the solutions  $v^*$  and corresponding solutions  $u_0 \in V$  for the cases in which  $f(x) = 0$  and  $f(x) = \sin(\pi x)/2$ .

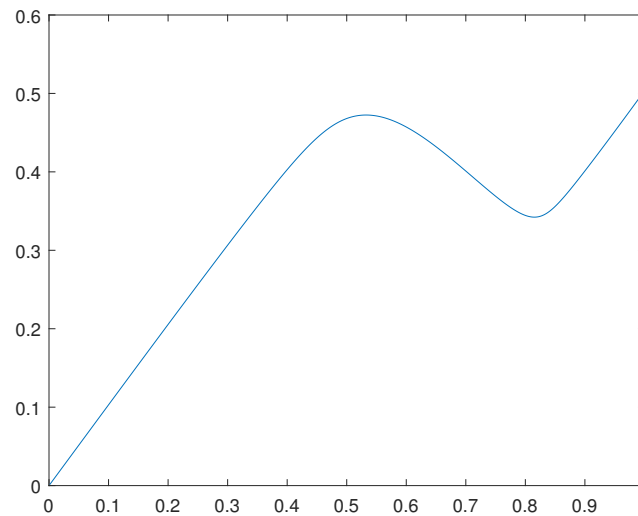
For the solution  $u_0(x)$  for the case in which  $f(x) = 0$ , please see Figure 3.

For the solution  $u_0(x)$  for the case in which  $f(x) = \sin(\pi x)/2$ , please see Figure 4.



**Figure 3.** solution  $u_0(x)$  for the case  $f(x) = 0$ .





**Figure 4.** solution  $u_0(x)$  for the case  $f(x) = \sin(\pi x)/2$ .

**Remark 12.1.** Observe that such solutions  $u_0$  obtained are not the global solutions for the related primal optimization problems. Indeed, such solutions reflect the average behavior of weak cluster points for concerning minimizing sequences.

### 13. A related numerical computation through the generalized method of lines

We start by recalling that the generalized method of lines was originally introduced in the book entitled "Topics on Functional Analysis, Calculus of Variations and Duality" [7], published in 2011.

Indeed, the present results are extensions and applications of previous ones which have been published since 2011, in books and articles such as [5,7–9]. About the Sobolev spaces involved we would mention [1]. Concerning the applications, related models in physics are addressed in [4,11].

We also emphasize that, in such a method, the domain of the partial differential equation in question is discretized in lines (or more generally, in curves) and the concerning solution is written on these lines as functions of boundary conditions and the domain boundary shape.

In fact, in its previous format, this method consists of an application of a kind of a partial finite differences procedure combined with the Banach fixed point theorem to obtain the relation between two adjacent lines (or curves).

In the present article, we propose an improvement concerning the way we truncate the series solution obtained through an application of the Banach fixed point theorem to find the relation between two adjacent lines. The results obtained are very good even as a typical parameter  $\varepsilon > 0$  is very small.

In the next lines and sections we develop in details such a numerical procedure.

#### 13.1. About a concerning improvement for the generalized method of lines

Let  $\Omega \subset \mathbb{R}^2$  where

$$\Omega = \{(r, \theta) \in \mathbb{R}^2 : 1 \leq r \leq 2, 0 \leq \theta \leq 2\pi\}.$$

Consider the problem of solving the partial differential equation

$$\begin{cases} -\varepsilon \left( \frac{\partial^2 u}{\partial r^2} + \frac{1}{r} \frac{\partial u}{\partial r} + \frac{1}{r^2} \frac{\partial^2 u}{\partial \theta^2} \right) + \alpha u^3 - \beta u = f, & \text{in } \Omega, \\ u = u_0(\theta), & \text{on } \partial\Omega_1, \\ u = u_f(\theta), & \text{on } \partial\Omega_2. \end{cases} \quad (80)$$

Here

$$\Omega = \{(r, \theta) \in \mathbb{R}^2 : 1 \leq r \leq 2, 0 \leq \theta \leq 2\pi\},$$

$$\partial\Omega_1 = \{(1, \theta) \in \mathbb{R}^2 : 0 \leq \theta \leq 2\pi\},$$

$$\partial\Omega_2 = \{(2, \theta) \in \mathbb{R}^2 : 0 \leq \theta \leq 2\pi\},$$

$\varepsilon > 0$ ,  $\alpha > 0$ ,  $\beta > 0$ , and  $f \equiv 1$ , on  $\Omega$ .

In a partial finite differences scheme, such a system stands for

$$-\varepsilon \left( \frac{u_{n+1} - 2u_n + u_{n-1}}{d^2} + \frac{1}{t_n} \frac{u_n - u_{n-1}}{d} + \frac{1}{t_n^2} \frac{\partial^2 u_n}{\partial \theta^2} \right) + \alpha u_n^3 - \beta u_n = f_n,$$

$\forall n \in \{1, \dots, N-1\}$ , with the boundary conditions

$$u_0 = 0,$$

and

$$u_N = 0.$$

Here  $N$  is the number of lines and  $d = 1/N$ .

In particular, for  $n = 1$  we have

$$-\varepsilon \left( \frac{u_2 - 2u_1 + u_0}{d^2} + \frac{1}{t_1} \frac{(u_1 - u_0)}{d} + \frac{1}{t_1^2} \frac{\partial^2 u_1}{\partial \theta^2} \right) + \alpha u_1^3 - \beta u_1 = f_1,$$

so that

$$u_1 = \left( u_2 + u_1 + u_0 + \frac{1}{t_1} (u_1 - u_0) d + \frac{1}{t_1^2} \frac{\partial^2 u_1}{\partial \theta^2} d^2 + (-\alpha u_1^3 + \beta u_1 - f_1) \frac{d^2}{\varepsilon} \right) / 3.0,$$

We solve this last equation through the Banach fixed point theorem, obtaining  $u_1$  as a function of  $u_2$ .

Indeed, we may set

$$u_1^0 = u_2$$

and

$$\begin{aligned} u_1^{k+1} = & \left( u_2 + u_1^k + u_0 + \frac{1}{t_1} (u_1^k - u_0) d + \frac{1}{t_1^2} \frac{\partial^2 u_1^k}{\partial \theta^2} d^2 \right. \\ & \left. + (-\alpha (u_1^k)^3 + \beta u_1^k - f_1) \frac{d^2}{\varepsilon} \right) / 3.0, \end{aligned} \quad (81)$$

$\forall k \in \mathbb{N}$ .

Thus, we may obtain

$$u_1 = \lim_{k \rightarrow \infty} u_1^k \equiv H_1(u_2, u_0).$$

Similarly, for  $n = 2$ , we have

$$\begin{aligned} u_2 = & \left( u_3 + u_2 + H_1(u_2, u_0) + \frac{1}{t_1} (u_2 - H_1(u_2, u_0)) d + \frac{1}{t_1^2} \frac{\partial^2 u_2}{\partial \theta^2} d^2 \right. \\ & \left. + (-\alpha u_2^3 + \beta u_2 - f_2) \frac{d^2}{\varepsilon} \right) / 3.0, \end{aligned} \quad (82)$$

We solve this last equation through the Banach fixed point theorem, obtaining  $u_2$  as a function of  $u_3$  and  $u_0$ .

Indeed, we may set

$$u_2^0 = u_3$$

and

$$\begin{aligned} u_2^{k+1} = & \left( u_3 + u_2^k + H_1(u_2^k, u_0) + \frac{1}{t_2}(u_2^k - H_1(u_2^k, u_0)) d + \frac{1}{t_2^2} \frac{\partial^2 u_2^k}{\partial \theta^2} d^2 \right. \\ & \left. + (-\alpha(u_2^k)^3 + \beta u_2^k - f_2) \frac{d^2}{\varepsilon} \right) / 3.0, \end{aligned} \quad (83)$$

$\forall k \in \mathbb{N}$ .

Thus, we may obtain

$$u_2 = \lim_{k \rightarrow \infty} u_2^k \equiv H_2(u_3, u_0).$$

Now reasoning inductively, having

$$u_{n-1} = H_{n-1}(u_n, u_0),$$

we may get

$$\begin{aligned} u_n = & \left( u_{n+1} + u_n + H_{n-1}(u_n, u_0) + \frac{1}{t_n}(u_n - H_{n-1}(u_n, u_0)) d + \frac{1}{t_n^2} \frac{\partial^2 u_n}{\partial \theta^2} d^2 \right. \\ & \left. + (-\alpha u_n^3 + \beta u_n - f_n) \frac{d^2}{\varepsilon} \right) / 3.0, \end{aligned} \quad (84)$$

We solve this last equation through the Banach fixed point theorem, obtaining  $u_n$  as a function of  $u_{n+1}$  and  $u_0$ .

Indeed, we may set

$$u_n^0 = u_{n+1}$$

and

$$\begin{aligned} u_n^{k+1} = & \left( u_{n+1} + u_n^k + H_{n-1}(u_n^k, u_0) + \frac{1}{t_n}(u_n^k - H_{n-1}(u_n^k, u_0)) d + \frac{1}{t_n^2} \frac{\partial^2 u_n^k}{\partial \theta^2} d^2 \right. \\ & \left. + (-\alpha(u_n^k)^3 + \beta u_n^k - f_n) \frac{d^2}{\varepsilon} \right) / 3.0, \end{aligned} \quad (85)$$

$\forall k \in \mathbb{N}$ .

Thus, we may obtain

$$u_n = \lim_{k \rightarrow \infty} u_n^k \equiv H_n(u_{n+1}, u_0).$$

We have obtained  $u_n = H_n(u_{n+1}, u_0), \forall n \in \{1, \dots, N-1\}$ .

In particular,  $u_N = u_f(\theta)$ , so that we may obtain

$$u_{N-1} = H_{N-1}(u_N, u_0) = H_{N-1}(0) \equiv F_{N-1}(u_N, u_0) = F_{N-1}(u_f(\theta), u_0(\theta)).$$

Similarly,

$$u_{N-2} = H_{N-2}(u_{N-1}, u_0) = H_{N-2}(H_{N-1}(u_N, u_0)) = F_{N-2}(u_N, u_0) = F_{N-1}(u_f(\theta), u_0(\theta)),$$

an so on, up to obtaining

$$u_1 = H_1(u_2) \equiv F_1(u_N, u_0) = F_1(u_f(\theta), u_0(\theta)).$$

The problem is then approximately solved.

### 13.2. Software in Mathematica for solving such an equation

We recall that the equation to be solved is a Ginzburg-Landau type one, where

$$\begin{cases} -\varepsilon \left( \frac{\partial^2 u}{\partial r^2} + \frac{1}{r} \frac{\partial u}{\partial r} + \frac{1}{r^2} \frac{\partial^2 u}{\partial \theta^2} \right) + \alpha u^3 - \beta u = f, & \text{in } \Omega, \\ u = 0, & \text{on } \partial\Omega_1, \\ u = u_f(\theta), & \text{on } \partial\Omega_2. \end{cases} \quad (86)$$

Here

$$\Omega = \{(r, \theta) \in \mathbb{R}^2 : 1 \leq r \leq 2, 0 \leq \theta \leq 2\pi\},$$

$$\partial\Omega_1 = \{(1, \theta) \in \mathbb{R}^2 : 0 \leq \theta \leq 2\pi\},$$

$$\partial\Omega_2 = \{(2, \theta) \in \mathbb{R}^2 : 0 \leq \theta \leq 2\pi\},$$

$\varepsilon > 0$ ,  $\alpha > 0$ ,  $\beta > 0$ , and  $f \equiv 1$ , on  $\Omega$ . In a partial finite differences scheme, such a system stands for

$$-\varepsilon \left( \frac{u_{n+1} - 2u_n + u_{n-1}}{d^2} + \frac{1}{t_n} \frac{u_n - u_{n-1}}{d} + \frac{1}{t_n^2} \frac{\partial^2 u_n}{\partial \theta^2} \right) + \alpha u_n^3 - \beta u_n = f_n,$$

$\forall n \in \{1, \dots, N-1\}$ , with the boundary conditions

$$u_0 = 0,$$

and

$$u_N = u_f[x].$$

Here  $N$  is the number of lines and  $d = 1/N$ .

At this point we present the concerning software for an approximate solution.

Such a software is for  $N = 10$  (10 lines) and  $u_0[x] = 0$ .

\*\*\*\*\*

```

1. m8 = 10; (N = 10 lines)
2. d = 1/m8;
3. e1 = 0.1; (ε = 0.1)
4. A = 1.0;
5. B = 1.0;
6. For[i = 1, i < m8, i++, f[i] = 1.0]; (f ≡ 1, on Ω)
7. a = 0.0;
8. For[i = 1, i < m8, i++,
  Clear[b, u];
  t[i] = 1 + i * d;
  b[x_] = u[i + 1][x];
9. For[k = 1, k < 30, k++, (we have fixed the number of iterations)
  z = (u[i + 1][x] + b[x] + a + 1/t[i] (b[x] - a) * d
  + 1/t[i]^2 D[b[x], {x, 2}] * d^2 + (-A * b[x]^3 + B * u[x] + f[i]) * d^2/e1) / 3.0;
  z =
  Series[z, {u[i + 1][x], 0, 3}, {u[i + 1]'[x], 0, 1}, {u[i + 1]''[x], 0, 1},
  {u[i + 1]'''[x], 0, 0}, {u[i + 1]''''[x], 0, 0}];
  z = Normal[z],

```

```

z = Expand[z];
b[x_] = z];
10. a1[i] = z;
11. Clear[b];
12. u[i + 1][x_] = b[x];
13. a = a1[i] ];
14. b[x_] = u_f[x];
15. For[i = 1, i < m8, i ++,
    A1 = a1[m8 - i];
    A1 = Series[A1, {u_f[x], 0, 3}, {u'_f[x], 0, 1}, {u''_f[x], 0, 1}, {u'''_f[x], 0, 0}, {u''''_f[x], 0, 0}];
    A1 = Normal[A1];
    A1 = Expand[A1];
    u[m8 - i][x_] = A1;
    b[x_] = A1];
Print[u[m8/2][x]];

```

\*\*\*\*\*

The numerical expressions for the solutions of the concerning  $N = 10$  lines are given by

$$\begin{aligned}
 u[1][x] = & 0.47352 + 0.00691u_f[x] - 0.00459u_f[x]^2 + 0.00265u_f[x]^3 + 0.00039(u''_f)[x] \\
 & - 0.00058u_f[x](u''_f)[x] + 0.00050u_f[x]^2(u''_f)[x] - 0.000181213u_f[x]^3(u''_f)[x]
 \end{aligned} \quad (87)$$

$$\begin{aligned}
 u[2][x] = & 0.76763 + 0.01301u_f[x] - 0.00863u_f[x]^2 + 0.00497u_f[x]^3 + 0.00068(u''_f)[x] \\
 & - 0.00103u_f[x](u''_f)[x] + 0.00088u_f[x]^2(u''_f)[x] - 0.00034u_f[x]^3(u''_f)[x]
 \end{aligned} \quad (88)$$

$$\begin{aligned}
 u[3][x] = & 0.91329 + 0.02034u_f[x] - 0.01342u_f[x]^2 + 0.00768u_f[x]^3 + 0.00095(u''_f)[x] \\
 & - 0.00144u_f[x](u''_f)[x] + 0.00122u_f[x]^2(u''_f)[x] - 0.00051u_f[x]^3(u''_f)[x]
 \end{aligned} \quad (89)$$

$$\begin{aligned}
 u[4][x] = & 0.97125 + 0.03623u_f[x] - 0.02328u_f[x]^2 + 0.01289u_f[x]^3 + 0.00147331(u''_f)[x] \\
 & - 0.00223u_f[x](u''_f)[x] + 0.00182u_f[x]^2(u''_f)[x] - 0.00074u_f[x]^3(u''_f)[x]
 \end{aligned} \quad (90)$$

$$\begin{aligned}
 u[5][x] = & 1.01736 + 0.09242u_f[x] - 0.05110u_f[x]^2 + 0.02387u_f[x]^3 + 0.00211(u''_f)[x] \\
 & - 0.00378u_f[x](u''_f)[x] + 0.00292u_f[x]^2(u''_f)[x] - 0.00132u_f[x]^3(u''_f)[x]
 \end{aligned} \quad (91)$$

$$\begin{aligned}
 u[6][x] = & 1.02549 + 0.21039u_f[x] - 0.09374u_f[x]^2 + 0.03422u_f[x]^3 + 0.00147(u''_f)[x] \\
 & - 0.00634u_f[x](u''_f)[x] + 0.00467u_f[x]^2(u''_f)[x] - 0.00200u_f[x]^3(u''_f)[x]
 \end{aligned} \quad (92)$$

$$u[7][x] = 0.93854 + 0.36459u_f[x] - 0.14232u_f[x]^2 + 0.04058u_f[x]^3 + 0.00259(u_f''[x]) \\ - 0.00747373u_f[x](u_f''[x]) + 0.0047969u_f[x]^2(u_f''[x]) - 0.00194u_f[x]^3(u_f''[x]) \quad (93)$$

$$u[8][x] = 0.74649 + 0.57201u_f[x] - 0.17293u_f[x]^2 + 0.02791u_f[x]^3 + 0.00353(u_f''[x]) \\ - 0.00658u_f[x](u_f''[x]) + 0.00407u_f[x]^2(u_f''[x]) - 0.00172u_f[x]^3(u_f''[x]) \quad (94)$$

$$u[9][x] = 0.43257 + 0.81004u_f[x] - 0.13080u_f[x]^2 + 0.00042u_f[x]^3 + 0.00294(u_f''[x]) \\ - 0.00398u_f[x](u_f''[x]) + 0.00222u_f[x]^2(u_f''[x]) - 0.00066u_f[x]^3(u_f''[x]) \quad (95)$$

### 13.3. Some plots concerning the numerical results

In this section we present the lines 2, 4, 6, 8 related to results obtained in the last section.

Indeed, we present such mentioned lines, in a first step, for the previous results obtained through the generalized of lines and, in a second step, through a numerical method which is combination of the Newton's one and the generalized method of lines. In a third step, we also present the graphs by considering the expression of the lines as those also obtained through the generalized method of lines, up to the numerical coefficients for each function term, which are obtained by the numerical optimization of the functional  $J$ , below specified. We consider the case in which  $u_0(x) = 0$  and  $u_f(x) = \sin(x)$ .

For the procedure mentioned above as the third step, recalling that  $N = 10$  lines, considering that  $u_f''(x) = -u_f(x)$ , we may approximately assume the following general line expressions:

$$u_n(x) = a(1, n) + a(2, n)u_f(x) + a(3, n)u_f(x)^3 + a(4, n)u_f(x)^3, \quad \forall n \in \{1, \dots, N-1\}.$$

Defining

$$W_n = -e_1 \frac{(u_{n+1}(x) - 2u_n(x) + u_{n-1}(x))}{d^2} - \frac{e_1}{t_n} \frac{(u_n(x) - u_{n-1}(x))}{d} - \frac{e_1}{t_n^2} u_n''(x) + u_n(x)^3 - u_n(x) - 1,$$

and

$$J(\{a(j, n)\}) = \sum_{n=1}^{N-1} \int_0^{2\pi} (W_n)^2 dx$$

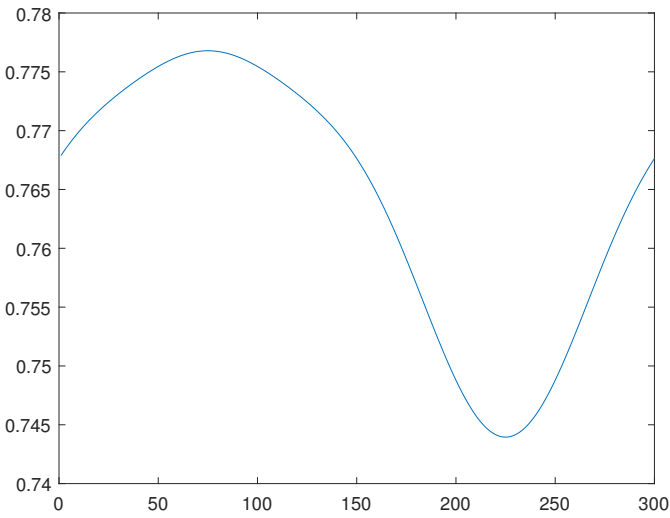
we obtain  $\{a(j, n)\}$  by numerically minimizing  $J$ .

Hence, we have obtained the following lines for these cases. For such graphs, we have considered 300 nodes in  $x$ , with  $2\pi/300$  as units in  $x \in [0, 2\pi]$ .

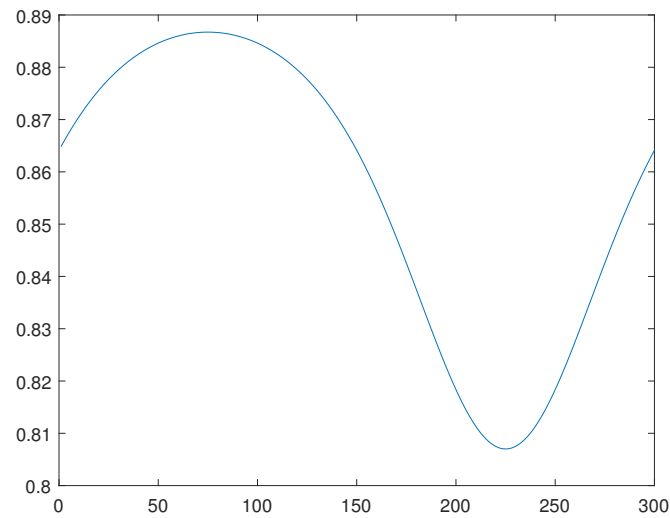
For the Lines 2, 4, 6, 8, through the generalized method of lines, please see Figures 5, 8, 11, 14.

For the Lines 2, 4, 6, 8, through a combination of the Newton's and the generalized method of lines, please see Figures 6, 9, 12, 15.

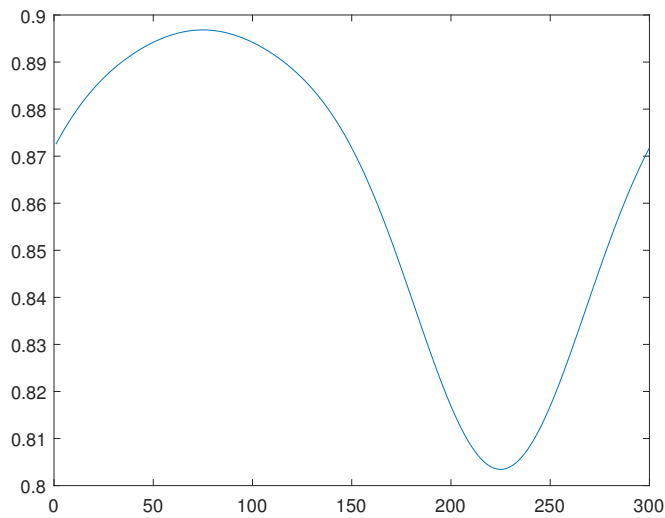
Finally, for the Line 2, 4, 6, 8 obtained through the minimization of the functional  $J$ , please see Figures 7, 10, 13, 16.



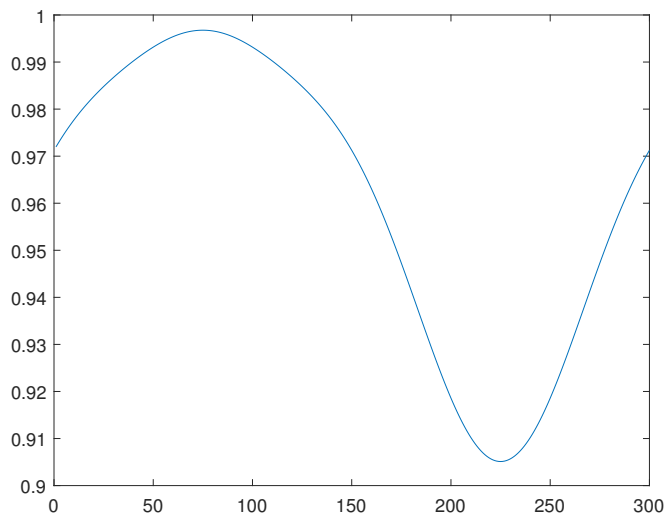
**Figure 5.** Line 2, solution  $u_2(x)$  through the general method of lines



**Figure 6.** Line 2, solution  $u_2(x)$  through the Newton's Method

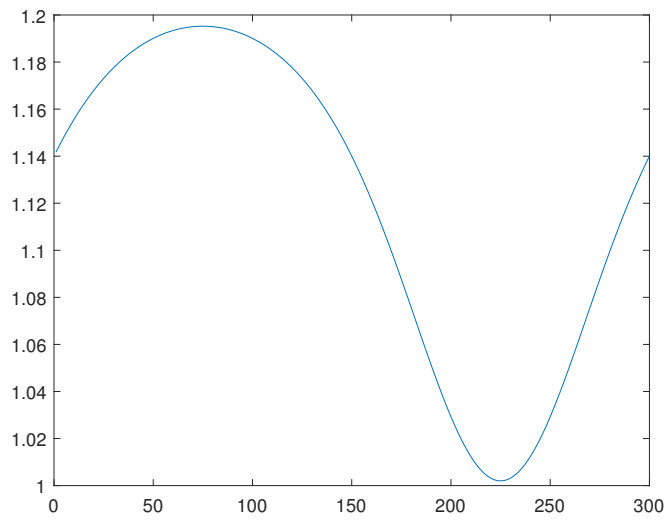


**Figure 7.** Line 2, solution  $u_2(x)$  through the minimization of functional  $J$

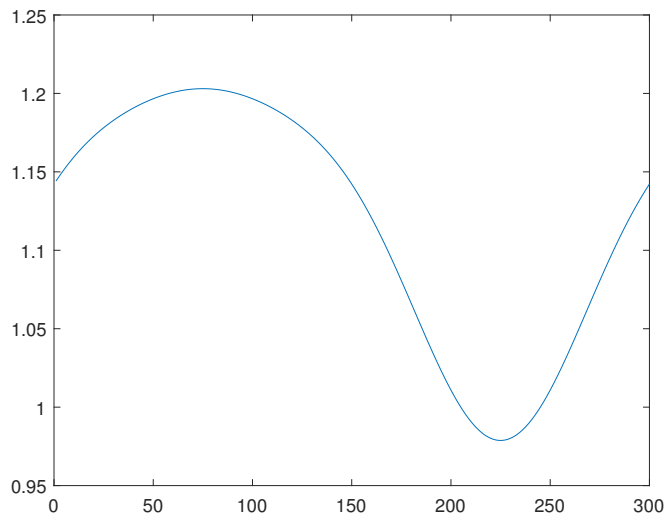


**Figure 8.** Line 4, solution  $u_4(x)$  through the general method of lines

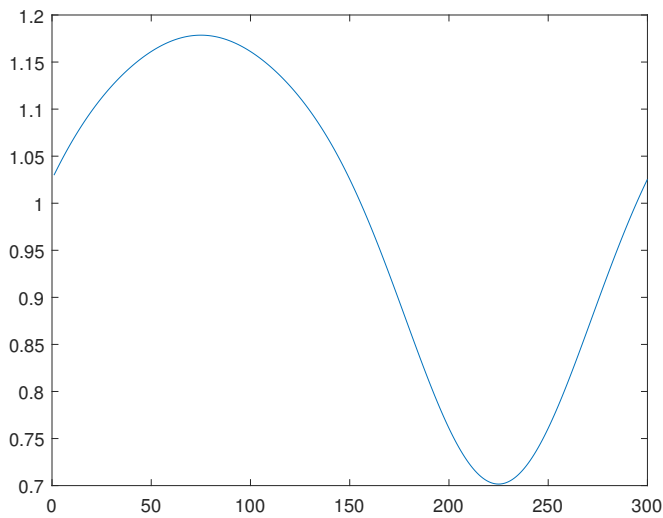




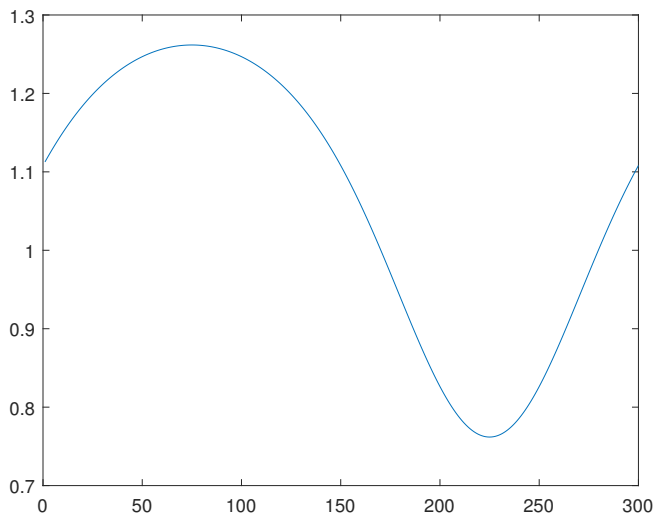
**Figure 9.** Line 4, solution  $u_4(x)$  through the Newton's Method



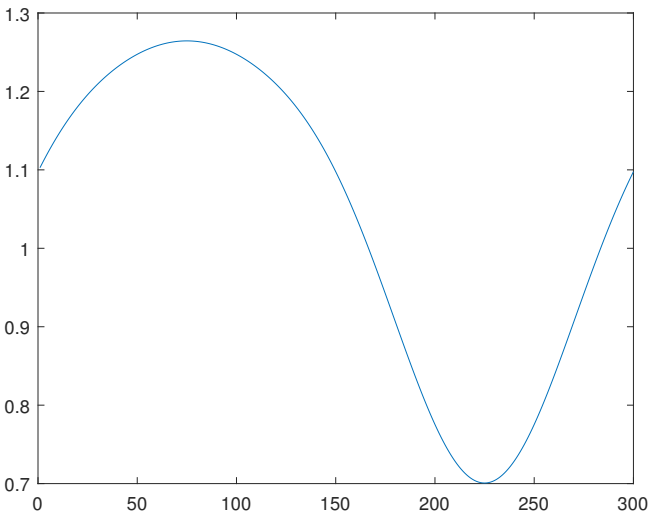
**Figure 10.** Line 4, solution  $u_4(x)$  through the minimization of functional  $J$



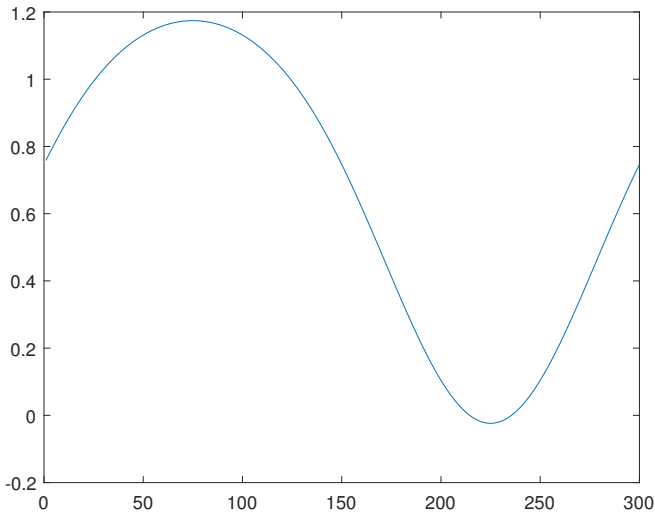
**Figure 11.** Line 6, solution  $u_6(x)$  through the general method of lines



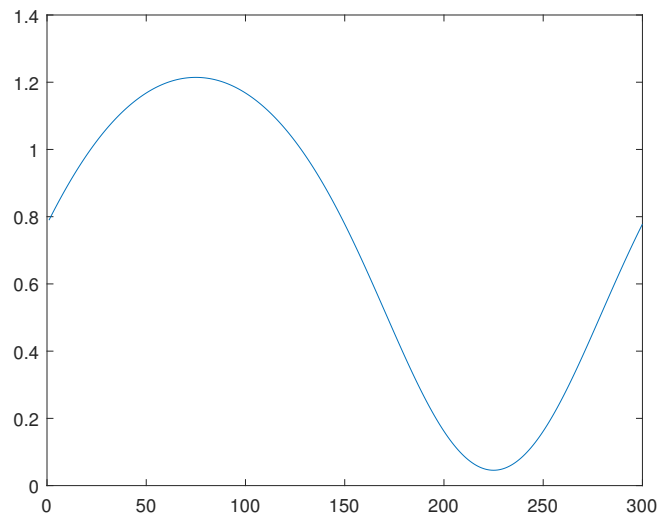
**Figure 12.** Line 6, solution  $u_6(x)$  through the Newton's Method



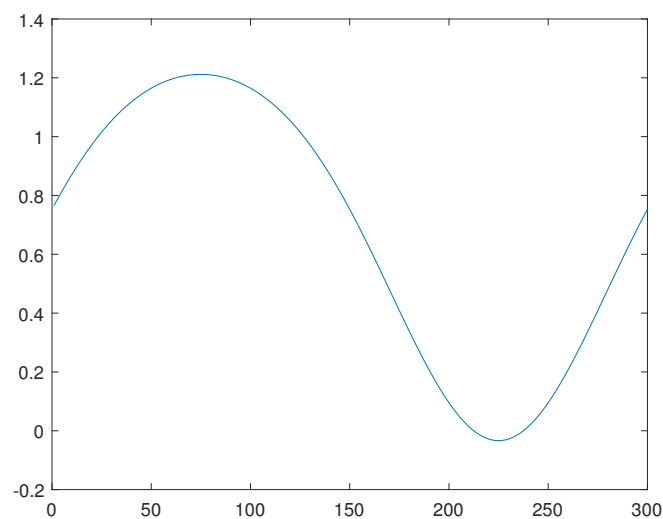
**Figure 13.** Line 6, solution  $u_6(x)$  through the minimization of functional  $J$



**Figure 14.** Line 8, solution  $u_8(x)$  through the general method of lines



**Figure 15.** Line 8, solution  $u_8(x)$  through the Newton's Method



**Figure 16.** Line 8, solution  $u_8(x)$  through the minimization of functional  $J$

#### 14. Conclusion

In the first part of this article we develop duality principles for non-convex variational optimization. In the final concerning sections we propose dual convex formulations suitable for a large class of models in physics and engineering. In the last article section, we present an advance concerning the computation of a solution for a partial differential equation through the generalized method of lines. In particular, in its previous versions, we used to truncate the series in  $d^2$  however, we have realized the results are much better by taking line solutions in series for  $u_f[x]$  and its derivatives, as it is indicated in the present software.

This is a little difference concerning the previous procedure, but with a great result improvement as the parameter  $\varepsilon > 0$  is small.

Indeed, with a sufficiently large  $N$  (number of lines), we may obtain very good qualitative results even as  $\varepsilon > 0$  is very small.

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