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Article

Duality Principles and Numerical Procedures for a Large Class of Non-Convex Models in the Calculus of Variations

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Abstract: This article develops duality principles and numerical results for a large class of non-convex variational models. The main results are based on fundamental tools of convex analysis, duality theory and calculus of variations. More specifically the approach is established for a class of non-convex functionals similar as those found in some models in phase transition. Moreover, we develop a general duality principle for quasi-convex relaxed formulations for some models in the vectorial calculus of variations. Concerning applications of such results are presented for a non-linear model of plates and for non-linear elasticity. Finally, in some sections we present concerning numerical examples and the respective softwares.

Keywords: duality theory; non-convex variational analysis; numerical method for a non-smooth model

MSC: 49N15; 35A15; 49J40

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1. Introduction

In this section we establish a dual formulation for a large class of models in non-convex optimization. It is worth highlighting the main duality principle is applied to double well models similar as those found in the phase transition theory.

Such results are based on the works of J.J. Telega and W.R. Bielski [1–4] and on a D.C. optimization approach developed in Toland [5]. About the other references, details on the Sobolev spaces involved are found in [6]. Related results on convex analysis and duality theory are addressed in [7–13].

Similar models on the superconductivity physics may be found in [14–16].

At this point we recall that the duality principles are important since the related dual variational formulations are either convex (in fact concave) or have a large region of convexity around their critical points. These features are relevant considering that, from a concerning strict convexity, the standard Newton, Newton type and similar methods are in general convergent. Moreover, the dual variational formulations are also relevant since in some situations, it is possible to assure the global optimality of some critical points which satisfy certain specific constraints theoretically established.

Among the main results here developed, we highlight the duality principles for the quasi-convex formulations in the context of the vectorial calculus of variations. An important example in non-linear elasticity is addressed along the text in details.

Also, for the applications in physics in the final sections, we believe to have found a path to connect the quantum approach with a more classical one in a unified framework.

Indeed, we have presented a path to model a great variety of chemical reactions through such a connection between the atomic and classical worlds.

Finally, in this text 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 1.1 (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*

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represented by another Banach space U^*, through a bilinear form $\langle \cdot, \cdot \rangle_U : U \times U^* \to \mathbb{R}$ (here we are referring to standard representations of dual spaces of Sobolev and Lebesgue spaces). Thus, given $f : U \to \mathbb{R}$ linear and continuous, we assume the existence of a unique $u^* \in U^*$ such that

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

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

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

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

2. A general duality principle non-convex optimization

In this section we present a duality principle applicable to a 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 $J : V \to \mathbb{R}$ where

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

and where

$$F(\nabla u_1, \cdots, \nabla u_N) = \int_\Omega f(\nabla u_1, \cdots, \nabla u_N) \, dx$$

$f : \mathbb{R}^{N \times n} \to \mathbb{R}$ is a three times Fréchet differentiable function not necessarily convex. Moreover,

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

$h = (h_1, \cdots, h_N) \in L^2(\Omega; \mathbb{R}^N)$, and $1 < p < +\infty$.

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

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

Furthermore, suppose G is 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.

Define $V_0 = W_0^{1,2}(\Omega; \mathbb{R}^N)$ and

$$V_0(u) = \{ \phi \in V_0 \ : \ \text{supp } \phi \subset B(u) \},$$

where

$$B(u) = \{ x \in \Omega \ : \ f^{**}(\nabla u(x)) < f(\nabla u(x)) \}.$$

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

$$\begin{aligned} F_1(u, \phi) \quad &= \quad F(\nabla u_1 + \nabla \phi_1, \cdots, \nabla u_N + \nabla \phi_N) + \frac{K}{2} \int_\Omega \nabla u_j \cdot \nabla u_j \, dx \\ &\quad + \frac{K_2}{2} \int_\Omega \nabla \phi_j \cdot \nabla \phi_j \, dx \end{aligned} \tag{3}$$

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and

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

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

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

and

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

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

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

Observe that

$$\begin{aligned}
J_1(u,\phi) &= F_1(u,\phi) + G_1(u) - G_2(\nabla u) - G_3(\nabla\phi) - G_4(u)\\
&\le F_1(u,\phi) + G_1(u) - \langle \nabla u, z_1^*\rangle_{L^2} - \langle \nabla\phi, z_2^*\rangle_{L^2} - \langle u, z_3^*\rangle_{L^2}\\
&\quad + \sup_{v_1\in Y_1}\{\langle v_1, z_1^*\rangle_{L^2} - G_2(v_1)\}\\
&\quad + \sup_{v_2\in Y_2}\{\langle v_2, z_2^*\rangle_{L^2} - G_3(v_2)\}\\
&\quad + \sup_{u\in V}\{\langle u, z_3^*\rangle_{L^2} - G_4(u)\}\\
&= F_1(u,\phi) + G_1(u) - \langle \nabla u, z_1^*\rangle_{L^2} - \langle \nabla\phi, z_2^*\rangle_{L^2} - \langle u, z_3^*\rangle_{L^2}\\
&\quad + G_2^*(z_1^*) + G_3^*(z_2^*) + G_4^*(z_3^*)\\
&= J_1^*(u,\phi,z^*),
\end{aligned} \tag{4}$$

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

From the general results in [5], we may infer that

$$\inf_{(u,\phi)\in V\times V_0(u)} J(u,\phi) = \inf_{(u,\phi,z^*)\in V\times V_0(u)\times Y^*} J_1^*(u,\phi,z^*). \tag{5}$$

On the other hand

$$\inf_{u\in V} J(u) \ge \inf_{(u,\phi)\in V\times V_0(u)} J_1(u,\phi).$$

From these last two results we may obtain

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

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

$$\begin{aligned}
\inf_{u\in V} J_1^*(u,\phi,z^*) &= \inf_{u\in V}\{F_1(u,\phi) + G_1(u)\\
&\quad - \langle \nabla u, z_1^*\rangle_{L^2} - \langle \nabla\phi, z_2^*\rangle_{L^2} - \langle u, z_3^*\rangle_{L^2}\\
&\quad + G_2^*(z_1^*) + G_3^*(z_2^*) + G_4^*(z_3^*)\}\\
&= \sup_{(v_1^*,v_2^*)\in C^*}\{-F_1^*(v_1^* + z_1^*,\phi) - G_1^*(v_2^* + z_3^*) - \langle \nabla\phi, z_2^*\rangle_{L^2}\\
&\quad + G_2^*(z_1^*) + G_3^*(z_2^*) + G_4^*(z_3^*)\},
\end{aligned} \tag{6}$$

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where

$$C^* = \{v^* = (v_1^*, v_2^*) \in Y_1^* \times Y_3^* \ : \ -\operatorname{div}(v_1^*)_i + (v_2^*)_i = \mathbf{0}, \forall i \in \{1, \cdots, N\}\},$$

$$F_1^*(v_1^* + z_1^*, \phi) = \sup_{u \in V}\{\langle u, -\operatorname{div}(z_1^* + v_1^*)\rangle_{L^2} - F_1(u, \phi)\},$$

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

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

we have got

$$\begin{aligned} \inf_{u \in V} J(u) &\geq \inf_{(u,\phi) \in V \times V_0} J_1(u, \phi) \\ &= \inf_{(u,\phi,z^*) \in V \times V_0(u) \times Y^*} J_1^*(u, \phi, z^*) \\ &= \inf_{z^* \in Y^*}\left\{\inf_{\phi \in V_0}\left\{\sup_{v^* \in C^*} J_2^*(\phi, z^*, v^*)\right\}\right\}. \end{aligned} \tag{7}$$

Finally, observe that

$$\begin{aligned} &\inf_{u \in V} J(u) \\ \geq\ & \inf_{z^* \in Y^*}\left\{\inf_{\phi \in V_0(u)}\left\{\sup_{v^* \in C^*} J_2^*(\phi, z^*, v^*)\right\}\right\} \\ \geq\ & \sup_{v^* \in C^*}\left\{\inf_{(z^*,\phi) \in Y^* \times V_0(u)} J_2^*(\phi, z^*, v^*)\right\}. \end{aligned} \tag{8}$$

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

3. 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 $J : V \to \mathbb{R}$ 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, $F : V \to \mathbb{R}$ and $F_1 : V \times V_0 \to \mathbb{R}$ by

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

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and

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

Observe that

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

In order to restrict the action of ϕ on the region where the primal functional is non-convex, we redefine a not relabeled

$$V_0 = \left\{\phi \in W_0^{1,4}(\Omega)\ :\ (\phi')^2 - 1 \leq 0,\ \text{in}\ \Omega\right\}$$

and define also

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

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

and

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

by

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

$$\begin{aligned} F_3(u,\phi) &= F_2(u,\phi) + \frac{K}{2}\int_\Omega (u')^2\, dx \\ &\quad + \frac{K_1}{2}\int_\Omega (\phi')^2\, dx \end{aligned} \tag{9}$$

and

$$\begin{aligned} G(u,\phi) &= \frac{K}{2}\int_\Omega (u')^2\, dx \\ &\quad + \frac{K_1}{2}\int_\Omega (\phi')^2\, dx \end{aligned} \tag{10}$$

Denoting $Y = Y^* = L^2(\Omega)$ we also define the polar functional $G^* : Y^* \times Y^* \to \mathbb{R}$ 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 $J_1^* : V \times V_0 \times [Y^*]^2 \to \mathbb{R}$, 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 (in order to obtain the concerning critical points, at first we have neglected the constraint $(\phi')^2 - 1 \leq 0$ in Ω).

1. Set $K \approx 0.1$ and $K_1 = 120.0$ and $0 < \varepsilon \ll 1$.
2. Choose $(u_1, \phi_1) \in V \times V_0$, such that $\|u_1\|_{1,\infty} < 1$ and $\|\phi_1\|_{1,\infty} < 1$.
3. Set $n = 1$.

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4. Calculate $(v_n^*, (v_0^*)_n)$ solution of the system of equations:

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

and

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

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}, ϕ_{n+1}) by solving the system of equations:

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

and

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

that is

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

and

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

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

At this point, we present the corresponding software in MAT-LAB, in finite differences and based on the one-dimensional version of the generalized method of lines.

Here the software.

****

1. clear all

```
m8=300;
d=1/m8;
K=0.1;
K1=120;
for i=1:m8
uo(i,1) = i^2 * d/2;
vo(i,1)=i*d/10;
yo(i,1)=sin(i*d*pi)/2;
end;
```

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```
k=1;
b12=1.0;
while (b12 > 10^(-4.3)) and (k < 230000)
k=k+1;
for i=1:m8-1
duo(i,1)=(uo(i+1,1)-uo(i,1))/d;
dvo(i,1)=(vo(i+1,1)-vo(i,1))/d;
end;
m9=zeros(2,2);
m9(1,1)=1;
i=1;
f1 = 6 * (duo(i,1) + dvo(i,1))^2 - 2;
m80(1,1,i)=-f1-K;
m80(1,2,i)=-f1;
m80(2,1,i)=-f1;
m80(2,2,i)=-f1-K1;
y11(1,i) = K * (uo(i+1,1) - 2 * uo(i,1))/d^2 - yo(i,1);
y11(2,i) = K1 * (vo(i+1,1) - 2 * vo(i,1))/d^2;
m12 = 2 * m80(:,:,i) - m9 * d^2;
m50(:,:,i)=m80(:,:,i)*inv(m12);
z(:,i)=inv(m12)*y11(:,i)*d^2;
for i=2:m8-1
f1 = 6 * (duo(i,1) + dvo(i,1))^2 - 2;
m80(1,1,i)=-f1-K;
m80(1,2,i)=-f1;
m80(2,1,i)=-f1;
m80(2,2,i)=-f1-K1;
y11(1,i) = K * (uo(i+1,1) - 2 * uo(i,1) + uo(i-1,1))/d^2 - yo(i,1);
y11(2,i) = K1 * (vo(i+1,1) - 2 * vo(i,1) + vo(i-1,1))/d^2;
m12 = 2 * m80(:,:,i) - m9 * d^2 - m80(:,:,i) * m50(:,:,i-1);
m50(:,:,i)=inv(m12)*m80(:,:,i);
z(:,i) = inv(m12) * (y11(:,i) * d^2 + m80(:,:,i) * z(:,i-1));
end;
U(1,m8)=1/2;
U(2,m8)=0.0;
for i=1:m8-1
U(:,m8-i)=m50(:,:,m8-i)*U(:,m8-i+1)+z(:,m8-i);
end;
for i=1:m8
```

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```
u(i,1)=U(1,i);
v(i,1)=U(2,i);
end;
b12=max(abs(u-uo))
uo=u;
vo=v;
u(m8/2,1)
end;
for i=1:m8
y(i)=i*d;
end;
plot(y,uo)
************************************
```

For the case in which $f(x) = 0$, we have obtained numerical results for $K = 0.1$ and $K_1 = 120$. 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 also for $K = 0.1$ and $K_1 = 120$. For such a concerning solution u_0 obtained, please see Figure 2.

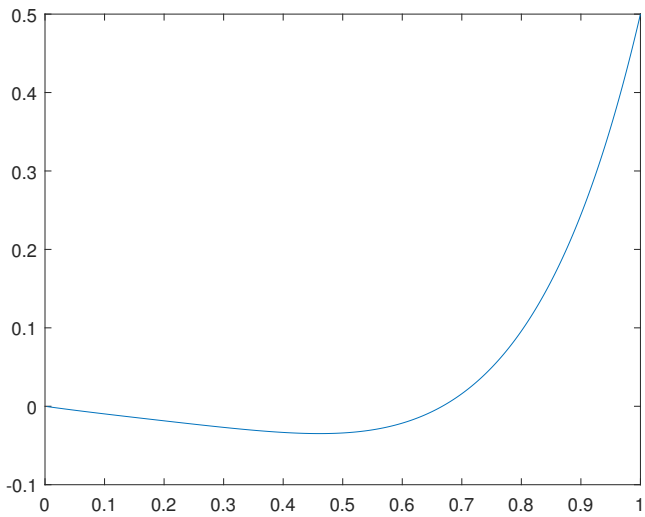

Figure 1. solution $u_0(x)$ for the case $f(x) = 0$.

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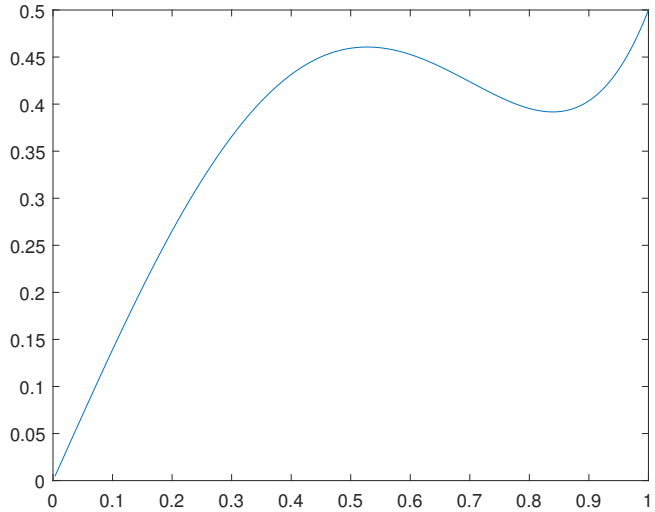

Figure 2. solution $u_0(x)$ for the case $f(x) = \sin(\pi x)/2$.

Remark 3.1. *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.*

3.1. *A general proposal for relaxation*

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

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

$$J(u) = F(\nabla u) + G(u) - \langle u, f_1 \rangle_{L^2},$$

where

$$V = \left\{ u \in W^{1,4}(\Omega; \mathbb{R}^N) \ : \ u = u_0 \text{ on } \partial\Omega \right\},$$

$$u_0 \in C^1(\Omega; \mathbb{R}^N),$$

$f_1 \in L^2(\Omega; \mathbb{R}^N)$, $G : V \to \mathbb{R}$ is convex and Fréchet differentiable, and

$$F(\nabla u) = \int_\Omega f(\nabla u)\, dx,$$

where $f : \mathbb{R}^{N\times n} \to \mathbb{R}$ is also Fréchet differentiable.

Assume there exists $\hat{N} \in \mathbb{N}$ such that

$$W_h \equiv \left\{ y \in \mathbb{R}^{N\times n} \ : \ f^{**}(y) < f(y) \right\} = \cup_{j=1}^{\hat{N}} W_j$$

where for each $j \in \{1, \cdots, \hat{N}\}$ $W_j \subset \mathbb{R}^{N\times n}$ is an open connected set such that ∂W_j is regular. We also suppose

$$\overline{W_j} \cap \overline{W_k} = \emptyset, \forall j \neq k.$$

Define

$$\hat{W}_j = \left\{ v_j \in W_0^{1,4}(\Omega; \mathbb{R}^N) \ ; \ \nabla v_j(x) \in W_j, \text{ a.e. in } \Omega \right\}$$

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and define also

$$W = \{v = (v_1, \cdots, v_{\hat{N}}) \ : \ v_j \in \hat{W}_j \ \forall j \in \{1, \cdots, \hat{N}\} \text{ and } \operatorname{supp} v_j \cap \operatorname{supp} v_k = \emptyset, \forall j \neq k\}.$$

At this point we define

$$h_5(u(x), v(x)) = \begin{cases} f(\nabla u(x) + \nabla v_j(x)), & \text{if } \nabla u(x) \in W_j, \\ f(\nabla u(x)), & \text{if } \nabla u(x) \notin W_h, \end{cases} \tag{11}$$

and

$$H(u) = \inf_{v \in W_u} \int_\Omega h_5(u, v)\, dx,$$

where

$$W_u = \{v \in W \ : \ \nabla u(x) + \nabla v_j(x) \in W_j, \text{ if } \nabla u(x) \in W_j, \text{ a.e. in } \Omega, \ \forall j \in \{1, \cdots, \hat{N}\}\}.$$

Moreover, we propose the relaxed functional

$$J_1(u) = H(u) + G(u) - \langle u, f_1 \rangle_{L^2}.$$

Observe that clearly

$$\inf_{u \in V} J_1(u) \leq \inf_{u \in V} J(u).$$

4. 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 $J : V \to \mathbb{R}$ 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, $F : V \to \mathbb{R}$ and $G : V \to \mathbb{R}$ by

$$\begin{aligned} F(u) &= \frac{1}{2} \int_\Omega \min\{(u' - 1)^2, (u' + 1)^2\}\, dx \\ &= \frac{1}{2} \int_\Omega (u')^2\, dx - \int_\Omega |u'|\, dx + 1/2 \\ &\equiv F_1(u'), \end{aligned} \tag{12}$$

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 $F_1^* : Y^* \to \mathbb{R}$ and $G^* : Y^* \to \mathbb{R}$ by

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$$\begin{aligned} F_1^*(v^*) &= \sup_{v\in Y}\{\langle v, v^*\rangle_{L^2} - F_1(v)\} \\ &= \frac{1}{2}\int_\Omega (v^*)^2\,dx + \int_\Omega |v^*|\,dx, \end{aligned} \tag{13}$$

and

$$\begin{aligned} G^*((v^*)') &= \sup_{u\in V}\{-\langle u', v^*\rangle_{L^2} - G(u)\} \\ &= \frac{1}{2}\int_\Omega ((v^*)' + f)^2\,dx - \frac{1}{2}v^*(1). \end{aligned} \tag{14}$$

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

$$\begin{cases} (v^*)'' + f' - v^* - \operatorname{sign}(v^*) = 0, & \text{in } \Omega, \\ (v^*)'(0) + f(0) = 0,\ (v^*)'(1) + f(1) = 1/2, \end{cases} \tag{15}$$

where $\operatorname{sign}(v^*(x)) = 1$ if $v^*(x) > 0$, $\operatorname{sign}(v^*(x)) = -1$, if $v^*(x) < 0$ and

$$-1 \le \operatorname{sign}(v^*(x)) \le 1,$$

if $v^*(x) = 0$.

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.

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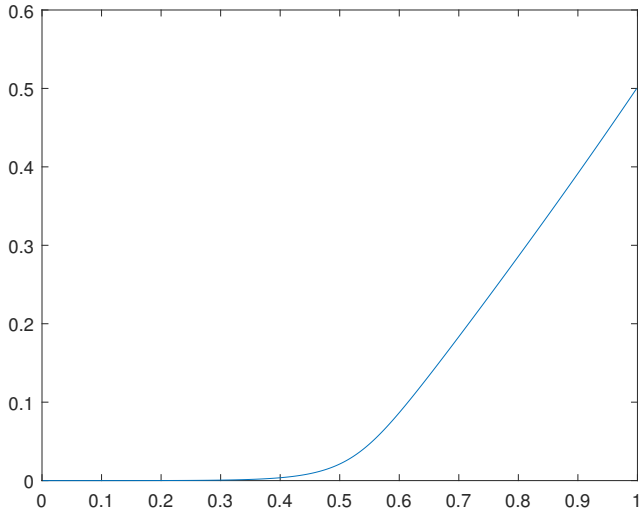

Figure 3. solution $u_0(x)$ for the case $f(x) = 0$.

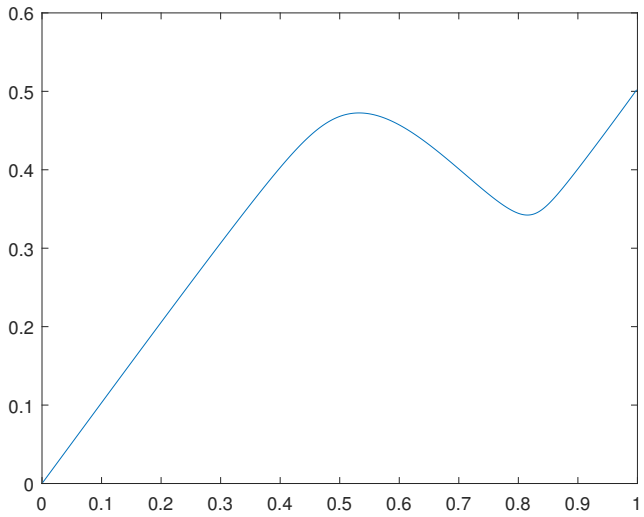

Figure 4. solution $u_0(x)$ for the case $f(x) = \sin(\pi x)/2$.

Remark 4.1. *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.*

4.1. The algorithm through which we have obtained the numerical results

In this subsection we present the software in MATLAB through which we have obtained the last numerical results.

This algorithm is for solving the concerning Euler-Lagrange equations for the dual problem, that is, for solving the equation

$$\begin{cases} (v^*)'' + f' - v^* - \operatorname{sign}(v^*) = 0, & \text{in } \Omega, \\ (v^*)'(0) = 0,\ (v^*)'(1) = 1/2. \end{cases} \tag{16}$$

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Here the concerning software in MATLAB. We emphasize to have used the smooth approximation

$$|v^*| \approx \sqrt{(v^*)^2 + e_1},$$

where a small value for e_1 is specified in the next lines.

****

1. clear all
2. $m_8 = 800$; (number of nodes)
3. $d = 1/m_8$;
4. $e_1 = 0.00001$;
5. $for\ i = 1 : m_8$

   $yo(i,1) = 0.01$;

   $y_1(i,1) = \sin(\pi * i/m_8)/2$;

   end;
6. $for\ i = 1 : m_8 - 1$

   $dy_1(i,1) = (y_1(i+1,1) - y_1(i,1))/d$;

   end;
7. $for\ k = 1 : 3000$ (we have fixed the number of iterations)

   $i = 1$;

   $h_3 = 1/\sqrt{vo(i,1)^2 + e_1}$;

   $m_{12} = 1 + d^2 * h_3 + d^2$;

   $m_{50}(i) = 1/m_{12}$;

   $z(i) = m_{50}(i) * (dy_1(i,1) * d^2)$;
8. $for\ i = 2 : m_8 - 1$

   $h_3 = 1/\sqrt{vo(i,1)^2 + e_1}$;

   $m_{12} = 2 + h_3 * d^2 + d^2 - m50(i-1)$;

   $m50(i) = 1/m_{12}$;

   $z(i) = m_{50}(i) * (z(i-1) + dy_1(i,1) * d^2)$;

   end;
9. $v(m_8,1) = (d/2 + z(m_8 - 1))/(1 - m_{50}(m_8 - 1))$;
10. $for\ i = 1 : m_8 - 1$

    $v(m_8 - i, 1) = m_{50}(m_8 - i) * v(m_8 - i + 1) + z(m_8 - i)$;

    end;
11. $v(m_8/2, 1)$
12. $vo = v$;

    end;
13. $for\ i = 1 : m_8 - 1$

    $u(i,1) = (v(i+1,1) - v(i,1))/d + y_1(i,1)$;

    end;
14. $for\ i = 1 : m_8 - 1$

    $x(i) = i * d$;

    end;

    $plot(x, u(:,1))$

****

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5. An improvement of the convexity conditions for a non-convex related model through an approximate primal formulation

In this section we develop an approximate primal dual formulation suitable for a large class of variational models.

Here, the applications are for the Kirchhoff-Love plate model, which may be found in Ciarlet, [17].

At this point we start to describe the primal variational formulation.

Let $\Omega \subset \mathbb{R}^2$ be an open, bounded, connected set which represents the middle surface of a plate of thickness h. The boundary of Ω, which is assumed to be regular (Lipschitzian), is denoted by $\partial\Omega$. The vectorial basis related to the cartesian system $\{x_1, x_2, x_3\}$ is denoted by $(\mathbf{a}_\alpha, \mathbf{a}_3)$, where $\alpha = 1, 2$ (in general Greek indices stand for 1 or 2), and where $\mathbf{a}_3$ is the vector normal to Ω, whereas $\mathbf{a}_1$ and $\mathbf{a}_2$ are orthogonal vectors parallel to Ω. Also, $\mathbf{n}$ is the outward normal to the plate surface.

The displacements will be denoted by

$$\hat{\mathbf{u}} = \{\hat{u}_\alpha, \hat{u}_3\} = \hat{u}_\alpha \mathbf{a}_\alpha + \hat{u}_3 \mathbf{a}_3.$$

The Kirchhoff-Love relations are

$$\begin{aligned} &\hat{u}_\alpha(x_1, x_2, x_3) = u_\alpha(x_1, x_2) - x_3 w(x_1, x_2)_{,\alpha} \\ &\text{and } \hat{u}_3(x_1, x_2, x_3) = w(x_1, x_2). \end{aligned} \tag{17}$$

Here $-h/2 \leq x_3 \leq h/2$ so that we have $u = (u_\alpha, w) \in U$ where

$$\begin{aligned} U &= \Big\{u = (u_\alpha, w) \in W^{1,2}(\Omega; \mathbb{R}^2) \times W^{2,2}(\Omega), \\ &\qquad u_\alpha = w = \frac{\partial w}{\partial \mathbf{n}} = 0 \ \text{ on } \partial\Omega\Big\} \\ &= W_0^{1,2}(\Omega; \mathbb{R}^2) \times W_0^{2,2}(\Omega). \end{aligned}$$

It is worth emphasizing that the boundary conditions here specified refer to a clamped plate.

We also define the operator $\Lambda : U \to Y \times Y$, where $Y = Y^* = L^2(\Omega; \mathbb{R}^{2\times 2})$, by

$$\Lambda(u) = \{\gamma(u), \kappa(u)\},$$

$$\gamma_{\alpha\beta}(u) = \frac{u_{\alpha,\beta} + u_{\beta,\alpha}}{2} + \frac{w_{,\alpha} w_{,\beta}}{2},$$

$$\kappa_{\alpha\beta}(u) = -w_{,\alpha\beta}.$$

The constitutive relations are given by

$$N_{\alpha\beta}(u) = H_{\alpha\beta\lambda\mu} \gamma_{\lambda\mu}(u), \tag{18}$$

$$M_{\alpha\beta}(u) = h_{\alpha\beta\lambda\mu} \kappa_{\lambda\mu}(u), \tag{19}$$

where: $\{H_{\alpha\beta\lambda\mu}\}$ and $\left\{h_{\alpha\beta\lambda\mu} = \frac{h^2}{12} H_{\alpha\beta\lambda\mu}\right\}$, are symmetric positive definite fourth order tensors. From now on, we denote $\{\overline{H}_{\alpha\beta\lambda\mu}\} = \{H_{\alpha\beta\lambda\mu}\}^{-1}$ and $\{\overline{h}_{\alpha\beta\lambda\mu}\} = \{h_{\alpha\beta\lambda\mu}\}^{-1}$.

Furthermore $\{N_{\alpha\beta}\}$ denote the membrane force tensor and $\{M_{\alpha\beta}\}$ the moment one. The plate stored energy, represented by $(G \circ \Lambda) : U \to \mathbb{R}$ is expressed by

$$(G \circ \Lambda)(u) = \frac{1}{2} \int_\Omega N_{\alpha\beta}(u) \gamma_{\alpha\beta}(u) \, dx + \frac{1}{2} \int_\Omega M_{\alpha\beta}(u) \kappa_{\alpha\beta}(u) \, dx \tag{20}$$

and the external work, represented by $F : U \to \mathbb{R}$, is given by

$$F(u) = \langle w, P \rangle_{L^2} + \langle u_\alpha, P_\alpha \rangle_{L^2}, \tag{21}$$

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where $P, P_1, P_2 \in L^2(\Omega)$ are external loads in the directions $\mathbf{a}_3$, $\mathbf{a}_1$ and $\mathbf{a}_2$ respectively. The potential energy, denoted by $J : U \to \mathbb{R}$ is expressed by:

$$J(u) = (G \circ \Lambda)(u) - F(u)$$

Define now $J_3 : \tilde{U} \to \mathbb{R}$ by

$$J_3(u) = J(u) + J_5(w).$$

where

$$J_5(w) = 10 \int_\Omega \frac{a^{K\,b\,w}}{\ln(a)\ K^{3/2}}\, dx + 10 \int_\Omega \frac{a^{-K(b\,w-1/100)}}{\ln(a)\ K^{3/2}}\, dx.$$

In such a case for $a = 2.71$, $K = 185$, $b = P/|P|$ in Ω and

$$\tilde{U} = \{u \in U \ : \ \|w\|_\infty \leq 0.01 \text{ and } P\ w \geq 0 \text{ a.e. in } \Omega\},$$

we get

$$\begin{aligned} \frac{\partial J_3(u)}{\partial w} &= \frac{\partial J(u)}{\partial w} + \frac{\partial J_5(u)}{\partial w} \\ &\approx \frac{\partial J(u)}{\partial w} + \mathcal{O}(\pm 3.0), \end{aligned} \tag{22}$$

and

$$\begin{aligned} \frac{\partial^2 J_3(u)}{\partial w^2} &= \frac{\partial^2 J(u)}{\partial w^2} + \frac{\partial^2 J_5(u)}{\partial w^2} \\ &\approx \frac{\partial^2 J(u)}{\partial w^2} + \mathcal{O}(850). \end{aligned} \tag{23}$$

This new functional J_3 has a relevant improvement in the convexity conditions concerning the previous functional J.

Indeed, we have obtained a gain in positiveness for the second variation $\frac{\partial^2 J(u)}{\partial w^2}$, which has increased of order $\mathcal{O}(700 - 1000)$.

Moreover the difference between the approximate and exact equation

$$\frac{\partial J(u)}{\partial w} = \mathbf{0}$$

is of order $\mathcal{O}(\pm 3.0)$ which corresponds to a small perturbation in the original equation for a load of $P = 1500\ N/m^2$, for example. Summarizing, the exact equation may be approximately solved in an appropriate sense.

5.1. A duality principle for the concerning quasi-convex envelope

In this section, denoting

$$V_1 = \{\phi = \phi(x, y) \in W^{1,2}(\Omega \times \Omega; \mathbb{R}^2) \ : \ \phi = 0 \text{ on } \Omega \times \partial\Omega\},$$

we define the functional $J_1 : U \times V_1 \to \mathbb{R}$, where

$$\begin{aligned} J_1(u, \phi) &= G_1(\{w_{,\alpha\beta}\}) + G_2\left(\left\{\frac{1}{2}(u_{\alpha,\beta} + u_{\beta,\alpha}) + \phi_{\alpha,y_\beta} + \frac{1}{2} w_{,\alpha} w_{,\beta}\right\}\right) \\ &\quad - \langle w, P\rangle_{L^2} - \langle u_\alpha, P_\alpha\rangle_{L^2}. \end{aligned} \tag{24}$$

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where

$$G_1(\{w_{,\alpha\beta}\}) = \frac{1}{2}\int_\Omega h_{\alpha\beta\lambda\mu} w_{,\alpha\beta} w_{,\lambda\mu}\, dx$$

and,

$$\begin{aligned} & G_2\left(\left\{\frac{1}{2}(u_{\alpha,\beta}+u_{\beta,\alpha})+\phi_{\alpha,y_\beta}+\frac{1}{2}w_{,\alpha}w_{,\beta}\right\}\right) \\ = & \frac{1}{2|\Omega|}\int_\Omega\int_\Omega H_{\alpha\beta\lambda\mu}\left(\frac{1}{2}(u_{\alpha,\beta}+u_{\beta,\alpha})+\phi_{\alpha,y_\beta}(x,y)+\frac{1}{2}w_{,\alpha}w_{,\beta}\right) \\ & \times\left(\frac{1}{2}(u_{\lambda,\mu}+u_{\lambda,\mu})+\phi_{\lambda,y_\mu}(x,y)+\frac{1}{2}w_{,\lambda}w_{,\mu}\right)\, dx\, dy \end{aligned}$$

We define also

$$J_2(\{u_\alpha\},\phi) = \inf_{w\in W_0^{2,2}(\Omega)} J_1(u,\phi),$$

and

$$J_3(\{u_\alpha\}) = \inf_{\phi\in V_1} J_2(\{u_\alpha\},\phi).$$

It is a well known result from the modern Calculus of Variations theory (please, see [18] for details) that

$$\inf_{u\in U} J(u) = \inf_{\{u_\alpha\}\in W_0^{1,2}(\Omega;\mathbb{R}^2)} J_3(\{u_\alpha\}).$$

At this point we denote

$$Y_1 = Y_1^* = Y_3 = Y_3^* \equiv L^2(\Omega\times\Omega;\mathbb{R}^4)$$

and

$$Y_2 = Y_2^* \equiv L^2(\Omega\times\Omega;\mathbb{R}^2).$$

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Observe that

$$
\begin{aligned}
& J(u) \\
= \; & G_1(\{w_{,\alpha\beta}\}) + G_2\left(\left\{\frac{1}{2}(u_{\alpha,\beta}+u_{\beta,\alpha}) + \phi_{\alpha,y_\beta} + \frac{1}{2}w_{,\alpha}w_{,\beta}\right\}\right) \\
& -\langle w, P\rangle_{L^2} - \langle u_\alpha, P_\alpha\rangle_{L^2} \\
= \; & G_1(\{w_{,\alpha\beta}\}) - \langle w_{,\alpha\beta}, M_{\alpha\beta}\rangle_{L^2} + \langle w_{,\alpha\beta}, M_{\alpha\beta}\rangle_{L^2} \\
& + \frac{1}{|\Omega|}\int_\Omega\int_\Omega w_{,\alpha}(x), Q_\alpha(x,y)\; dx\; dy - \langle w, P\rangle_{L^2} \\
& - \frac{1}{|\Omega|}\int_\Omega\int_\Omega w_{,\alpha}(x), Q_\alpha(x,y)\; dx\; dy + G_2\left(\left\{\frac{1}{2}(u_{\alpha,\beta}+u_{\beta,\alpha}) + \phi_{\alpha,y_\beta} + \frac{1}{2}w_{,\alpha}w_{,\beta}\right\}\right) \\
& - \frac{1}{|\Omega|}\int_\Omega\int_\Omega \left(\frac{1}{2}(u_{\alpha,\beta}+u_{\beta,\alpha}) + \phi_{\alpha,y_\beta} + \frac{1}{2}w_{,\alpha}w_{,\beta}\right), v^*_{\alpha\beta}(x,y)\; dx\; dy \\
& + \frac{1}{|\Omega|}\int_\Omega\int_\Omega \left(\frac{1}{2}(u_{\alpha,\beta}+u_{\beta,\alpha}) + \phi_{\alpha,y_\beta} + \frac{1}{2}w_{,\alpha}w_{,\beta}\right), v^*_{\alpha\beta}(x,y)\; dx\; dy - \langle u_\alpha, P_\alpha\rangle_{L^2} \\
\geq \; & \inf_{v_3\in Y_3}\{-\langle (v_3)_{\alpha\beta}, M_{\alpha\beta}\rangle_{L^2} + G_1((v_3)_{\alpha\beta})\} \\
& + \inf_{w\in W_0^{2,2}(\Omega)}\left\{\langle w_{,\alpha\beta}, M_{\alpha\beta}\rangle_{L^2} + \frac{1}{|\Omega|}\int_\Omega\int_\Omega w_{,\alpha}(x)\; Q_\alpha(x,y)\; dx\; dy - \langle w, P\rangle_{L^2}\right\} \\
& + \inf_{v\in Y_1}\left\{-\frac{1}{|\Omega|}\int_\Omega\int_\Omega v_{\alpha\beta}\; v^*_{\alpha\beta}\; dx\; dy + G_2(\{v_{\alpha\beta}\})\right\} \\
& + \inf_{(v_2,\{u_\alpha\})\in Y_2\times W_0^{1,2}(\Omega;\mathbb{R}^2)}\left\{\frac{1}{|\Omega|}\int_\Omega\int_\Omega\left(\frac{1}{2}(u_{\alpha,\beta}+u_{\beta,\alpha}) + \phi_{\alpha,y_\beta} + \frac{1}{2}(v_2)_\alpha(x,y)(v_2)_\beta(x,y)\right)\right. \\
& \left.\times v^*_{\alpha\beta}(x,y)\; dx\; dy - \langle u_\alpha, P_\alpha\rangle_{L^2} + \frac{1}{|\Omega|}\int_\Omega\int_\Omega (v_2)_\alpha(x,y) Q_\alpha(x,y)\; dx\; dy\right\} \\
\geq \; & -G_1^*(M) - \frac{1}{2|\Omega|}\int_\Omega\int_\Omega \left(\overline{v^*_{\alpha\beta}}\right)\; Q_\alpha\; Q_\beta\; dx\; dy - \frac{1}{2|\Omega|}\int_\Omega\int_\Omega \overline{H}_{\alpha\beta\lambda\mu} v^*_{\alpha\beta} v^*_{\lambda\mu}\; dx\; dy,
\end{aligned}
\tag{25}
$$

$\forall u \in U,\ (M,Q) \in C^*, v = \{v_{\alpha\beta}\} \in A^*$ where $A^* = A_1^* \cap A_2^* \cap B^*$,

$$A_1^* = \{\{v^*_{\alpha\beta}\} \in Y_1^* \;:\; (v^*_{\alpha\beta})_{,y_\beta} = 0, \text{ in } \Omega\},$$

$$A_2^* = \left\{\{v^*_{\alpha\beta}\} \in Y_1^* \;:\; \frac{1}{|\Omega|}\left(\int_\Omega v^*_{\alpha\beta}\; dy\right)_{,x_\beta} + P_\alpha = 0, \text{ in } \Omega\right\},$$

$$B^* = \left\{\{v^*_{\alpha\beta}\} \in Y_1^* \;:\; \left\{v^*_{\alpha\beta}(x,y)\right\} \text{ is positive definite in } \Omega\times\Omega\right\}.$$

and

$$C^* = \left\{(M,Q) \in Y_3^* \times Y_2^* \;:\; M_{\alpha\beta,\alpha\beta} - \left(\int_\Omega Q_\alpha\; dy\right)_{,x_\alpha} - P = 0, \text{ in } \Omega\right\}.$$

Also

$$\left\{\overline{v^*_{\alpha\beta}}\right\} = \left\{v^*_{\alpha\beta}\right\}^{-1},$$

and

$$\{\overline{H}_{\alpha\beta\lambda\mu}\} = \{H_{\alpha\beta\lambda\mu}\}$$

in an appropriate tensor sense.

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Here it is worth highlighting we have denoted,

$$\begin{aligned} G_1^*(M) &= \sup_{v_3 \in Y_3} \{ \langle (v_3)_{\alpha\beta}, M_{\alpha\beta} \rangle_{L^2} - G_1(v_3) \} \\ &= \frac{1}{2} \int_\Omega \overline{h}_{\alpha\beta\lambda\mu} M_{\alpha\beta} M_{\lambda\mu} \, dx, \end{aligned} \tag{26}$$

where we recall that

$$\{\overline{h}_{\alpha\beta\lambda\mu}\} = \{h_{\alpha\beta\lambda\mu}\}^{-1}$$

in an appropriate tensorial sense.

Summarizing, defining $J^* : C^* \times A^* \to \mathbb{R}$ by

$$\begin{aligned} J^*((M,Q),v^*) &= -G_1^*(M) - \frac{1}{2|\Omega|} \int_\Omega \int_\Omega \left(\overline{v^*_{\alpha\beta}} \right) \, Q_\alpha \, Q_\beta \, dx \, dy \\ &\quad - \frac{1}{2|\Omega|} \int_\Omega \int_\Omega \overline{H}_{\alpha\beta\lambda\mu} v^*_{\alpha\beta} v^*_{\lambda\mu} \, dx \, dy, \end{aligned} \tag{27}$$

we have got

$$\inf_{u \in U} J(u) \geq \sup_{((M,Q),v^*) \in C^* \times A^*} J^*((M,Q),v^*).$$

Remark 5.1. *This last dual functional is concave and such a concerning inequality corresponds a duality principle for the relaxed primal formulation.*

We emphasize such results are extensions and in some sense complement the original duality principles in the works of Telega and Bielski, [1–3].

Moreover, if $((M_0,Q_0),v_0^*) \in C^* \times A^*$ is such that

$$\delta J^*((M_0,Q_0),v_0^*) = \mathbf{0},$$

it is a well known result from the Legendre transform proprieties that the corresponding $(u_0,\phi_0) \in V \times V_1$ such that

$$(w_0)_{,\alpha\beta} = \overline{h}_{\alpha\beta\lambda\mu} (M_0)_{\lambda\mu},$$

and

$$(v_0^*)_{\alpha\beta} = H_{\alpha\beta\lambda} \left(\frac{(u_0)_{\lambda,\mu} + (u_0)_{\mu,\lambda}}{2} + \frac{(\phi_0)_{\lambda,y_\mu} + (\phi_0)_{\mu,y_\lambda}}{2} + \frac{1}{2} (v_{2_0})_\lambda (v_{2_0})_\mu \right),$$

$$(v_0^*)_{\alpha\beta,y_\beta} = \mathbf{0},$$

is also such that

$$\delta J_1(u_0,\phi_0) = \mathbf{0}$$

and

$$J_1(u_0,\phi_0) = J^*((M_0,Q_0),v_0^*).$$

From this and

$$\inf_{u \in V} J(u) = \inf_{(u,\phi) \in V \times V_1} J_1(u,\phi) \geq \sup_{((M,Q),v^*) \in C^* \times A^*} J^*((M,Q),v^*),$$

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we obtain

$$\begin{aligned} J_1(u_0,\phi_0) &= \inf_{(u,\phi)\in V\times V_1} J_1(u,\phi) \\ &= \sup_{((M,Q),v^*)\in C^*\times A^*} J^*((M,Q),v^*) \\ &= J^*((M_0,Q_0),v_0^*) \\ &= \inf_{u\in V} J(u). \end{aligned} \tag{28}$$

Also, from the modern calculus of variations theory, there exists a sequence $\{u_n\} \subset V$ *such that*

$$u_n \rightharpoonup u_0, \text{ weakly in } V,$$

and

$$J(u_n) \to J_1(u_0,\phi_0) = \inf_{u\in V} J(u).$$

From this and the Ekeland variational principle, there exists $\{v_n\} \subset V$ *such that*

$$\|u_n - v_n\|_V \leq 1/n,$$

$$J(v_n) \leq \inf_{u\in V} J(u) + 1/n,$$

and

$$\|\delta J(v_n)\|_{V^*} \leq 1/n, \ \forall n \in \mathbb{N},$$

so that

$$v_n \rightharpoonup u_0, \text{ weakly in } V,$$

and

$$J(v_n) \to J_1(u_0,\phi_0) = \inf_{u\in V} J(u).$$

Assume now we are dealing with a finite dimensional version of such a model, in a finite elements of finite differences context, for example.

In such a case we have

$$v_n \to u_0, \text{ strongly in } \mathbb{R}^N$$

for an appropriate $N \in \mathbb{N}$.

From continuity we obtain

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

$$J(v_n) \to J(u_0).$$

Summarizing, we have got

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

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

Here we highlight such last results are valid just for this finite-dimensional model version.

6. A duality principle for a related relaxed formulation concerning the vectorial approach in the calculus of variations

In this section we develop a duality principle for a related vectorial model in the calculus of variations.

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

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For $1 < p < +\infty$, consider a functional $J : V \to \mathbb{R}$ where

$$J(u) = G(\nabla u) + F(u) - \langle u, f \rangle_{L^2},$$

where

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

$u_0 \in C^1(\overline{\Omega}; \mathbb{R}^N)$ and $f \in L^2(\Omega; \mathbb{R}^N)$.

We assume $G : Y \to \mathbb{R}$ and $F : V \to \mathbb{R}$ are Fréchet differentiable and F is also convex.

Also

$$G(\nabla u) = \int_\Omega g(\nabla u)\, dx,$$

where $g : \mathbb{R}^{N\times n} \to \mathbb{R}$ it is supposed to be Fréchet differentiable. Here we have denoted $Y = L^p(\Omega; \mathbb{R}^{N\times n})$.

We define also $J_1 : V \times Y_1 \to \mathbb{R}$ by

$$J_1(u, \phi) = G_1(\nabla u + \nabla_y \phi) + F(u) - \langle u, f \rangle_{L^2},$$

where

$$Y_1 = W^{1,p}(\Omega \times \Omega; \mathbb{R}^N)$$

and

$$G_1(\nabla u + \nabla_y \phi) = \frac{1}{|\Omega|} \int_\Omega \int_\Omega g(\nabla u(x) + \nabla_y \phi(x, y))\, dx\, dy.$$

Moreover, we define the relaxed functional $J_2 : V \to \mathbb{R}$ by

$$J_2(u) = \inf_{\phi \in V_0} J_1(u, \phi),$$

where

$$V_0 = \{\phi \in Y_1 \ : \ \phi(x, y) = 0, \ \text{ on } \Omega \times \partial\Omega\}.$$

Now observe that

$$\begin{aligned}
J_1(u,\phi) &= G_1(\nabla u + \nabla_y \phi) + F(u) - \langle u, f \rangle_{L^2} \\
&= -\frac{1}{|\Omega|} \int_\Omega \int_\Omega v^*(x,y) \cdot (\nabla u + \nabla_y \phi(x,y))\, dy\, dx + G_1(\nabla u + \nabla_y \phi) \\
&\quad + \frac{1}{|\Omega|} \int_\Omega \int_\Omega v^*(x,y) \cdot (\nabla u + \nabla_y \phi(x,y))\, dy\, dx + F(u) - \langle u, f \rangle_{L^2} \\
&\geq \inf_{v \in Y_2} \left\{ -\frac{1}{|\Omega|} \int_\Omega \int_\Omega v^*(x,y) \cdot v(x,y)\, dy\, dx + G_1(v) \right\} \\
&\quad + \inf_{(v,\phi) \in V \times V_0} \left\{ \frac{1}{|\Omega|} \int_\Omega \int_\Omega v^*(x,y) \cdot (\nabla u + \nabla_y \phi(x,y))\, dy\, dx + F(u) - \langle u, f \rangle_{L^2} \right\} \\
&= -G_1^*(v^*) - F^* \left(\operatorname{div}_x \left(\frac{1}{|\Omega|} \int_\Omega v^*(x,y)\, dy \right) + f \right) \\
&\quad + \frac{1}{|\Omega|} \int_{\partial\Omega} \left(\int_\Omega v^*(x,y)\, dy \right) \otimes \mathbf{n} u_0\, d\Gamma,
\end{aligned} \tag{29}$$

$\forall (u, \phi) \in V \times V_0, v^* \in A^*$, where

$$A^* = \{v^* \in Y_2^* \ : \ \operatorname{div}_y v^*(x, y) = 0, \text{ in } \Omega\}.$$

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Here we have denoted

$$G_1^*(v^*) = \sup_{v \in Y_2} \left\{ \frac{1}{|\Omega|} \int_\Omega \int_\Omega v^*(x,y) \cdot v(x,y)\, dy\, dx - G_1(v) \right\},$$

where $Y_2 = L^p(\Omega \times \Omega; \mathbb{R}^{N\times n})$, $Y_2^* = L^q(\Omega \times \Omega; \mathbb{R}^{N\times n})$, and where

$$\frac{1}{p} + \frac{1}{q} = 1.$$

Furthermore, for $v^* \in A^*$, we have

$$\begin{aligned} & F^*\left(\mathrm{div}_x\left(\frac{1}{|\Omega|}\int_\Omega v^*(x,y)\, dy\right) + f\right) - \frac{1}{|\Omega|}\int_{\partial\Omega}\left(\int_\Omega v^*(x,y)\, dy\right) \otimes \mathbf{n} u_0\, d\Gamma \\ = & \sup_{(v,\phi)\in V\times V_0} \left\{ -\frac{1}{|\Omega|}\int_\Omega\int_\Omega v^*(x,y)\cdot(\nabla u + \nabla_y \phi(x,y))\, dy\, dx - F(u) + \langle u, f\rangle_{L^2} \right\}, \end{aligned} \tag{30}$$

Therefore, denoting $J_3^* : Y_2^* \to \mathbb{R}$ by

$$J_3^*(v^*) = -G_1^*(v^*) - F^*\left(\mathrm{div}_x\left(\int_\Omega v^*(x,y)\, dy\right) + f\right) + \frac{1}{|\Omega|}\int_{\partial\Omega}\left(\int_\Omega v^*(x,y)\, dy\right) \otimes \mathbf{n} u_0\, d\Gamma,$$

we have got

$$\inf_{u\in V} J_2(u) \geq \sup_{v^*\in A^*} J_3^*(v^*).$$

Finally, we highlight such a dual functional J_3^* is convex (in fact concave).

6.1. *An example in finite elasticity*

In this section we develop an application of results obtained in the last section to a model in non-linear elasticity.

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

Concerning a standard model in non-linear elasticity, consider a functional $J : V \to \mathbb{R}$ where

$$\begin{aligned} & J(u) \\ = & \frac{1}{2}\int_\Omega H_{ijkl}\left(\frac{u_{i,j}+u_{j,i}}{2} + \frac{1}{2}u_{m,i}u_{m,j}\right)\left(\frac{u_{k,l}+u_{j,i}}{2} + \frac{1}{2}u_{m,k}u_{m,l}\right)\, dx \\ & -\langle u_i, f_i\rangle_{L^2} \end{aligned} \tag{31}$$

where $f \in L^2(\Omega;\mathbb{R}^3)$ and $V = W_0^{1,2}(\Omega;\mathbb{R}^3)$.

Here $\{H_{ijkl}\}$ is a fourth-order and positive definite symmetric tensor (in an appropriate standard sense). Moreover, $u = (u_1, u_2, u_3) \in V$ is a field of displacements resulting from the f load field action on the volume comprised by Ω.

At this point, we define the functional $J_1 : V \times V_1 \to \mathbb{R}$, where

$$\begin{aligned} & J_1(u,\phi) \\ = & \frac{1}{2|\Omega|}\int_\Omega\int_\Omega H_{ijkl}\left(\frac{u_{i,j}+u_{j,i}}{2} + \frac{\phi_{i,y_j}+\phi_{j,y_i}}{2}\frac{1}{2}(u_{m,i}+\phi_{m,y_i})(u_{m,j}+\phi_{m,y_j})\right) \\ & \times\left(\frac{u_{k,l}+u_{l,k}}{2} + \frac{\phi_{k,y_l}+\phi_{l,y_k}}{2} + \frac{1}{2}(u_{m,k}+\phi_{m,y_k})(u_{m,l}+\phi_{m,y_l})\right)\, dx\, dy \\ & -\langle u_i, f_i\rangle_{L^2}, \end{aligned} \tag{32}$$

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where

$$V_1 = \{\phi \in W^{1,2}(\Omega \times \Omega; \mathbb{R}^3) \ : \ \phi = 0 \text{ on } \Omega \times \partial\Omega\}.$$

We define also the quasi-convex envelop of J, denoted by $Q_J : V \to \mathbb{R}$, as

$$Q_J(u) = \inf_{\phi \in V_1} J_1(u, \phi).$$

It is a well known result from the modern calculus of variations theory (please see [18] for details), that

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

Observe now that, denoting $Y_1 = Y_1^* = L^2(\Omega \times \Omega; \mathbb{R}^9)$, $Y_2 = Y_2^* = L^2(\Omega \times \Omega; \mathbb{R}^3)$, and

$$\begin{aligned} & G_1\left(\frac{u_{i,j}+u_{j,i}}{2} + \frac{\phi_{i,y_j}+\phi_{j,y_i}}{2} + \frac{1}{2}(u_{m,i}+\phi_{m,y_i})(u_{m,j}+\phi_{m,y_j})\right) \\ = \ & \frac{1}{2|\Omega|}\int_\Omega\int_\Omega H_{ijkl}\left(\frac{u_{i,j}+u_{j,i}}{2} + \frac{\phi_{i,y_j}+\phi_{j,y_i}}{2} + \frac{1}{2}(u_{m,i}+\phi_{m,y_i})(u_{m,j}+\phi_{m,y_j})\right) \\ & \times\left(\frac{u_{k,l}+u_{l,k}}{2} + \frac{\phi_{k,y_l}+\phi_{l,y_k}}{2} + \frac{1}{2}(u_{m,k}+\phi_{m,y_k})(u_{m,l}+\phi_{m,y_l})\right) dx\, dy \end{aligned} \tag{33}$$

we have that

$$\begin{aligned} & J_1(u,\phi) \\ = \ & G_1\left(\frac{u_{i,j}+u_{j,i}}{2} + \frac{\phi_{i,y_j}+\phi_{j,y_i}}{2} + \frac{1}{2}(u_{m,i}+\phi_{m,y_i})(u_{m,j}+\phi_{m,y_j})\right) - \langle u_i, f_i\rangle_{L^2} \\ = \ & -\frac{1}{|\Omega|}\int_\Omega\int_\Omega\left(\frac{u_{i,j}+u_{j,i}}{2} + \frac{\phi_{i,y_j}+\phi_{j,y_i}}{2} + \frac{1}{2}(u_{m,i}+\phi_{m,y_i})(u_{m,j}+\phi_{m,y_j})\right)\sigma_{ij}\, dx\, dy \\ & +G_1\left(\frac{u_{i,j}+u_{j,i}}{2} + \frac{\phi_{i,y_j}+\phi_{j,y_i}}{2} + \frac{1}{2}(u_{m,i}+\phi_{m,y_i})(u_{m,j}+\phi_{m,y_j})\right) \\ & +\frac{1}{|\Omega|}\int_\Omega\int_\Omega\left(\frac{u_{i,j}+u_{j,i}}{2} + \frac{\phi_{i,y_j}+\phi_{j,y_i}}{2} + \frac{1}{2}(u_{m,i}+\phi_{m,y_i})(u_{m,j}+\phi_{m,y_j})\right)\sigma_{ij}\, dx\, dy - \langle u_i, f_i\rangle_{L^2} \\ \geq \ & \inf_{v \in Y_1}\left\{-\frac{1}{|\Omega|}\int_\Omega\int_\Omega v_{ij}\sigma_{ij}\, dx\, dy - G_1\left(\{v_{ij}\}\right)\right\} \\ & + \inf_{v_2 \in Y_1}\left\{-\frac{1}{|\Omega|}\int_\Omega\int_\Omega (v_2)_{ij}\, Q_{ij}\, dx\, dy + \frac{1}{|\Omega|}\int_\Omega\int_\Omega\left(\sigma_{ij}\,\frac{1}{2}((v_2)_{mi}(v_2)_{mj})\right) dx\, dy\right\} \\ & + \inf_{(u,\phi)\in V\times V_1}\left\{\frac{1}{|\Omega|}\int_\Omega\int_\Omega(\sigma_{ij}+Q_{ij})\left(\frac{u_{i,j}+u_{j,i}}{2} + \frac{\phi_{i,y_j}+\phi_{j,y_i}}{2}\right) dx\, dy - \langle u_i, f_i\rangle_{L^2}\right\} \\ \geq \ & -\frac{1}{2|\Omega|}\int_\Omega\int_\Omega \overline{H}_{ijkl}\,\sigma_{ij}\,\sigma_{kl}\, dx\, dy \\ & -\frac{1}{2|\Omega|}\int_\Omega\int_\Omega \overline{\sigma_{ij}}\, Q_{mi}\, Q_{mk}\, dx\, dy, \end{aligned} \tag{34}$$

$\forall (u,\phi) \in V \times V_1, (\sigma, Q) \in A^*$, where $A^* = A_1^* \cap A_2^* \cap A_3^*$,

$$A_1^* = \{(\sigma, Q) \in Y_1^* \times Y_1^* \ : \ \sigma_{ij,y_j} + Q_{ij,y_j} = 0, \text{ in } \Omega \times \Omega\}.$$

$$A_2^* = \left\{(\sigma, Q) \in Y_1^* \times Y_1^* \ : \ \frac{1}{|\Omega|}\left(\int_\Omega(\sigma_{ij})\, dy\right)_{x_j} + \frac{1}{|\Omega|}\left(\int_\Omega(Q_{ij})\, dy\right)_{x_j} + f_i = 0, \text{ in } \Omega\right\},$$

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$$A_3^* = \{(\sigma, Q) \in Y_1^* \times Y_1^* \ : \ \{\sigma_{ij}\} \text{ is positive definite in } \Omega \times \Omega\}.$$

Hence, denoting

$$J^*(\sigma, Q) = -\frac{1}{2|\Omega|} \int_\Omega \int_\Omega \overline{H}_{ijkl}\, \sigma_{ij}\, \sigma_{kl}\, dx\, dy - \frac{1}{2|\Omega|} \int_\Omega \int_\Omega \overline{\sigma_{ij}}\, Q_{mi}\, Q_{mk}\, dx\, dy,$$

we have obtained

$$\inf_{u \in V} J(u) \geq \sup_{(\sigma, Q) \in A^*} J^*(\sigma, Q).$$

Remark 6.1. *This last dual functional is concave and such a concerning inequality corresponds a duality principle for the relaxed primal formulation.*

We emphasize again such results are also extensions and in some sense complement the original duality principles in the works of Telega and Bielski, [1–3].

Moreover, if $(\sigma_0, Q_0) \in A^*$ is such that

$$\delta J^*(\sigma_0, Q_0) = \mathbf{0},$$

it is a well known result from the Legendre transform proprieties that the corresponding $(u_0, \phi_0) \in V \times V_1$ such that

$$(\sigma_0)_{ij} = H_{ijkl} \left(\frac{u_{k,l} + u_{l,k}}{2} + \frac{\phi_{k,y_l} + \phi_{l,y_k}}{2} + \frac{1}{2}(u_{m,k} + \phi_{m,y_k})(u_{m,l} + \phi_{m,y_l}) \right)$$

and

$$(Q_0)_{ij} = (\sigma_0)_{im} (v_{2_0})_{mj},$$

is also such that

$$\delta J_1(u_0, \phi_0) = \mathbf{0}$$

and

$$J_1(u_0, \phi_0) = J^*(\sigma_0, Q_0).$$

From this and

$$\inf_{u \in V} J(u) = \inf_{(u, \phi) \in V \times V_1} J_1(u, \phi) \geq \sup_{(\sigma, Q) A^*} J^*(\sigma, Q),$$

we obtain

$$\begin{aligned} J_1(u_0, \phi_0) &= \inf_{(u, \phi) \in V \times V_1} J_1(u, \phi) \\ &= \sup_{(\sigma, Q) \in A^*} J^*(\sigma, Q) \\ &= J^*(\sigma_0, Q_0) \\ &= \inf_{u \in V} J(u). \end{aligned} \tag{35}$$

Also, from the modern calculus of variations theory, there exists a sequence $\{u_n\} \subset V$ such that

$$u_n \rightharpoonup u_0, \text{ weakly in } V,$$

and

$$J(u_n) \to J_1(u_0, \phi_0) = \inf_{u \in V} J(u).$$

From this and the Ekeland variational principle, there exists $\{v_n\} \subset V$ such that

$$\|u_n - v_n\|_V \leq 1/n,$$

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$$J(v_n) \leq \inf_{u \in V} J(u) + 1/n,$$

and

$$\|\delta J(v_n)\|_{V^*} \leq 1/n, \ \forall n \in \mathbb{N},$$

so that

$$v_n \rightharpoonup u_0, \text{ weakly in } V,$$

and

$$J(v_n) \to J_1(u_0, \phi_0) = \inf_{u \in V} J(u).$$

Assume now we are dealing with a finite dimensional version of such a model, in a finite elements of finite differences context, for example.

In such a case we have

$$v_n \to u_0, \text{ strongly in } \mathbb{R}^N$$

for an appropriate $N \in \mathbb{N}$.

From continuity we obtain

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

$$J(v_n) \to J(u_0).$$

Summarizing, we have got

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

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

Here we highlight such last results are valid just for this finite-dimensional model version.

7. An exact convex dual variational formulation for a non-convex primal one

In this section we develop a convex dual variational formulation suitable to compute a critical point for the corresponding primal one.

Let $\Omega \subset \mathbb{R}^2$ be an open, bounded, connected set with a regular (Lipschitzian) boundary denoted by $\partial\Omega$.

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

$$J(u) = F(u_x, u_y) - \langle u, f \rangle_{L^2},$$

$V = W_0^{1,2}(\Omega)$ and $f \in L^2(\Omega)$.

Here we denote $Y = Y^* = L^2(\Omega)$ and $Y_1 = Y_1^* = L^2(\Omega) \times L^2(\Omega)$.

Defining

$$V_1 = \{u \in V \ : \ \|u\|_{1,\infty} \leq K_1\}$$

for some appropriate $K_1 > 0$, suppose also F is twice Fréchet differentiable and

$$\det \left\{ \frac{\partial^2 F(u_x, u_y)}{\partial v_1 \partial v_2} \right\} \neq 0,$$

$\forall u \in V_1$.

Define now $F_1 : V \to \mathbb{R}$ and $F_2 : V \to \mathbb{R}$ by

$$F_1(u_x, u_y) = F(u_x, u_y) + \frac{\varepsilon}{2} \int_\Omega u_x^2 \, dx + \frac{\varepsilon}{2} \int_\Omega u_y^2 \, dx,$$

and

$$F_2(u_x, u_y) = \frac{\varepsilon}{2} \int_\Omega u_x^2 \, dx + \frac{\varepsilon}{2} \int_\Omega u_y^2 \, dx,$$

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where here we denote $dx = dx_1 dx_2$.

Moreover, we define the respective Legendre transform functionals F_1^* and F_2^* as

$$F_1^*(v^*) = \langle v_1, v_1^* \rangle_{L^2} + \langle v_2, v_2^* \rangle_{L^2} - F_1(v_1, v_2),$$

where $v_1, v_2 \in Y$ are such that

$$v_1^* = \frac{\partial F_1(v_1, v_2)}{\partial v_1},$$

$$v_2^* = \frac{\partial F_1(v_1, v_2)}{\partial v_2},$$

and

$$F_2^*(v^*) = \langle v_1, v_1^* + f_1 \rangle_{L^2} + \langle v_2, v_2^* \rangle_{L^2} - F_2(v_1, v_2),$$

where $v_1, v_2 \in Y$ are such that

$$v_1^* + f_1 = \frac{\partial F_2(v_1, v_2)}{\partial v_1},$$

$$v_2^* = \frac{\partial F_2(v_1, v_2)}{\partial v_2}.$$

Here f_1 is any function such that

$$(f_1)_x = f, \text{ in } \Omega.$$

Furthermore, we define

$$\begin{aligned} J^*(v^*) &= -F_1^*(v^*) + F_2^*(v^*) \\ &= -F_1^*(v^*) + \frac{1}{2\varepsilon} \int_\Omega (v_1^* + f_1)^2 \, dx + \frac{1}{2\varepsilon} \int_\Omega (v_2^*)^2 \, dx. \end{aligned} \tag{36}$$

Observe that through the target conditions

$$v_1^* + f_1 = \varepsilon u_x,$$

$$v_2^* = \varepsilon u_y,$$

we may obtain the compatibility condition

$$(v_1^* + f_1)_y - (v_2^*)_x = 0.$$

Define now

$$A^* = \{v^* = (v_1^*, v_2^*) \in B_r(0,0) \subset Y_1^* \ : \ (v_1^* + f_1)_y - (v_2^*)_x = 0, \text{ in } \Omega\},$$

for some appropriate $r > 0$ such that J^* is convex in $B_r(0,0)$.

Consider the problem of minimizing J^* subject to $v^* \in A^*$.

Assuming $r > 0$ is large enough so that the restriction in r is not active, at this point we define the associated Lagrangian

$$J_1^*(v^*, \varphi) = J^*(v^*) + \langle \varphi, (v_1^* + f)_y - (v_2^*)_x \rangle_{L^2},$$

where φ is an appropriate Lagrange multiplier.

Therefore

$$\begin{aligned} J_1^*(v^*) &= -F_1^*(v^*) + \frac{1}{2\varepsilon} \int_\Omega (v_1^* + f_1)^2 \, dx + \frac{1}{2\varepsilon} \int_\Omega (v_2^*)^2 \, dx \\ &\quad + \langle \varphi, (v_1^* + f)_y - (v_2^*)_x \rangle_{L^2}. \end{aligned} \tag{37}$$

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The optimal point in question will be a solution of the corresponding Euler-Lagrange equations for J_1^*.

From the variation of J_1^* in v_1^* we obtain

$$-\frac{\partial F_1^*(v^*)}{\partial v_1^*}+\frac{v_1^*+f}{\varepsilon}-\frac{\partial \varphi}{\partial y}=0. \tag{38}$$

From the variation of J_1^* in v_2^* we obtain

$$-\frac{\partial F_1^*(v^*)}{\partial v_2^*}+\frac{v_2^*}{\varepsilon}+\frac{\partial \varphi}{\partial x}=0. \tag{39}$$

From the variation of J_1^* in φ we have

$$(v_1^*+f)_y-(v_2^*)_x=0.$$

From this last equation, we may obtain $u \in V$ such that

$$v_1^*+f=\varepsilon u_x,$$

and

$$v_2^*=\varepsilon u_y.$$

From this and the previous extremal equations indicated we have

$$-\frac{\partial F_1^*(v^*)}{\partial v_1^*}+u_x-\frac{\partial \varphi}{\partial y}=0,$$

and

$$-\frac{\partial F_1^*(v^*)}{\partial v_2^*}+u_y+\frac{\partial \varphi}{\partial x}=0.$$

so that

$$v_1^*+f=\frac{\partial F_1(u_x-\varphi_y,u_y+\varphi_x)}{\partial v_1},$$

and

$$v_2^*=\frac{\partial F_1(u_x-\varphi_y,u_y+\varphi_x)}{\partial v_2}.$$

From this and equation (38) and (39) we have

$$\begin{aligned} & -\varepsilon\left(\frac{\partial F_1^*(v^*)}{\partial v_1^*}\right)_x-\varepsilon\left(\frac{\partial F_1^*(v^*)}{\partial v_2^*}\right)_y \\ & +(v_1^*+f_1)_x+(v_2^*)_y \\ = \quad & -\varepsilon u_{xx}-\varepsilon u_{yy}+(v_1^*)_x+(v_2^*)_y+f=0. \end{aligned} \tag{40}$$

Replacing the expressions of v_1^* and v_2^* into this last equation, we have

$$-\varepsilon u_{xx}-\varepsilon u_{yy}+\left(\frac{\partial F_1(u_x-\varphi_y,u_y+\varphi_x)}{\partial v_1}\right)_x+\left(\frac{\partial F_1(u_x-\varphi_y,u_y+\varphi_x)}{\partial v_2}\right)_y+f=0,$$

so that

$$\left(\frac{\partial F(u_x-\varphi_y,u_y+\varphi_x)}{\partial v_1}\right)_x+\left(\frac{\partial F(u_x-\varphi_y,u_y+\varphi_x)}{\partial v_2}\right)_y+f=0, \text{ in } \Omega. \tag{41}$$

Observe that if

$$\nabla^2\varphi=0$$

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then there exists $\hat{u}$ such that u and φ are also such that

$$u_x - \varphi_y = \hat{u}_x$$

and

$$u_y + \varphi_x = \hat{u}_y.$$

The boundary conditions for φ must be such that $\hat{u} \in W_0^{1,2}$.

From this and equation (41) we obtain

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

Summarizing, we may obtain a solution $\hat{u} \in W_0^{1,2}$ of equation $\delta J(\hat{u}) = \mathbf{0}$ by minimizing J^* on A^*.

Finally, observe that clearly J^* is convex in an appropriate large ball $B_r(0,0)$ for some appropriate $r > 0$

8. Another primal dual formulation for a related model

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

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

$$\begin{aligned} J(u) &= \frac{\gamma}{2}\int_\Omega \nabla u \cdot \nabla u \, dx + \frac{\alpha}{2}\int_\Omega (u^2 - \beta)^2 \, dx \\ &\quad - \langle u, f \rangle_{L^2}, \end{aligned} \tag{42}$$

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

Denoting $Y = Y^* = L^2(\Omega)$, define now $J_1^* : V \times Y^* \to \mathbb{R}$ by

$$\begin{aligned} J_1^*(u, v_0^*) &= -\frac{\gamma}{2}\int_\Omega \nabla u \cdot \nabla u \, dx - \langle u^2, v_0^* \rangle_{L^2} \\ &\quad + \frac{K_1}{2}\int_\Omega (-\gamma\nabla^2 u + 2v_0^* u - f)^2 \, dx + \langle u, f \rangle_{L^2} \\ &\quad + \frac{1}{2\alpha}\int_\Omega (v_0^*)^2 \, dx + \beta \int_\Omega v_0^* \, dx, \end{aligned} \tag{43}$$

Define also

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

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

and

$$V_1 = V_2 \cap A^+$$

for some appropriate $K_3 > 0$ to be specified.

Moreover define

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

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

Observe that, denoting

$$\varphi = -\gamma\nabla^2 u + 2v_0^* u - f$$

we have

$$\frac{\partial^2 J_1^*(u, v_0^*)}{\partial (v_0^*)^2} = \frac{1}{\alpha} + 4K_1 u^2$$

$$\frac{\partial^2 J_1^*(u, v_0^*)}{\partial u^2} = \gamma\nabla^2 - 2v_0^* + K_1(-\gamma\nabla^2 + 2v_0^*)^2$$

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and

$$\frac{\partial^2 J_1^*(u,v_0^*)}{\partial u \partial v_0^*} = K_1(2\varphi + 2(-\gamma\nabla^2 u + 2v_0^* u)) - 2u$$

so that

$$\begin{aligned} & \det\{\delta^2 J_1^*(u,v_0^*)\} \\ = & \frac{\partial^2 J_1^*(u,v_0^*)}{\partial (v_0^*)^2}\frac{\partial^2 J_1^*(u,v_0^*)}{\partial u^2} - \left(\frac{\partial^2 J_1^*(u,v_0^*)}{\partial u \partial v_0^*}\right)^2 \\ = & \frac{K_1(-\gamma\nabla^2 + 2v_0^*)^2}{\alpha} - \frac{\gamma\nabla^2 + 2v_0^* + 4\alpha u^2}{\alpha} \\ & -4K_1^2\varphi^2 - 8K_1\varphi(-\gamma\nabla^2 + 2v_0^*)u + 8K_1\varphi u \\ & +4K_1(-\gamma\nabla^2 u + 2v_0^* u)u. \end{aligned} \tag{44}$$

Observe now that a critical point $\varphi = 0$ and $(-\gamma\nabla^2 u + 2v_0^* u)u = fu \geq 0$ in Ω. Therefore, for an appropriate large $K_1 > 0$, also at a critical point, we have

$$\begin{aligned} & \det\{\delta^2 J_1^*(u,v_0^*)\} \\ = & 4K_1 fu - \frac{\delta^2 J(u)}{\alpha} + K_1\frac{(-\gamma\nabla^2 + 2v_0^*)^2}{\alpha} > \mathbf{0}. \end{aligned} \tag{45}$$

Remark 8.1. *From this last equation we may observe that J_1^* has a large region of convexity about any critical point $(u_0, \hat{v}_0^*)$, that is, there exists a large $r > 0$ such that J_1^* is convex on $B_r(u_0, \hat{v}_0^*)$.*

With such results in mind, we may easily prove the following theorem.

Theorem 8.2. *Assume $K_1 \gg \max\{1, K, K_3\}$ and suppose $(u_0, \hat{v}_0^*) \in V_1 \times B^*$ is such that*

$$\delta J_1^*(u_0, \hat{v}_0^*) = \mathbf{0}.$$

Under such hypotheses, there exists $r > 0$ such that J_1^* is convex in $E^* = B_r(u_0, \hat{v}_0^*) \cap (V_1 \times B^*)$,

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

and

$$-J(u_0) = J_1(u_0, \hat{v}_0^*) = \inf_{(u,v_0^*)\in E^*} J_1^*(u, v_0^*).$$

9. A third primal dual formulation for a related model

Let $\Omega \subset \mathbb{R}^3$ be an open, bounded and connected set with a regular boundary denoted by $\partial\Omega$. Consider the functional $J : V \to \mathbb{R}$ where

$$\begin{aligned} J(u) = & \frac{\gamma}{2}\int_\Omega \nabla u \cdot \nabla u \, dx + \frac{\alpha}{2}\int_\Omega (u^2 - \beta)^2 \, dx \\ & -\langle u, f\rangle_{L^2}, \end{aligned} \tag{46}$$

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

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Denoting $Y = Y^* = L^2(\Omega)$, define now $J_1^* : V \times Y^* \times Y^* \to \mathbb{R}$ by

$$\begin{aligned} J_1^*(u, v_0^*, v_1^*) &= \frac{\gamma}{2}\int_\Omega \nabla u \cdot \nabla u \, dx + \frac{1}{2}\int_\Omega K\, u^2 \, dx \\ &\quad -\langle u, v_1^*\rangle_{L^2} + \frac{1}{2}\int_\Omega \frac{(v_1^*)^2}{(-2v_0^* + K)}\, dx \\ &\quad + \frac{1}{2(\alpha+\varepsilon)}\int_\Omega (v_0^* - \alpha(u^2 - \beta))^2 \, dx + \langle u, f\rangle_{L^2} \\ &\quad - \frac{1}{2\alpha}\int_\Omega (v_0^*)^2 \, dx - \beta \int_\Omega v_0^* \, dx, \end{aligned} \tag{47}$$

where $\varepsilon > 0$ is a small real constant.

Define also

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

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

and

$$V_1 = V_2 \cap A^+$$

for some appropriate $K_3 > 0$ to be specified.

Moreover define

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

and

$$D^* = \{v_1^* \in Y^* \ : \ \|v_1^*\| \leq K_5\},$$

for some appropriate real constants $K_4, K_5 > 0$ to be specified.

Remark 9.1. *Define now*

$$H_1(u, v_0^*) = -\gamma\nabla^2 + 2v_0^* + 4\alpha u^2$$

For an appropriate function (or, in a more general fashion, an appropriate bounded operator) M_1 define

$$B_1^* = \{v_0^* \in B^* \ : \ 2v_0^* + M_1 \geq \varepsilon_1\},$$

for some small parameter $\varepsilon_1 > 0$.

Moreover, define

$$E^* = \{u \in V_1 \ : \ \sqrt{4\alpha}|u| \geq \sqrt{|M_1 + \gamma\nabla^2|}.$$

Since for $(u, v_0^*) \in V_1 \times B_1^*$ we have $u\, f \geq 0$, in Ω, so that for $u_1, u_2 \in V_1$ we have

$$sign\ (u_1) = \ sign\ (u_2) \text{ in } \Omega,$$

we may infer that E^* is a convex set.

Moreover if $(u, v_0^*) \in E^* \times B_1^*$, then

$$\sqrt{4\alpha}|u| \geq \sqrt{|M_1 + \gamma\nabla^2|}$$

so that

$$4\alpha u^2 \geq M_1 + \gamma\nabla^2$$

and

$$2v_0^* + M_1 \geq \varepsilon_1$$

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so that

$$H_1(u, v_0^*) = -\gamma\nabla^2 + 2v_0^* + 4\alpha u^2 \geq \varepsilon_1.$$

Such a result we will be used many times in the next sections.

Observe that, defining

$$\varphi = v_0^* - \alpha(u^2 - \beta)$$

we may obtain

$$\frac{\partial^2 J_1^*(u, v_0^*, v_1^*)}{\partial u^2} = -\gamma\nabla^2 + K + \frac{\alpha}{\alpha+\varepsilon}4u^2 - 2\varphi\frac{\alpha}{\alpha+\varepsilon}$$

$$\frac{\partial^2 J_1^*(u, v_0^*, v_1^*)}{\partial (v_1^*)^2} = \frac{1}{-2v_0^* + K}$$

and

$$\frac{\partial^2 J_1^*(u, v_0^*, v_1^*)}{\partial u \partial v_1^*} = -1$$

so that

$$\begin{aligned}
& \det\left\{\frac{\partial^2 J_1^*(u, v_0^*, v_1^*)}{\partial u \partial v_1^*}\right\} \\
= \; & \frac{\partial^2 J_1^*(u, v_1^*, v_0^*)}{\partial (v_1^*)^2}\frac{\partial^2 J_1^*(u, v_1^*, v_0^*)}{\partial u^2} - \left(\frac{\partial^2 J_1^*(u, v_1^*, v_0^*)}{\partial u \partial v_1^*}\right)^2 \\
= \; & \frac{-\gamma\nabla^2 + 2v_0^* + 4\frac{\alpha^2}{\alpha+\varepsilon}u^2 - 2\frac{\alpha}{\alpha+\varepsilon}\varphi}{-2v_0^* + K} \\
\equiv \; & H(u, v_0^*). \qquad (48)
\end{aligned}$$

However, at a critical point, we have $\varphi = \mathbf{0}$ so that, for a fixed $v_0^* \in B^*$ we define the non-active but convex restriction

$$(C_1)_{v_0^*}^* = \{u \in V_1 \; : \; (\varphi)^2 \leq \varepsilon\},$$

for a small parameter $\varepsilon > 0$.

From such results, assuming $K \gg \max\{K_3, K_4, K_5\}$, and $0 < \varepsilon \ll \varepsilon_1 \ll 1$, we have that

$$H(u, v_0^*) > \mathbf{0},$$

for $v_0^* \in B_1^*$ and $u \in E^* \cap (C_1)_{v_0^*}^*$.

With such results in mind, we may easily prove the following theorem.

Theorem 9.2. *Suppose* $(u_0, \hat{v}_1^*, \hat{v}_0^*) \in (E^* \cap (C_1)_{\hat{v}_0^*}^*) \times D^* \times B_1^*$ *is such that*

$$\delta J_1^*(u_0, \hat{v}_1^*, \hat{v}_0^*) = \mathbf{0}.$$

Under such hypotheses, we have that

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

and

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$$\begin{aligned} J(u_0) &= \inf_{u \in (C_1)^*_{\hat{v}_0^*}} J(u) \\ &= J_1^*(u_0, \hat{v}_1^*, \hat{v}_0^*) \\ &= \inf_{(u,v_1^*) \in (C_1)^*_{\hat{v}_0^*} \times D^*} \left\{ \sup_{v_0^* \in B^*} J_1^*(u, v_1^*, v_0^*) \right\} \\ &= \sup_{v_0^* \in B^*} \left\{ \inf_{(u,v_1^*) \in (C_1)^*_{\hat{v}_0^*} \times D^*} J_1^*(u, v_1^*, v_0^*) \right\}. \end{aligned} \tag{49}$$

Proof. The proof that

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

and

$$J(u_0) = J_1^*(u_0, \hat{v}_1^*, \hat{v}_0^*)$$

may be easily made similarly as in the previous sections.

Moreover, observe that for $K > 0$ sufficiently large, we have

$$\frac{\partial^2 J_1^*(u_0, \hat{v}_1^*, v_0^*)}{\partial (v_0^*)^2} < \mathbf{0}, \ \forall v_0^* \in B^*$$

so that this and the other hypotheses, we have also

$$J_1^*(u_0, \hat{v}_1^*, \hat{v}_0^*) = \inf_{(u,v_1^*) \in (C_1)^*_{\hat{v}_0^*} \times D^*} J_1^*(u, v_1^*, \hat{v}_0^*)$$

and

$$J_1^*(u_0, \hat{v}_1^*, \hat{v}_0^*) = \sup_{v_0^* \in B^*} J_1^*(u_0, \hat{v}_1^*, v_0^*).$$

From this, from a standard saddle point theorem and the remaining hypotheses, we may infer that

$$\begin{aligned} J(u_0) &= J_1^*(u_0, \hat{v}_1^*, \hat{v}_0^*) \\ &= \inf_{(u,v_1^*) \in (C_1)^*_{\hat{v}_0^*} \times D^*} \left\{ \sup_{v_0^* \in B^*} J_1^*(u, v_1^*, v_0^*) \right\} \\ &= \sup_{v_0^* \in B^*} \left\{ \inf_{(u,v_1^*) \in (C_1)^*_{\hat{v}_0^*} \times D^*} J_1^*(u, v_1^*, v_0^*) \right\}. \end{aligned} \tag{50}$$

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Moreover, observe that

$$\begin{aligned}
J_1^*(u_0,\hat{v}_1^*,\hat{v}_0^*) &= \inf_{(u,v_1^*)\in(C_1)^*_{\hat{v}_0^*}\times D^*} J_1^*(u,v_1^*,\hat{v}_0^*) \\
&\leq \frac{\gamma}{2}\int_\Omega \nabla u\cdot\nabla u\,dx + \frac{K}{2}\int_\Omega u^2\,dx \\
&\quad +\langle u^2,\hat{v}_0^*\rangle_{L^2} - \frac{K}{2}\int_\Omega u^2\,dx \\
&\quad -\frac{1}{2\alpha}\int_\Omega(\hat{v}_0^*)^2\,dx - \beta\int_\Omega \hat{v}_0^*\,dx \\
&\quad +\frac{1}{2(\alpha+\varepsilon)}\int_\Omega(\hat{v}_0^*-\alpha(u^2-\beta))^2\,dx - \langle u,f\rangle_{L^2} \\
&\leq \sup_{v_0^*\in Y^*}\left\{\frac{\gamma}{2}\int_\Omega \nabla u\cdot\nabla u\,dx + \langle u^2,v_0^*\rangle\right. \\
&\quad -\frac{1}{2\alpha}\int_\Omega(v_0^*)^2\,dx - \beta\int_\Omega v_0^*\,dx \\
&\quad \left.+\frac{1}{2(\alpha+\varepsilon)}\int_\Omega(v_0^*-\alpha(u^2-\beta))^2\,dx - \langle u,f\rangle_{L^2}\right\} \\
&= \frac{\gamma}{2}\int_\Omega \nabla u\cdot\nabla u\,dx + \frac{\alpha}{2}\int_\Omega(u^2-\beta)^2\,dx \\
&\quad -\langle u,f\rangle_{L^2},\ \forall u\in(C_1)^*_{\hat{v}_0^*}.
\end{aligned} \tag{51}$$

Summarizing, we have got

$$J(u_0) = J_1^*(u_0,\hat{v}_1^*,\hat{v}_0^*) \leq \inf_{u\in(C_1)^*_{\hat{v}_0^*}} J(u).$$

From such results, we may infer that

$$\begin{aligned}
J(u_0) &= \inf_{u\in(C_1)^*_{\hat{v}_0^*}} J(u) \\
&= J_1^*(u_0,\hat{v}_1^*,\hat{v}_0^*) \\
&= \inf_{(u,v_1^*)\in(C_1)^*_{\hat{v}_0^*}\times D^*}\left\{\sup_{v_0^*\in B^*} J_1^*(u,v_1^*,v_0^*)\right\} \\
&= \sup_{v_0^*\in B^*}\left\{\inf_{(u,v_1^*)\in(C_1)^*_{\hat{v}_0^*}\times D^*} J_1^*(u,v_1^*,v_0^*)\right\}.
\end{aligned} \tag{52}$$

The proof is complete. □

10. An algorithm for a related model in shape optimization

The next two subsections have been previously published by Fabio Silva Botelho and Alexandre Molter in [8], Chapter 21.

10.1. Introduction

Consider an elastic solid which the volume corresponds to an open, bounded, connected set, denoted by $\Omega\subset\mathbb{R}^3$ with a regular (Lipschitzian) boundary denoted by $\partial\Omega = \Gamma_0\cup\Gamma_t$ where $\Gamma_0\cap\Gamma_t = \emptyset$. Consider also the problem of minimizing the functional $\hat{J}: U\times B\to\mathbb{R}$ where

$$\hat{J}(u,t) = \frac{1}{2}\langle u_i,f_i\rangle_{L^2(\Omega)} + \frac{1}{2}\langle u_i,\hat{f}_i\rangle_{L^2(\Gamma_t)},$$

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subject to

$$\begin{cases} (H_{ijkl}(t)e_{kl}(u))_{,j} + f_i = 0 \text{ in } \Omega, \\ \\ H_{ijkl}(t)e_{kl}(u)n_j - \hat{f}_i = 0, \text{ on } \Gamma_t, \ \forall i \in \{1,2,3\}. \end{cases} \tag{53}$$

Here $\mathbf{n} = (n_1, n_2, n_3)$ denotes the outward normal to $\partial\Omega$ and

$$U = \{u = (u_1, u_2, u_3) \in W^{1,2}(\Omega; \mathbb{R}^3) \ : \ u = (0,0,0) = \mathbf{0} \text{ on } \Gamma_0\},$$

$$B = \left\{ t : \Omega \to [0,1] \text{ measurable } \ : \ \int_\Omega t(x)\, dx = t_1|\Omega| \right\},$$

where

$$0 < t_1 < 1$$

and $|\Omega|$ denotes the Lebesgue measure of Ω.

Moreover $u = (u_1, u_2, u_3) \in W^{1,2}(\Omega; \mathbb{R}^3)$ is the field of displacements relating the cartesian system $(0, x_1, x_2, x_3)$, resulting from the action of the external loads $f \in L^2(\Omega; \mathbb{R}^3)$ and $\hat{f} \in L^2(\Gamma_t; \mathbb{R}^3)$.

We also define the stress tensor $\{\sigma_{ij}\} \in Y^* = Y = L^2(\Omega; \mathbb{R}^{3\times 3})$, by

$$\sigma_{ij}(u) = H_{ijkl}(t)e_{kl}(u),$$

and the strain tensor $e : U \to L^2(\Omega; \mathbb{R}^{3\times 3})$ by

$$e_{ij}(u) = \frac{1}{2}(u_{i,j} + u_{j,i}), \ \forall i, j \in \{1,2,3\}.$$

Finally,

$$\{H_{ijkl}(t)\} = \{tH^0_{ijkl} + (1-t)H^1_{ijkl}\},$$

where H^0 corresponds to a strong material and H^1 to a very soft material, intending to simulate voids along the solid structure.

The variable t is the design one, which the optimal distribution values along the structure are intended to minimize its inner work with a volume restriction indicated through the set B.

The duality principle obtained is developed inspired by the works in [1,2]. Similar theoretical results have been developed in [7], however we believe the proof here presented, which is based on the min-max theorem is easier to follow (indeed we thank an anonymous referee for his suggestion about applying the min-max theorem to complete the proof). We highlight throughout this text we have used the standard Einstein sum convention of repeated indices.

Moreover, details on the Sobolev spaces addressed may be found in [6]. In addition, the primal variational development of the topology optimization problem has been described in [7].

The main contributions of this work are to present the detailed development, through duality theory, for such a kind of optimization problems. We emphasize that to avoid the check-board standard and obtain appropriate robust optimized structures without the use of filters, it is necessary to discretize more in the load direction, in which the displacements are much larger.

10.2. Mathematical formulation of the topology optimization problem

Our mathematical topology optimization problem is summarized by the following theorem.

Theorem 10.1. *Consider the statements and assumptions indicated in the last section, in particular those refereing to Ω and the functional $\hat{J} : U \times B \to \mathbb{R}$.*

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Define $J_1 : U \times B \to \mathbb{R}$ *by*

$$J_1(u,t) = -G(e(u),t) + \langle u_i, f_i \rangle_{L^2(\Omega)} + \langle u_i, \hat{f}_i \rangle_{L^2(\Gamma_t)},$$

where

$$G(e(u),t) = \frac{1}{2}\int_\Omega H_{ijkl}(t) e_{ij}(u) e_{kl}(u)\, dx,$$

and where

$$dx = dx_1 dx_2 dx_3.$$

Define also $J^* : U \to \mathbb{R}$ *by*

$$\begin{aligned} J^*(u) &= \inf_{t\in B}\{J_1(u,t)\} \\ &= \inf_{t\in B}\{-G(e(u),t) + \langle u_i, f_i \rangle_{L^2(\Omega)} + \langle u_i, \hat{f}_i \rangle_{L^2(\Gamma_t)}\}. \end{aligned} \tag{54}$$

Assume there exists $c_0, c_1 > 0$ *such that*

$$H^0_{ijkl} z_{ij} z_{kl} > c_0 z_{ij} z_{ij}$$

and

$$H^1_{ijkl} z_{ij} z_{kl} > c_1 z_{ij} z_{ij},\ \forall z = \{z_{ij}\} \in \mathbb{R}^{3\times 3},\ \text{ such that } z \neq \mathbf{0}.$$

Finally, define $J : U \times B \to \mathbb{R} \cup \{+\infty\}$ *by*

$$J(u,t) = \hat{J}(u,t) + Ind(u,t),$$

where

$$Ind(u,t) = \begin{cases} 0, & \text{if } (u,t) \in A^*, \\ +\infty, & \text{otherwise}, \end{cases} \tag{55}$$

where $A^* = A_1 \cap A_2$,

$$A_1 = \{(u,t) \in U \times B \ :\ (\sigma_{ij}(u))_{,j} + f_i = 0,\ \text{in } \Omega,\ \forall i \in \{1,2,3\}\}$$

and

$$A_2 = \{(u,t) \in U \times B \ :\ \sigma_{ij}(u) n_j - \hat{f}_i = 0,\ \text{on } \Gamma_t,\ \forall i \in \{1,2,3\}\}.$$

Under such hypotheses, there exists $(u_0, t_0) \in U \times B$ *such that*

$$\begin{aligned} J(u_0,t_0) &= \inf_{(u,t)\in U\times B} J(u,t) \\ &= \sup_{\hat{u}\in U} J^*(\hat{u}) \\ &= J^*(u_0) \\ &= \hat{J}(u_0,t_0) \\ &= \inf_{(t,\sigma)\in B\times C^*} G^*(\sigma,t) \\ &= G^*(\sigma(u_0),t_0), \end{aligned} \tag{56}$$

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where

$$\begin{aligned} G^*(\sigma,t) &= \sup_{v\in Y}\{\langle v_{ij},\sigma_{ij}\rangle_{L^2(\Omega)} - G(v,t)\} \\ &= \frac{1}{2}\int_\Omega \overline{H}_{ijkl}(t)\sigma_{ij}\sigma_{kl}\,dx, \end{aligned} \tag{57}$$

$$\{\overline{H}_{ijkl}(t)\} = \{H_{ijkl}(t)\}^{-1}$$

and $C^* = C_1 \cap C_2$, *where*

$$C_1 = \{\sigma \in Y^* \ : \ \sigma_{ij,j} + f_i = 0, \ in\ \Omega, \ \forall i \in \{1,2,3\}\}$$

and

$$C_2 = \{\sigma \in Y^* \ : \ \sigma_{ij}n_j - \hat{f}_i = 0, \ on\ \Gamma_t, \ \forall i \in \{1,2,3\}\}.$$

Proof. Observe that

$$\begin{aligned} \inf_{(u,t)\in U\times B} J(u,t) &= \inf_{t\in B}\left\{\inf_{u\in U} J(u,t)\right\} \\ &= \inf_{t\in B}\left\{\sup_{\hat{u}\in U}\left\{\inf_{u\in U}\left\{\frac{1}{2}\int_\Omega H_{ijkl}(t)e_{ij}(u)e_{kl}(u)\,dx\right.\right.\right. \\ &\quad +\langle \hat{u}_i, (H_{ijkl}(t)e_{kl}(u))_{,j} + f_i\rangle_{L^2(\Omega)} \\ &\quad \left.\left.\left. -\langle \hat{u}_i, H_{ijkl}(t)e_{kl}(u)n_j - \hat{f}_i\rangle_{L^2(\Gamma_t)}\right\}\right\}\right\} \\ &= \inf_{t\in B}\left\{\sup_{\hat{u}\in U}\left\{\inf_{u\in U}\left\{\frac{1}{2}\int_\Omega H_{ijkl}(t)e_{ij}(u)e_{kl}(u)\,dx\right.\right.\right. \\ &\quad - \int_\Omega H_{ijkl}(t)e_{ij}(\hat{u})e_{kl}(u)\,dx \\ &\quad \left.\left.\left. +\langle \hat{u}_i, f_i\rangle_{L^2(\Omega)} + \langle \hat{u}_i, \hat{f}_i\rangle_{L^2(\Gamma_t)}\right\}\right\}\right\} \\ &= \inf_{t\in B}\left\{\sup_{\hat{u}\in U}\left\{-\int_\Omega H_{ijkl}(t)e_{ij}(\hat{u})e_{kl}(\hat{u})\,dx\right.\right. \\ &\quad \left.\left. \langle \hat{u}_i, f_i\rangle_{L^2(\Omega)} + \langle \hat{u}_i, \hat{f}_i\rangle_{L^2(\Gamma_t)}\right\}\right\} \\ &= \inf_{t\in B}\left\{\inf_{\sigma\in C^*} G^*(\sigma,t)\right\}. \end{aligned} \tag{58}$$

Also, from this and the min-max theorem, there exist $(u_0,t_0) \in U \times B$ such that

$$\begin{aligned} \inf_{(u,t)\in U\times B} J(u,t) &= \inf_{t\in B}\left\{\sup_{\hat{u}\in U} J_1(u,t)\right\} \\ &= \sup_{u\in U}\left\{\inf_{t\in B} J_1(u,t)\right\} \\ &= J_1(u_0,t_0) \\ &= \inf_{t\in B} J_1(u_0,t) \\ &= J^*(u_0). \end{aligned} \tag{59}$$

Finally, from the extremal necessary condition

$$\frac{\partial J_1(u_0,t_0)}{\partial u} = \mathbf{0}$$

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we obtain

$$(H_{ijkl}(t_0)e_{kl}(u_0))_{,j} + f_i = 0 \text{ in } \Omega,$$

and

$$H_{ijkl}(t_0)e_{kl}(u_0)n_j - \hat{f}_i = 0 \text{ on } \Gamma_t, \ \forall i \in \{1,2,3\},$$

so that

$$G(e(u_0)) = \frac{1}{2}\langle (u_0)_i, f_i\rangle_{L^2(\Omega)} + \frac{1}{2}\langle (u_0)_i, \hat{f}_i\rangle_{L^2(\Gamma_t)}.$$

Hence $(u_0, t_0) \in A^*$ so that $Ind(u_0, t_0) = 0$ and $\sigma(u_0) \in C^*$.
Moreover

$$\begin{aligned} J^*(u_0) &= -G(e(u_0)) + \langle (u_0)_i, f_i\rangle_{L^2(\Omega)} + \langle (u_0)_i, \hat{f}_i\rangle_{L^2(\Gamma_t)} \\ &= G(e(u_0)) \\ &= G(e(u_0)) + Ind(u_0, t_0) \\ &= J(u_0, t_0) \\ &= G^*(\sigma(u_0), t_0). \end{aligned} \tag{60}$$

This completes the proof. □

10.3. *About a concerning algorithm and related numerical method*

For numerically solve this optimization problem in question, we present the following algorithm

1. Set $t_1 = 0.5$ in Ω and $n = 1$.
2. Calculate $u_n \in U$ such that
$$J_1(u_n, t_n) = \sup_{u \in U} J_1(u, t_n).$$
3. Calculate $t_{n+1} \in B$ such that
$$J_1(u_n, t_{n+1}) = \inf_{t \in B} J_1(u_n, t).$$
4. If $\|t_{n+1} - t_n\|_\infty < 10^{-4}$ or $n > 100$ then stop, else set $n := n + 1$ and go to item 2.

We have developed a software in finite differences for solving such a problem.
Here the software.
****

1. clear all

```
global P m8 d w u v Ea Eb Lo d1 z1 m9 du1 du2 dv1 dv2 c3
m8=27;
m9=24;
c3=0.95;
d=1.0/m8;
d1=0.5/m9;
Ea=210 * 10^5; (stronger material)
Eb=1000; (softer material simulating voids)
w=0.30;
P=-42000000;
z1=(m8-1)*(m9-1);
A3=zeros(z1,z1);
```

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```
for i=1:z1
A3(1,i)=1.0;
end;
b=zeros(z1,1);
uo=0.000001*ones(z1,1);
u1=ones(z1,1);
b(1,1)=c3*z1;
for i=1:m9-1
for j=1:m8-1
Lo(i,j)=c3;
end; end;
for i=1:z1
x1(i)=c3*z1;
end;
for i=1:2*m8*m9
xo(i)=0.000;
end;
xw=xo;
xv=Lo;
for k2=1:24
c3=0.98*c3;
b(1,1)=c3*z1;
k2
b14=1.0;
k3=0;
while (b14 > 10^-3.5) and (k3 < 5)
k3=k3+1;
b12=1.0;
k=0;
while (b12 > 10^-4.0) and (k < 120)
k=k+1;
k2
k3
k
X=fminunc('funbeam',xo);
xo=X;
b12=max(abs(xw-xo));
xw=X;
end;
```

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```
for i=1:m9-1
for j=1:m8-1
E1 = Lo(i,j)^2 * (Ea - Eb);
ex=du1(i,j);
ey=dv2(i,j);
exy=1/2*(dv1(i,j)+du2(i,j));
Sx = E1 * (ex + w * ey)/(1 - w^2);
Sy = E1 * (w * ex + ey)/(1 - w^2);
Sxy=E1/(2*(1+w))*exy;
dc3(i,j)=-(Sx*ex+Sy*ey+2*Sxy*exy);
end;
end;
for i=1:m9-1
for j=1:m8-1
f(j+(i-1)*(m8-1))=dc3(i,j);
end;
end;
for k1=1:1
k1
X1=linprog(f,[ ],[ ],A3,b,uo,u1,x1);
x1=X1;
end;
for i=1:m9-1
for j=1:m8-1
Lo(i,j)=X1(j+(m8-1)*(i-1));
end;
end;
b14=max(max(abs(Lo-xv)))
xv=Lo;
colormap(gray); imagesc(-Lo); axis equal; axis tight; axis off;pause(1e-6)
end;
end;
```

****

Here the auxiliary Function 'funbeam'

```
function S=funbeam(x)
global P m8 d w u v Ea Eb Lo d1 m9 du1 du2 dv1 dv2
for i=1:m9
for j=1:m8
u(i,j)=x(j+(m8)*(i-1));
v(i,j)=x(m8*m9+(i-1)*m8+j);
```

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```
end;
end;
for i=1:m9
end;
u(m9-1,1)=0;
v(m9-1,1)=0;
u(m9-1,m8-1)=0;
v(m9-1,m8-1)=0;
for i=1:m9-1
for j=1:m8-1
du1(i,j)=(u(i,j+1)-u(i,j))/d;
du2(i,j)=(u(i+1,j)-u(i,j))/d1;
dv1(i,j)=(v(i,j+1)-v(i,j))/d;
dv2(i,j)=(v(i+1,j)-v(i,j))/d1;
end;
end;
S=0;
for i=1:m9-1
for j=1:m8-1
E1 = Lo(i,j)^3 * Ea + (1 - Lo(i,j)^3) * Eb;
ex=du1(i,j);
ey=dv2(i,j);
exy=1/2*(dv1(i,j)+du2(i,j));
Sx = E1 * (ex + w * ey)/(1 - w^2);
Sy = E1 * (w * ex + ey)/(1 - w^2);
Sxy=E1/(2*(1+w))*exy;
S=S+1/2*(Sx*ex+Sy*ey+2*Sxy*exy);
end;
end;
S=S*d*d1-P*v(2,(m8)/3)*d*d1;
```

****

For a two dimensional beam of dimensions $1m \times 0.5m$ and $t_1 = 0.63$ we have obtained the following results:

1. Case A: For the optimal shape for a clamped beam at left (cantilever) and load $P = -4\ 10^6 N\mathbf{j}$ at $(x, y) = (1, 0.25)$, please Figure 5.
2. Case B :For the optimal shape for a simply supported beam at $(0, 0)$ and $(1, 0)$ and load $P = -4\ 10^6 N\mathbf{j}$ at $(x, y) = (1/3, 0.5)$, please Figure 6.

   In the first case the mesh was 28×24. In the second one the mesh was 27×24

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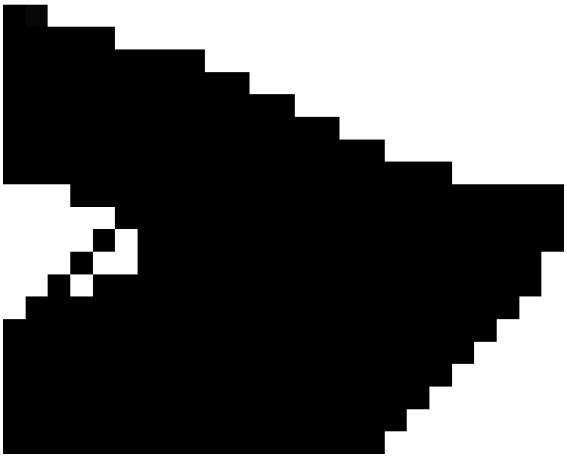

Figure 5. Density $t(x, y)$ for the Case A.

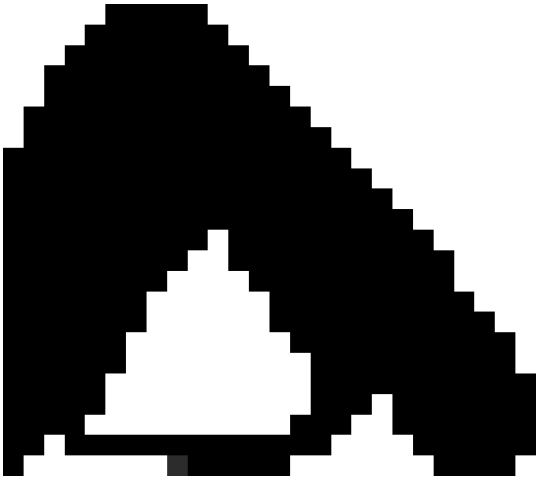

Figure 6. Density $t(x, y)$ for the Case B.

11. A duality principle for a general vectorial case in the calculus of variations

In this section we develop a duality principle for a general vectorial case in variational optimization.

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

$$J(u) = G(\nabla u_1, \cdots, \nabla u_N) - \langle u, f \rangle_{L^2},$$

where

$$V = W_0^{1,2}(\Omega; \mathbb{R}^N)$$

and

$$f = (f_1, \cdots, f_N) \in L^2(\Omega; \mathbb{R}^N).$$

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Here we have denoted $u = (u_1, \cdots, u_N) \in V$ and

$$\langle u, f \rangle_{L^2} = \langle u_i, f_i \rangle_{L^2},$$

so that we may also denote

$$J(u) = G(\nabla u) - \langle u, f \rangle_{L^2}.$$

Assume

$$G(\nabla u) = \int_\Omega g(\nabla u)\, dx$$

where $g : \mathbb{R}^{3N} \to \mathbb{R}$ is a differentiable function such that

$$g(y) \to +\infty$$

as $|y| \to \infty$. Moreover, suppose there exists $\alpha \in \mathbb{R}$ such that

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

It is well known that

$$\begin{aligned} \alpha &= \inf_{u \in V} J(u) \\ &= \inf_{u \in V} J^{**}(u) \\ &= \inf_{u \in V} \{(G \circ \nabla)^{**}(u) - \langle u, f \rangle_{L^2}\}. \end{aligned} \tag{61}$$

Under some mild hypotheses, from convexity, we have that

$$\begin{aligned} &\inf_{u \in V} \{(G \circ \nabla)^{**}(u) - \langle u, f \rangle_{L^2}\} \\ = &\sup_{v^* \in A^*} \{-(G \circ \nabla)^*(-div\, v^*)\} = -(G \circ \nabla)^*(f), \end{aligned} \tag{62}$$

where

$$A^* = \{v^* \in Y = Y^* = L^2(\Omega; \mathbb{R}^{3N}) \ : \ div\, v^* + f = 0\}.$$

Now observe that the restriction $v = \nabla u$ for some $u \in V$ is equivalent to the restriction

$$\text{curl}\, v_i = \mathbf{0}, \text{ in } \Omega$$

where $v = \{v_i\} = \{v_{ij}\}_{j=1}^3, \forall i \in \{1, \cdots, N\}$, with appropriate boundary conditions, so that with an appropriate Lagrange multiplier $\phi = \{\phi_i\}$, we obtain

$$\begin{aligned} (G \circ \nabla)^*(-div\, v^*) &= \sup_{u \in V} \{\langle u, -div\, v^* \rangle_{L^2} - G(\nabla u)\} \\ &= \sup_{u \in V} \{\langle \nabla u, v^* \rangle_{L^2} - G(\nabla u)\} \\ &\leq \inf_{\phi \in Y^*} \left\{ \sup_{v \in Y} \{\langle v, v^* \rangle_{L^2} - G(v) + \langle \phi, \text{curl}\, v \rangle_{L^2} \right\} \\ &= \inf_{\phi \in Y^*} G^*(v^* + \text{curl}\, \phi). \end{aligned} \tag{63}$$

where we have denoted

$$\text{curl}\, v = \{\text{curl}\, v_i\}$$

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and

$$\text{curl}\,\phi = \{\text{curl}\,\phi_i\}.$$

Joining the pieces, we have got

$$\begin{aligned} \inf_{u\in V} J(u) &= \inf_{u\in V}\{G(\nabla u) - \langle u, f\rangle_{L^2}\} \\ &\geq \sup_{(v^*,\phi)\in A^*\times Y^*} \{-G^*(v^* + \text{curl}\,\phi)\}, \end{aligned} \tag{64}$$

where we recall that $Y = Y^* = L^2(\Omega;\mathbb{R}^{3N})$.

We emphasize such a dual formulation in (v^*, ϕ) is convex (in fact concave).

12. A note on the Galerkin Functional

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

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

$$\begin{aligned} J(u) &= \frac{\gamma}{2}\int_\Omega \nabla u\cdot\nabla u\,dx + \frac{\alpha}{4}\int_\Omega u^4\,dx \\ &\quad -\frac{\beta}{2}\int_\Omega u^2\,dx - \langle u, f\rangle_{L^2} \end{aligned} \tag{65}$$

Here $V = W_0^{1,2}(\Omega)$, $\gamma > 0,\ \alpha > 0,\ \beta > 0$.

We denote also

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

At this point we define

$$A^+ = \{u \in V\ :\ u\,f \geq 0,\ \text{in}\ \Omega\},$$

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

for some appropriate real constant $K_3 > 0$ and

$$V_1 = A^+ \cap V_2.$$

Observe that

$$J'(u) = -\gamma\nabla^2 u + \alpha u^3 - \beta - f,$$

so that we define the Galerkin functional $J_1 : V \to \mathbb{R}$ by

$$J_1(u) = \frac{1}{2}\|J'(u)\|_2^2 = \frac{1}{2}\int_\Omega(-\gamma\nabla^2 u + \alpha u^3 - \beta u - f)^2\,dx.$$

From this, we get

$$\begin{aligned} \frac{\partial^2 J_1(u)}{\partial u^2} &= (-\gamma\nabla u + \alpha u^3 - \beta u - f)6\alpha u \\ &\quad +(-\gamma\nabla^2 + 3\alpha u^2 - \beta)^2. \end{aligned} \tag{66}$$

Define now

$$\varphi_2 = (-\gamma\nabla^2 u + \alpha u^3 - \beta u - f)^2.$$

At this point, for an appropriate small real constant $\varepsilon_1 > 0$ and bounded constant operator $M_1 > \varepsilon_1$, we set the intended non-active restriction

$$\sqrt{3\alpha}|u| \geq \sqrt{|M_1 + \gamma\nabla^2 + \beta|},$$

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and define

$$B_1 = \{u \in V_1 \ : \ \sqrt{3\alpha}|u| \geq \sqrt{|M_1 + \gamma\nabla^2 + \beta|}\}.$$

Observe that since for $u \in V_1$ we have $u\ f \geq 0$ in Ω so that if $u_1, u_2 \in V_1$ then

$$\text{sign}(u_1) = \text{sign}(u_2), \text{in } \Omega,$$

we may infer that B_1 is a convex set.

Furthermore, if $u \in B_1$, then

$$\sqrt{3\alpha}|u| \geq \sqrt{|M_1 + \gamma\nabla^2 + \beta|},$$

so that

$$3\alpha u^2 \geq M_1 + \gamma\nabla^2 + \beta,$$

and hence

$$\delta^2 J(u) = -\gamma\nabla^2 + 3\alpha u^2 - \beta \geq M_1 > \varepsilon_1 > \mathbf{0}.$$

For a small parameter $\varepsilon > 0$ we define the intended non-active restriction

$$\varphi_2 \leq \varepsilon, \text{ in } \Omega,$$

and define

$$B_2 = \{u \in V_1 \ : \ \varphi_2 \leq \varepsilon, \text{ in } \Omega\}.$$

Observe that for $\alpha > 0$ and $\beta > 0$ sufficiently large φ_2 is convex in V_1 (positive definite Hessian) so that B_2 is a convex set. Assuming $0 < \varepsilon \ll \varepsilon_1 \ll 1$, define $B_3 = B_1 \cap B_2$, which is a convex set.

Summarizing, if $u \in B_3$, then

$$\delta^2 J_1(u) \geq \mathbf{0}.$$

With such results in mind, we define the following convex optimization problem for finding a critical point of J.

Minimize

$$J_1(u) = \frac{1}{2}\|J'(u)\|_2^2 = \frac{1}{2}\int_\Omega (-\gamma\nabla^2 u + \alpha u^3 - \beta u - f)^2\, dx,$$

subject to

$$u \in B_3.$$

Observe that a critical point $u_0 \in B_3$ of J_1, from such a concerning convexity of J_1 on the convex set B_1, is also such that

$$J(u_0) = \min_{u \in B_3} J_1(u).$$

Finally, we may also define the convex optimization problem of minimizing

$$\begin{aligned} J_3(u) &= K_1 J_1(u) + J(u) \\ &= \frac{K_1}{2}\int_\Omega (-\gamma\nabla^2 u + \alpha u^3 - \beta u - f)^2\, dx \\ &\quad + \frac{\gamma}{2}\int_\Omega \nabla u \cdot \nabla u\, dx + \frac{\alpha}{4}\int_\Omega u^4\, dx \\ &\quad - \frac{\beta}{2}\int_\Omega u^2\, dx - \langle u, f\rangle_{L^2}, \end{aligned} \tag{67}$$

subject to

$$u \in B_3.$$

Here $K_1 > 0$ is a large real constant.

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Such a functional J_3 is also convex on B_3 so that a critical point $u_0 \in B_3$ of J is also a critical point of J_3, and thus

$$J_3(u_0) = \min_{u \in B_3} J_3(u).$$

13. A note on the Legendre-Galerkin functional

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

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

$$\begin{aligned} J(u) &= \frac{\gamma}{2}\int_\Omega \nabla u \cdot \nabla u \, dx + \frac{\alpha}{4}\int_\Omega u^4 \, dx \\ &\quad -\frac{\beta}{2}\int_\Omega u^2 \, dx - \langle u, f\rangle_{L^2} \end{aligned} \tag{68}$$

Here $V = W_0^{1,2}(\Omega)$, $\gamma > 0,\ \alpha > 0,\ \beta > 0$.

We denote also

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

and $F_1 : V \to \mathbb{R}$, $F_2 : V \to \mathbb{R}$ and $F_3 : V \to \mathbb{R}$ by

$$F_1(u) = \frac{\gamma}{2}\int_\Omega \nabla u \cdot \nabla u \, dx,$$

$$F_2(u) = \frac{\alpha}{4}\int_\Omega u^4 \, dx,$$

$$F_3(u) = \frac{\beta}{2}\int_\Omega u^2 \, dx.$$

Moreover, we define $F_1^*, F_2^*, F_3^* : Y^* \to \mathbb{R}$ by

$$\begin{aligned} F_1^*(v_1^*) &= \sup_{u \in V}\{\langle u, v_1^*\rangle_{L^2} - F_1(u)\} \\ &= \frac{1}{2}\int_\Omega \frac{(v_1^*)^2}{-\gamma\nabla^2} \, dx, \end{aligned} \tag{69}$$

$$\begin{aligned} F_2^*(v_2^*) &= \sup_{u \in V}\{\langle u, v_2^*\rangle_{L^2} - F_2(u)\} \\ &= \frac{3}{4}\int_\Omega \frac{(v_2^*)^{4/3}}{\alpha^{1/3}} \, dx, \end{aligned} \tag{70}$$

$$\begin{aligned} F_3^*(v_3^*) &= \sup_{u \in V}\{\langle u, v_3^*\rangle_{L^2} - F_3(u)\} \\ &= \frac{1}{2\beta}\int_\Omega (v_3^*)^2 \, dx. \end{aligned} \tag{71}$$

Observe now that these three last suprema are attained through the equations,

$$v_1^* = \frac{\partial F_1(u)}{\partial u} = -\gamma\nabla^2 u,$$

$$v_2^* = \frac{\partial F_2(u)}{\partial u} = \alpha u^3$$

$$v_3^* = \frac{\partial F_3(u)}{\partial u} = \beta u.$$

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From such results, at a critical point, we obtain the following compatibility conditions

$$u = \frac{v_1^*}{-\gamma\nabla^2} = \left(\frac{v_2^*}{\beta}\right)^{1/3} = \frac{v_3^*}{\beta}.$$

From such relations we have

$$\frac{v_1^*}{-\gamma\nabla^2} = \frac{v_3^*}{\beta},$$

and

$$v_2^* = \alpha\left(\frac{v_3^*}{\beta}\right)^3,$$

so that

$$v_1^* = -\gamma\nabla^2\left(\frac{v_3^*}{\beta}\right),$$

and

$$v_2^* = \alpha\left(\frac{v_3^*}{\beta}\right)^3.$$

Moreover, we define the functional $F_4^* : Y^* \to \mathbb{R}$, by

$$F_4^*(v^*) = \sup_{u\in V}\{\langle u, v_1^* + v_2^* - v_3^*\rangle_{L^2} - \langle u, f\rangle_{L^2}\}.$$

Therefore

$$F_4^*(v^*) = \begin{cases} 0, & \text{if } v_1^* + v_2^* - v_3^* - f = 0, \text{ in } \Omega, \\ +\infty, & \text{otherwise.} \end{cases} \tag{72}$$

Hence, a critical point of J corresponds to the solution of the following system of equations

$$v_1^* = -\gamma\nabla^2\left(\frac{v_3^*}{\beta}\right),$$

$$v_2^* = \alpha\left(\frac{v_3^*}{\beta}\right)^3,$$

and

$$v_1^* + v_2^* - v_3^* - f = 0, \text{ in } \Omega.$$

From this last equation we may obtain

$$v_1^* = -v_2^* + v_3^* + f,$$

so that the final equations to be solved are

$$-v_2^* + v_3^* + f + \gamma\nabla^2\left(\frac{v_3^*}{\beta}\right) = 0$$

and

$$v_2^* - \alpha\left(\frac{v_3^*}{\beta}\right)^3 = 0, \text{ in } \Omega,$$

with the boundary conditions

$$u = \frac{v_3^*}{\beta} = 0, \text{ on } \partial\Omega.$$

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With such results in mind, we define the Legendre-Galerkin functional $J^* : [Y^*]^2 \to \mathbb{R}$, where

$$\begin{aligned} J^*(v^*) &= \frac{1}{2}\int_\Omega \left(-v_2^* + v_3^* + f + \frac{\gamma\nabla^2 v_3^*}{\beta}\right)^2 dx \\ &+ \frac{1}{2}\int_\Omega \left(v_2^* - \alpha\left(\frac{v_3^*}{\beta}\right)^3\right)^2 dx. \end{aligned} \tag{73}$$

At this point, defining

$$\varphi = v_2^* - \alpha\left(\frac{v_3^*}{\beta}\right)^3,$$

we obtain

$$\frac{\partial^2 J^*(v^*)}{\partial (v_2^*)^2} = 2;$$

$$\frac{\partial^2 J^*(v^*)}{\partial (v_3^*)^2} = \left(-1 - \frac{\gamma\nabla^2}{\beta}\right)^2 + \frac{9\alpha^2 (v_3^*)^4}{\beta^6} + \mathcal{O}(\varphi),$$

$$\frac{\partial^2 J^*(v^*)}{\partial v_2^* \partial v_3^*} = \frac{-3\alpha (v_3^*)^2}{\beta^3} + \left(-1 - \frac{\gamma\nabla^2}{\beta}\right).$$

From such results we may infer that

$$\begin{aligned} \det\left(\frac{\partial^2 J^*(v^*)}{\partial v_2^* \partial v_3^*}\right) &= \frac{\partial^2 J^*(v^*)}{\partial (v_2^*)^2}\frac{\partial^2 J^*(v^*)}{\partial (v_3^*)^2} - \left(\frac{\partial^2 J^*(v^*)}{\partial v_2^* \partial v_3^*}\right)^2 \\ &= \left(-1 - \frac{\gamma\nabla^2}{\beta} + 3\alpha\frac{(v_3^*)^2}{\beta^3}\right)^2 + \mathcal{O}(\varphi) \end{aligned} \tag{74}$$

Observe that a critical point $\varphi = 0$ so that $\delta^2 J^*(v^*) > \mathbf{0}$ at a neighborhood of any critical point. At this point we define

$$A^+ = \left\{v^* = (v_2^*, v_3^*) \in [Y^*]^2 \ : \ \frac{v_3^*}{\beta} f \geq 0, \text{ in } \Omega\right\},$$

$$D^* = \{v^* = (v_2^*, v_3^*) \in [Y^*]^2 \ : \ \|v^*\|_\infty \leq K\},$$

for an appropriate real constant $K > 0$.

Define now $E^* = A^+ \cap D^*$,

$$C_1^* = \{v^* = (v_2^*, v_3^*) \in E^* \ : \ \varphi^2 \leq \varepsilon, \text{ in } \Omega\},$$

for a small real constant $\varepsilon > 0$,

$$C_2^* = \left\{v^* = (v_2^*, v_3^*) \in E^* \ : \ \left(-1 - \frac{\gamma\nabla^2}{\beta} + 3\alpha\frac{(v_3^*)^2}{\beta^3}\right) \geq \varepsilon_1\right\},$$

and

$$C^* = C_1^* \cap C_2^*.$$

Similarly as done in the previous section, we may prove that C^* is a convex set.

Furthermore, for $0 < \varepsilon \ll \varepsilon_1 \ll 1$, we have that J^* is convex on C^*.

Summarizing, we may define the following convex optimization problem to obtain a critical point of the primal functional J,

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$$\text{Minimize } J^*(v_2^*, v_3^*) \text{ subject to } v^* = (v_2^*, v_3^*) \in C^*.$$

We call J^* the Legendre-Galerkin functional associated to J.

13.1. Numerical examples

We have obtained numerical solutions for two one-dimensional examples.

1. For $\gamma = 1.0$, $\alpha = 3.0$, $\beta = 30.0$, $f \equiv 10$, in $\Omega = [0, 1]$.

   For the respective solution please see Figure 7.
2. For $\gamma = 0.01$, $\alpha = 3.0$, $\beta = 30.0$, $f \equiv 10$, in $\Omega = [0, 1]$.

   For the respective solution please see Figure 8.

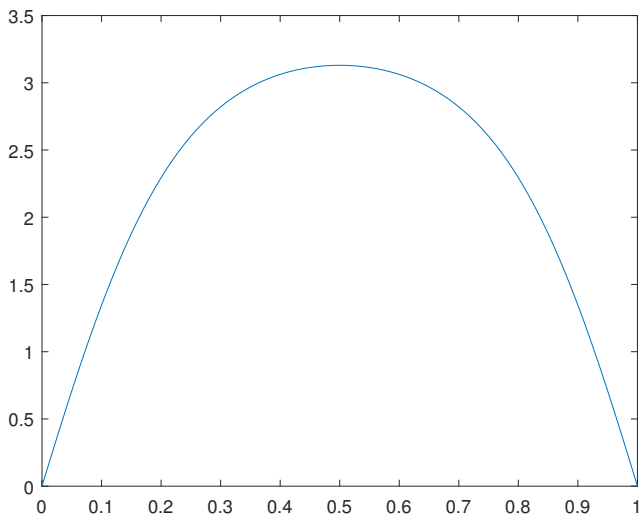

Figure 7. Solution $u(x) = v_3^*(x)/\beta$ for the example 1.

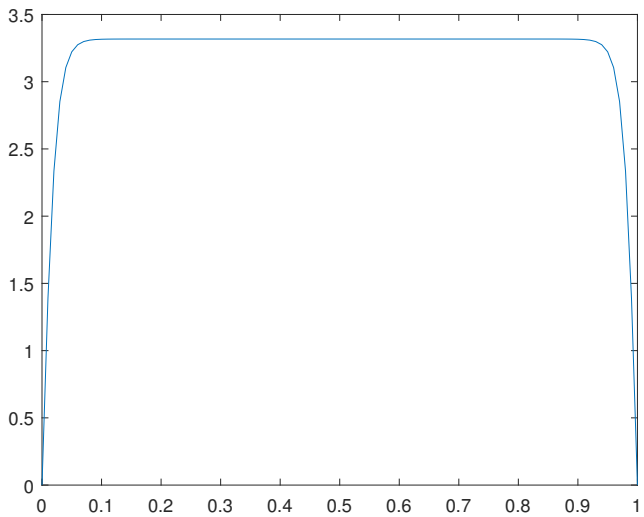

Figure 8. Solution $u(x) = v_3^*(x)/\beta$ for the example 2.

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14. A general concave dual variational formulation for global optimization

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

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

$$J(u) = G(u) - \langle u, f\rangle_{L^2}, \ \forall u \in V.$$

Here $V = W_0^{1,2}(\Omega)$, $f \in L^2(\Omega)$ and we also denote $Y = Y^* = L^2(\Omega)$.

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

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

Furthermore, suppose G is three times Fréchet differentiable and there exists $K > 0$ such that

$$\frac{\partial^2 G(u)}{\partial u^2} + K > \mathbf{0}, \forall u \in V.$$

Define now $J_1 : V \times Y \to \mathbb{R}$ where,

$$J_1(u, v) = G_1(u, v) + F(u),$$

where

$$G_1(u, v) = G(v) - \frac{\varepsilon}{2}\int_\Omega v^2\, dx + \frac{K}{2}\int_\Omega (v - u)^2\, dx,$$

and

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

Moreover, we define the polar functionals $G_1^* : Y^* \times V \to \mathbb{R}$ and $F^* : Y^* \to \mathbb{R}$, where

$$\begin{aligned} G_1^*(v^*, u) &= \sup_{v\in Y}\{\langle v, v^*\rangle_{L^2} - G_1(u, v)\} \\ &= -G_{K_\varepsilon}^*(v^* + Ku) + \frac{K}{2}\int_\Omega u^2\, dx, \end{aligned} \tag{75}$$

$$G_{K_\varepsilon}^*(v^* + Ku) = \sup_{v\in Y}\left\{\langle v, v^*\rangle_{L^2} - G(v) - \frac{K}{2}\int_\Omega v^2\, dx + \frac{\varepsilon}{2}\int_\Omega v^2\, dx\right\},$$

and

$$\begin{aligned} F^*(-v^*) &= \sup_{u\in V}\{-\langle u, v^*\rangle_{L^2} - F(u)\} \\ &= \frac{1}{2\varepsilon}\int_\Omega (v^* - f)^2\, dx. \end{aligned} \tag{76}$$

At this point we define the functional $J_2^* : Y^* \times V \to \mathbb{R}$ by

$$J_2^*(v^*, u) = -G_{K_\varepsilon}^*(v^* + Ku) + \frac{K}{2}\int_\Omega u^2\, dx - F^*(-v^*).$$

With such results in mind we define

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

and

$$D^* = \{v^* \in Y^* \ : \ \|v^*\|_\infty \le K_4\},$$

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for appropriated real constants $K_3 > 0$ and $K_4 > 0$.

Moreover, we define also the penalized functional $J_3^* : Y^* \times V \to \mathbb{R}$ where

$$J_3^*(v^*, u) = J_2^*(v^*, u) - \frac{K_1}{2} \int_\Omega \left(v^* - \frac{\partial G(u)}{\partial u} + \varepsilon u \right)^2 dx.$$

Finally, we remark that for $\varepsilon > 0$ sufficiently small and $K_1 > 0$ sufficiently large, J_3^* is concave in $D^* \times V_1$ around a concerning critical point. We recall that a critical point

$$v^* - \frac{\partial G(u)}{\partial u} + \varepsilon u = 0, \text{ in } \Omega.$$

15. A related restricted problem in phase transition

In this section we develop a convex (in fact concave) dual variational for a model similar to those found in phase transition problems.

Let $\Omega = [0, 1] \subset \mathbb{R}$. Consider the functional $J : V \to \mathbb{R}$ where

$$\begin{aligned} J(u) &= \frac{1}{2} \int_\Omega \min\{(u'+1)^2, (u'-1)^2\}\, dx \\ &\quad + \frac{1}{2} \int_\Omega u^2\, dx - \langle u, f \rangle_{L^2} \\ &= \frac{1}{2} \int_\Omega (u')^2\, dx - \int_\Omega |u'|\, dx + 1/2 \\ &\quad + \frac{1}{2} \int_\Omega u^2\, dx - \langle u, f \rangle_{L^2}. \end{aligned} \tag{77}$$

Here

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

We also denote $V_1 = W_0^{1,2}(\Omega)$, and $Y = Y^* = L^2(\Omega)$.

Furthermore, we define the functionals G and $F : V \times V_1 \to \mathbb{R}$ by

$$G(u', v') = \frac{1}{2} \int_\Omega (u' + v')^2\, dx - \int_\Omega |u' + v'|\, dx + 1/2,$$

and

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

Moreover we define $J_1 : V \times V_1 \to \mathbb{R}$ by

$$J_1(u, v) = G(u', v') + F(u, v),$$

and consider the problem of minimizing J_1 on the set

$$A = \{(u, v) \in V \times V_1 \ : \ (v')^2 \leq K_2, \text{ in } \Omega\}.$$

Already including the Lagrange multiplier ϕ concerning such restrictions, we define

$$J_2(u, v, \phi) = J_1(u, v) + \frac{1}{2} \langle \phi^2, (v')^2 - K_2 \rangle_{L^2}.$$

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Observe now that

$$\begin{aligned}
J_2(u,v,\phi) &= J_1(u,v) + \frac{1}{2}\langle \phi^2, (v')^2 - K_2\rangle_{L^2} \\
&= G(u',v') + \frac{1}{2}\langle \phi^2, (v')^2 - K_2\rangle_{L^2} \\
&\quad + F(u,v) \\
&= -\langle u', v_1^*\rangle_{L^2} - \langle v', v_2^*\rangle_{L^2} + G(u',v') \\
&\quad + \frac{1}{2}\langle \phi^2, (v')^2 - K_2\rangle_{L^2} \\
&\quad \langle u', v_1^*\rangle_{L^2} + \langle v', v_2^*\rangle_{L^2} + F(u,v) \\
&\geq \inf_{(v_1,v_2)\in Y\times Y} \{-\langle v_1, v_1^*\rangle_{L^2} - \langle v_2, v_2^*\rangle_{L^2} + G_1(v_1,v_2,\phi) \\
&\quad + \frac{1}{2}\langle \phi^2, (v_2)^2 - K_2\rangle_{L^2}\Big\} \\
&\quad + \inf_{(u,v)\in V\times V_1} \{\langle u', v_1^*\rangle_{L^2} + \langle v', v_2^*\rangle_{L^2} + F(u,v)\} \\
&= -G_1^*(v_1^*, v_2^*, \phi) - \tilde{F}^*(v_1^*, v_2^*),\ \forall (u,v)\in V\times V_1, (v_1^*, v_2^*, \phi)\in [Y^*]^3,
\end{aligned} \tag{78}$$

where

$$G_1(u',v',\phi) = G(u',v') + \frac{1}{2}\langle \phi^2, (v')^2 - K_2\rangle_{L^2}.$$

Also,

$$\begin{aligned}
G_1^*(v_1^*, v_2^*, \phi) &= \sup_{(v_1,v_2)\in Y\times Y} \{\langle v_1, v_1^*\rangle_{L^2} + \langle v_1, v_1^*\rangle_{L^2} - G_1(v_1,v_2,\phi)\} \\
&= \frac{1}{2}\int_\Omega (v_1^*)^2\, dx \\
&\quad + \int_\Omega |v_1^*|\, dx + \frac{1}{2}\int_\Omega \frac{(v_1^* - v_2^*)^2}{\phi^2} \\
&\quad + \frac{K_2}{2}\int_\Omega \phi^2\, dx,
\end{aligned} \tag{79}$$

where

$$\tilde{F}^*(v^*) = \begin{cases} \frac{1}{2}\int_\Omega ((v_1^*)' + f)^2\, dx - v_1^*(1)u(1), & \text{if } (v_2^*)' = 0, \text{ in } \Omega, \\ +\infty, & \text{otherwise.} \end{cases} \tag{80}$$

From this we may infer that $v_2^* = c$, in Ω, for some $c \in \mathbb{R}$.
Summarizing, denoting $v^* = (v_1^*, v_2^*) = (v_1^*, c)$, and

$$J^*(v^*, \phi) = -G_1^*(v^*, \phi) - \tilde{F}^*(v^*)$$

we have got

$$\inf_{(u,v)\in A} J_1(u,v) \geq \sup_{(v^*,\phi)\in Y^*\times\mathbb{R}\times Y^*} J^*(v^*\phi).$$

We have developed numerical results by maximizing the dual functional J^* for two examples, namely.

1. Example A: In this case, we consider $f(x) = \cos(\pi x)/2$, $K_2 = 10^{-4}$.

   For the optimal

$$u_0 = (v_1^*)' + f,$$

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please see Figure 9.

2. Example B: In this case, we consider $f(x) = \cos(\pi x)/2$, $K_2 = 30$.

   For the optimal
$$u_0 = (v_1^*)' + f,$$
   please see Figure 10.

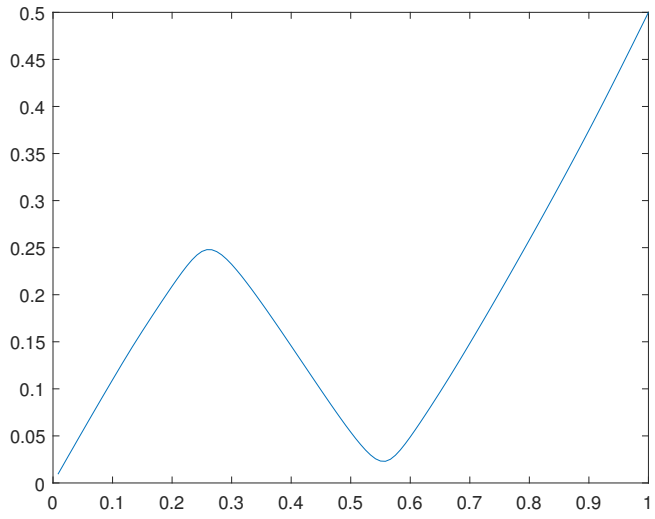

Figure 9. Solution $u_0(x)$ for the example A.

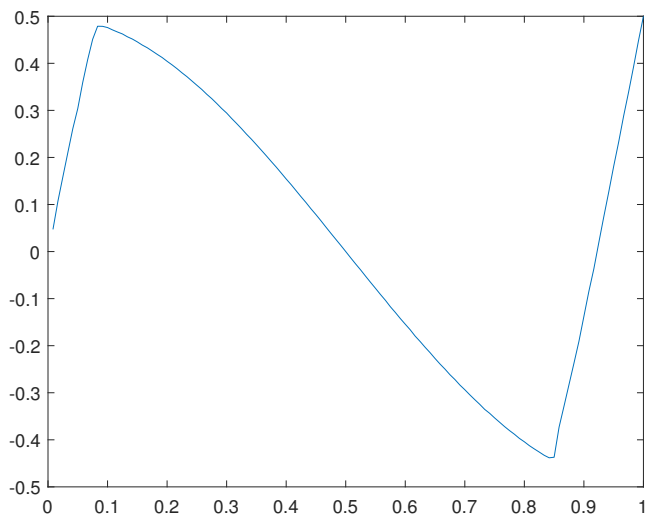

Figure 10. Solution $u_0(x)$ for the example B.

16. One more dual variational formulation

In this section we develop one more dual variational formulation for a related model. Let $\Omega = [0,1] \subset \mathbb{R}$ and consider the functional $J : V \to \mathbb{R}$ defined by

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

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where

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

We define also the relaxed functional $J_1 : V \times V_0 \to \mathbb{R}$, already including a concerning restriction and corresponding non-negative Lagrange multiplier Λ^2, where

$$J_1(u, v, \Lambda) = \frac{1}{2}\int_\Omega ((u' + v')^2 - 1)^2 \, dx + \frac{1}{2}\int_\Omega u^2 \, dx - \langle u, f\rangle_{L^2} + \langle \Lambda^2, (v')^2 - K\rangle_{L^2}.$$

where

$$V_0 = \{v \in W_0^{1,4}(\Omega) \ : \ (v')^2 - K \leq 0 \text{ in } \Omega\}.$$

Observe that

$$\begin{aligned}
& \frac{1}{2}\int_\Omega ((u' + v')^2 - 1)^2 \, dx + \frac{1}{2}\int_\Omega u^2 \, dx - \langle u, f\rangle_{L^2} + \langle \Lambda^2, (v')^2 - K\rangle_{L^2} \\
= \ & -\langle v_0^*, (u' + v')^2 - 1\rangle_{L^2} + \frac{1}{2}\int_\Omega ((u' + v')^2 - 1)^2 \, dx \\
& + \langle v_0^*, (u' + v')^2 - 1\rangle_{L^2} + \langle \Lambda^2, (v')^2 - K\rangle_{L^2} - \langle u', v_1^*\rangle_{L^2} - \langle v', v_2^*\rangle_{L^2} \\
& + \langle u', v_1^*\rangle_{L^2} + \langle v', v_2^*\rangle_{L^2} + \frac{1}{2}\int_\Omega u^2 \, dx - \langle u, f\rangle_{L^2} \\
\geq \ & \inf_{w \in Y} \left\{ -\langle v_0^*, w\rangle_{L^2} + \frac{1}{2}\int_\Omega (w)^2 \, dx \right\} \\
& \inf_{(v_1, v_2) \in Y \times Y} \left\{ \langle v_0^*, (v_1 + v_2)^2 - 1\rangle_{L^2} + \langle \Lambda^2, (v_2)^2 - K\rangle_{L^2} - \langle v_1, v_1^*\rangle_{L^2} - \langle v_2, v_2^*\rangle_{L^2} \right\} \\
& + \inf_{(u, v) \in V \times V_0} \left\{ \langle u', v_1^*\rangle_{L^2} + \langle v', v_2^*\rangle_{L^2} + \frac{1}{2}\int_\Omega u^2 \, dx - \langle u, f\rangle_{L^2} \right\} \\
= \ & -\frac{1}{2}\int_\Omega (v_0^*)^2 \, dx - \int_\Omega v_0^* \, dx \\
& -\frac{1}{4}\int_\Omega \frac{(v_1^*)^2}{v_0^*} \, dx - \frac{1}{2}\int_\Omega \frac{(v_1^* - v_2^*)^2}{2\Lambda^2} \, dx \\
& -\frac{1}{2}\int_\Omega ((v_1^*)' + f)^2 \, dx - \frac{1}{2}\int_\Omega K\Lambda^2 \, dx + v_1^*(1)u(1).
\end{aligned} \tag{81}$$

Here, we highlight $v_2^* = c \in \mathbb{R}$ in Ω, for some real constant c.
Hence, denoting

$$\begin{aligned}
J_1^*(v^*, \Lambda) \ = \ & -\frac{1}{2}\int_\Omega (v_0^*)^2 \, dx - \int_\Omega v_0^* \, dx \\
& -\frac{1}{4}\int_\Omega \frac{(v_1^*)^2}{v_0^*} \, dx - \frac{1}{2}\int_\Omega \frac{(v_1^* - v_2^*)^2}{2\Lambda^2} \, dx \\
& -\frac{1}{2}\int_\Omega ((v_1^*)' + f)^2 \, dx - \frac{1}{2}\int_\Omega K\Lambda^2 \, dx + v_1^*(1)u(1)
\end{aligned} \tag{82}$$

and

$$J_2(u, v) = \frac{1}{2}\int_\Omega ((u' + v')^2 - 1)^2 \, dx + \frac{1}{2}\int_\Omega u^2 \, dx - \langle u, f\rangle_{L^2},$$

we have obtained

$$\inf_{(u,v) \in V \times V_0} J_2(u, v)\} \geq \sup_{(v^*, \Lambda) \in A^* \times [Y^*] \times \mathbb{R} \times Y^*} J_1^*(v^*, \Lambda).$$

Finally, for

$$A^* = \{v_0^* \in Y^* \ : \ v_0^* \geq \varepsilon \text{ in } \Omega\}$$

we emphasize J_1^* is concave on $A^* \times [Y^*] \times \mathbb{R} \times Y^*$.

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Here $\varepsilon > 0$ is a small regularizing real constant.

Remark 16.1. *The constraint $(v')^2 - K \leq 0$, in Ω is included to restrict the action of v on the region where the primal functional is non-convex, through an appropriate constant $K > 0$.*

17. A model in superconductivity through an eigenvalue approach

In this section we intend to model superconductivity through a two phase eigenvalue approach.

Let $\Omega = [0,5] \subset \mathbb{R}$ be a straight wire corresponding to a one-dimensional super-conducting sample.

Consider the functional $J : V \times V \times \mathbb{R} \to \mathbb{R}$ where

$$\begin{aligned} J(u,v,E) \quad = \quad & \frac{\gamma_1}{2}\int_\Omega \nabla u \cdot \nabla u \, dx + \frac{\alpha_1}{2}\int_\Omega |u|^4 \, dx \\ & -\frac{\omega^2}{2}\int_\Omega |u|^2 \, dx \\ & +\frac{\gamma_2}{2}\int_\Omega \nabla v \cdot \nabla v \, dx + \frac{\alpha_2}{2}\int_\Omega |v|^4 \, dx \\ & -\frac{\omega_1^2}{2K_3^2}\int_\Omega |v|^2 \, dx \\ & -\frac{E}{2}\left(\int_\Omega (|u|^2 + |v|^2) \, dx - m_T\right). \end{aligned} \tag{83}$$

Here, in atomic units, m_T is the total electronic charge, $V = W_0^{1,2}(\Omega)$ and we set $\alpha_1 = 10^4$ corresponding to higher self-interacting energy which is related to a normal phase. We also set $\alpha_2 = 10^{-1}$ corresponding to a lower self-interacting energy which is related to a super-conducting phase and respective super-currents.

Moreover, we set $\gamma_1 = \gamma_2 = 1$, and initially $\omega = 1.8$ which is gradually decreased to $\omega = 1.0$.

Furthermore, we define

$$|\phi_N|^2 = \frac{|u|^2}{|u|^2 + |v|^2}$$

and

$$|\phi_S|^2 = \frac{|v|^2}{|u|^2 + |v|^2}$$

where ϕ_N corresponds to a normal phase and ϕ_S to a super-conducting one.

At this point we observe that the temperature $T = T(x,t)$ is proportional the frequency $\omega/(2\pi)$ of vibration for the normal phase.

We start the process with $\omega = 1.8$ which in atomic units corresponds to a higher temperature and gradually decreases it to the value $\omega = 1.0$

Between $\omega = 1.2$ and $\omega = 1.0$ the system changes from an almost total normal phase to an almost total super-conducting phase, as expected.

We highlight that the temperature is proportional to the vibrational kinetics energy

$$E_1(t) = \frac{1}{2}\int_\Omega |u|^2 \frac{\partial \mathbf{r}_N(x,t)}{\partial t} \cdot \frac{\partial \mathbf{r}_N(x,t)}{\partial t} \, dx$$

so that for

$$\mathbf{r}_N(x,t) = e^{i\omega t}\mathbf{w}_5(x)$$

and for a suitable vectorial function $\mathbf{w}_5$, we have

$$T \propto E_1 \propto \omega^2$$

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so that we may model the decreasing of temperature T through the decreasing of ω^2.

For $\omega = 1.8$, for the corresponding normal phase ϕ_N and super-conducting phase ϕ_S, please se Figures 11 and 12, respectively.

For $\omega = 1.0$, for the corresponding normal phase ϕ_N and super-conducting phase ϕ_S, please se Figures 13 and 14, respectively.

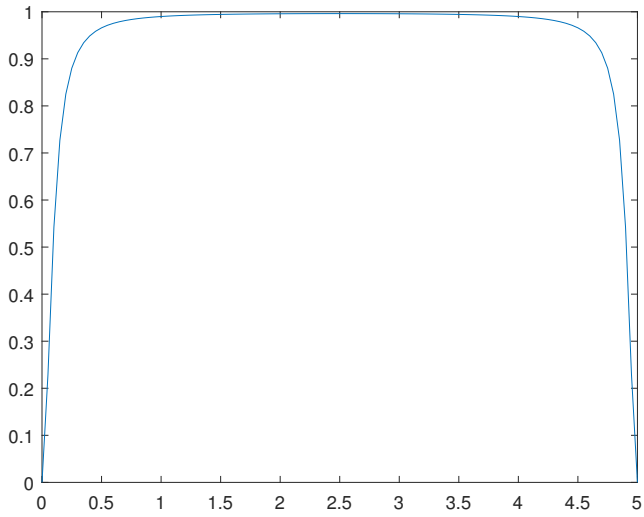

Figure 11. Solution $\phi_N(x)$ for the $\omega = 1.8$.

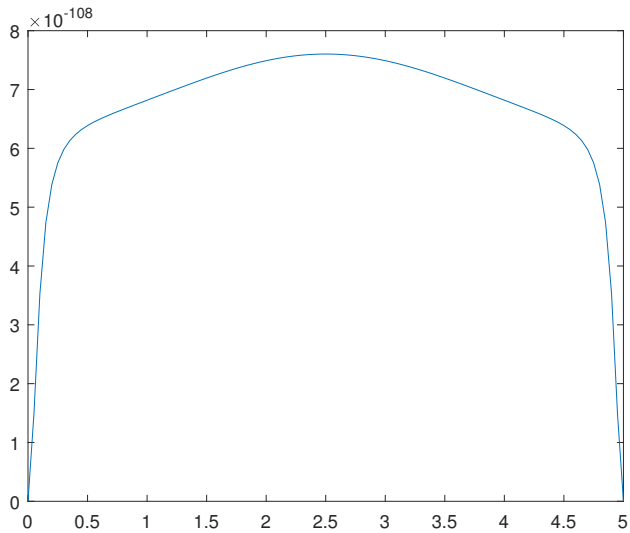

Figure 12. Solution $\phi_S(x)$ for the $\omega = 1.8$.

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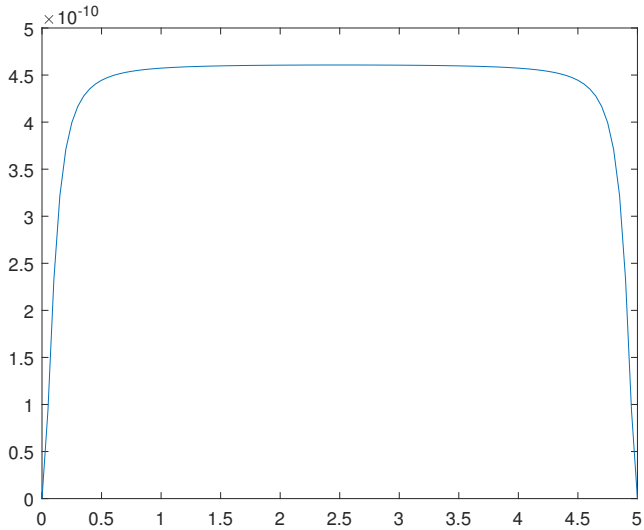

Figure 13. Solution $\phi_N(x)$ for the $\omega = 1.0$.

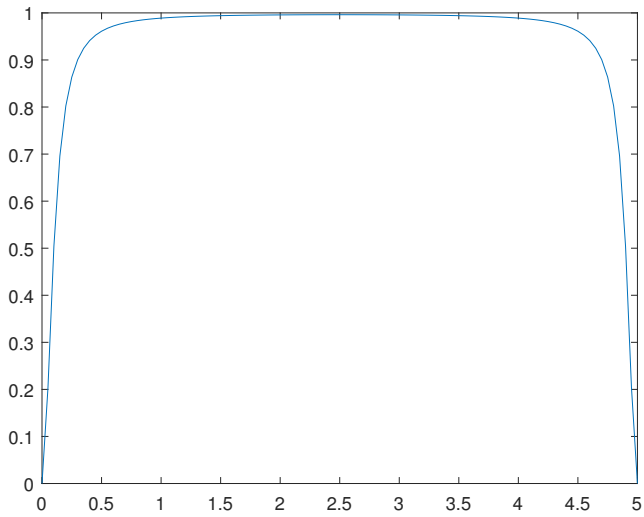

Figure 14. Solution $\phi_S(x)$ for the $\omega = 1.0$.

Finally, we have set $\omega_1/K_3 \approx 1$ which for large ω_1 corresponds to the super-currents.

18. A simplified qualitative many body model for the hydrogen nuclear fusion

In this section we develop a qualitative simple model for the hydrogen nuclear fusion.

Let $\Omega = [0, L]^3 \subset \mathbb{R}^3$ be a box in which is confined a gas comprised by an amount of ionized deuterium and tritium isotopes of hydrogen.

Though a suitable increasing in temperature, we intend to develop the following nuclear reaction

$$\text{Deuterium}^+ + \text{Tritium}^+ \to \text{Helium}^{++} + \text{Neutron (energetic)}.$$

We recall that the ionized Deuterium atom comprises a proton and a neutron and the ionized Tritium atom comprises a proton and two neutrons.

Under certain conditions and at a suitable high temperature the ionized Deuterium and Tritium atoms react chemically resulting in an ionized Helium atom, comprised by two protons and two

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neutrons and resulting also in one more single energetic neutron. We emphasize the higher kinetics neutron energy level has many potential practical applications, including its conversion in electric energy.

At this point we denote by $m_D,\ m_T,\ m_{H_e}$ and m_N the masses of the ionized Deuterium, Tritium and Helium atoms, and the single neutron, respectively.

Therefore, we have the following mass relation

$$m_D + m_T = m_{H_e} + m_N.$$

To simplify our analysis, in such a chemical reaction, denoting the total masses of ionized Deuterium, Tritium, Helium and single Neutrons by $(m_D)_T,\ (m_T)_T,\ (m_{H_e})_T$ and $(m_N)_T$ we assume there is a real constant $c > 0$ such that

$$(m_D)_T = c\, m_D,\ (m_T)_T = c\, m_T,\ (m_{H_e})_T = c\, m_{H_e},\ (m_N)_T = c\, m_N.$$

With such statements and definitions in mind, we define the following functional J, where

$$J(\phi, \mathbf{r}) = J(\phi_D, \phi_T, \phi_{H_e}, \phi_N, \mathbf{r}) = G(\nabla\phi) + F(\phi) + E_c(\phi, \mathbf{r}),$$

where, in a simplified many body context,

$$|\phi_D(x,y)|^2 = |\phi_p^D(y)|^2 + |\phi_N^D(x,y)|^2 |\phi_p^D(y)|^2 \frac{1}{m_p},$$

$$|\phi_T(x,y)|^2 = |\phi_p^T(y)|^2 + (|\phi_{N_1}^T(x,y)|^2 + |\phi_{N_2}^T(x,y)|^2)|\phi_p^T(y)|^2 \frac{1}{m_p},$$

$$|\phi_{H_e}(x,y)|^2 = |\phi_{2P}^{H_e}(y)|^2 + (|\phi_{N_1}^{H_e}(x,y)|^2 + |\phi_{N_2}^{H_e}(x,y)|^2)|\phi_{2P}^{H_e}(y)|^2 \frac{1}{2\, m_p},$$

$$\phi_N = \phi_N(x).$$

Here $x, y \in \Omega \subset \mathbb{R}^3$ refers to the particle densities.

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Furthermore, we assume $\gamma_p^D > 0,\ \gamma_p^T > 0,\ \gamma_N^D > 0,\ \gamma_{N_1}^T > 0,\ \gamma_{N_2}^T > 0,\ \gamma_{2p}^{H_e} > 0,\ \gamma_{N_1}^{H_e} > 0,$ $\gamma_{N_2}^{H_e} > 0,\ \gamma_N > 0,$ and $\alpha_D > 0,\ \alpha_T > 0,\ \alpha_{H_e} > 0,\ \alpha_N > 0\ , \alpha_{DT} > 0,\ \alpha_{H_e\,N} > 0,$ so that

$$\begin{aligned}
G(\nabla\phi) \quad = \quad & \frac{\gamma_p^D}{2}\int_\Omega (\nabla\phi_p^D)\cdot(\nabla\phi_p^D)\,dy \\
& +\frac{\gamma_N^D}{2}\int_\Omega (\nabla\phi_N^D)\cdot(\nabla\phi_N^D)\,dx\,dy \\
& \frac{\gamma_p^T}{2}\int_\Omega (\nabla\phi_p^T)\cdot(\nabla\phi_p^T)\,dy \\
& +\frac{\gamma_{N_1}^T}{2}\int_\Omega (\nabla\phi_{N_1}^T)\cdot(\nabla\phi_{N_1}^T)\,dx\,dy \\
& +\frac{\gamma_{N_2}^T}{2}\int_\Omega (\nabla\phi_{N_2}^T)\cdot(\nabla\phi_{N_2}^T)\,dx\,dy \\
& +\frac{\gamma_{2p}^{H_e}}{2}\int_\Omega (\nabla\phi_{2p}^{H_e})\cdot(\nabla\phi_{2p}^{H_e})\,dy \\
& +\frac{\gamma_{N_1}^{H_e}}{2}\int_\Omega (\nabla\phi_{N_1}^{H_e})\cdot(\nabla\phi_{N_1}^{H_e})\,dx\,dy \\
& +\frac{\gamma_{N_2}^{H_e}}{2}\int_\Omega (\nabla\phi_{N_2}^{H_e})\cdot(\nabla\phi_{N_2}^{H_e})\,dx\,dy \\
& +\frac{\gamma_N}{2}\int_\Omega (\nabla\phi_N)\cdot(\nabla\phi_N)\,dx,
\end{aligned} \tag{84}$$

and,

$$\begin{aligned}
F(\phi) \quad = \quad & \frac{\alpha_D}{2}\int_\Omega \frac{|\phi_D(x-\xi_1,y-\xi_2)|^2|\phi_D(\xi_1,\xi_2)|^2}{|(x,y)-(\xi_1,\xi_2)|}\,dx\,dy\,d\xi_1\,d\xi_2 \\
& +\frac{\alpha_T}{2}\int_\Omega \frac{|\phi_T(x-\xi_1,y-\xi_2)|^2|\phi_T(\xi_1,\xi_2)|^2}{|(x,y)-(\xi_1,\xi_2)|}\,dx\,dy\,d\xi_1\,d\xi_2 \\
& +\frac{\alpha_{DT}}{2}\int_\Omega \frac{|\phi_D(x-\xi_1,y-\xi_2)|^2|\phi_T(\xi_1,\xi_2)|^2}{|(x,y)-(\xi_1,\xi_2)|}\,dx\,dy\,d\xi_1\,d\xi_2 \\
& +\frac{\alpha_{H_e}}{2}\int_\Omega \frac{|\phi_{H_e}(x-\xi_1,y-\xi_2)|^2|\phi_{H_e}(\xi_1,\xi_2)|^2}{|(x,y)-(\xi_1,\xi_2)|}\,dx\,dy\,d\xi_1\,d\xi_2 \\
& +\frac{\alpha_N}{2}\int_0^{t_f}\int_\Omega \frac{|\phi_N(x-\xi)|^2|\phi_N(\xi)|^2}{|x-\xi|}\,dx\,d\xi \\
& +\sum_{j=1}^{2}\frac{\alpha_{H_e\,N}}{2}\int_\Omega \frac{|\phi_{H_e}(x_1-\xi_1,y-\xi_2)|^2|\phi_N(\xi_j)|^2}{|(x,y)-(\xi_1,\xi_2)|}\,dx\,dy\,d\xi_1\,d\xi_2
\end{aligned} \tag{85}$$

and the kinetics energy is expressed by

$$\begin{aligned}
E_c(\phi,\mathbf{r}) \quad = \quad & \frac{1}{2}\int_\Omega |\phi_D|^2\,\frac{\partial\mathbf{r}_D}{\partial t}\cdot\frac{\partial\mathbf{r}_D}{\partial t}\,dx\,dy \\
& +\frac{1}{2}\int_\Omega |\phi_T|^2\,\frac{\partial\mathbf{r}_T}{\partial t}\cdot\frac{\partial\mathbf{r}_T}{\partial t}\,dx\,dy \\
& +\frac{1}{2}\int_\Omega |\phi_{H_e}|^2\,\frac{\partial\mathbf{r}_{H_e}}{\partial t}\cdot\frac{\partial\mathbf{r}_{H_e}}{\partial t}\,dx\,dy \\
& +\frac{1}{2}\int_\Omega |\phi_N|^2\,\frac{\partial\mathbf{r}_N}{\partial t}\cdot\frac{\partial\mathbf{r}_N}{\partial t}\,dx\,dy,
\end{aligned} \tag{86}$$

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where we also assume

$$\mathbf{r}_D \approx e^{i\omega t}\mathbf{w}_5(x,y),$$
$$\mathbf{r}_T \approx e^{i\omega t}\mathbf{w}_6(x,y),$$

so that considering such a vibrational motion, the temperature T is proportional to ω^2, that is

$$T \propto \omega^2.$$

Therefore, an increasing in T corresponds to a proportional increasing in ω^2.

Summarizing, we have supposed

$$E_c(\phi,\mathbf{r}) \approx \frac{1}{2}\omega^2 \int_\Omega |\phi_D|^2 + |\phi_T|^2\, dx\, C_1 + \frac{1}{2}\omega_1^2 \int_\Omega |\phi_N|^2\, dx\, C_2,$$

so that we represent the increasing in T through an increasing in ω^2.

Moreover, we denote by m_N the mass of a single neutron and by m_p the mass of a single proton.

Thus, denoting also by $\lambda_1,\ \lambda_2$ the proportion of non-reacted and reacted masses respectively, we have the following constraints.

1. $$\int_\Omega |\phi_N^D(x,y)|^2\, dx = m_N,$$
2. $$\int_\Omega |\phi_{N_1}^T(x,y)|^2\, dx = m_N,$$
3. $$\int_\Omega |\phi_{N_2}^T(x,y)|^2\, dx = m_N,$$
4. $$\int_\Omega |\phi_{N_1}^{H_e}(x,y)|^2\, dx = m_N,$$
5. $$\int_\Omega |\phi_{N_2}^{H_e}(x,y)|^2\, dx = m_N,$$
6. $$\int_\Omega |\phi_p^D(y)|^2\, dy = \lambda_1\, cm_p,$$
7. $$\int_\Omega |\phi_p^T(y)|^2\, dy = \lambda_1\, cm_p,$$
8. $$\int_\Omega |\phi_{2P}^{H_e}(y)|^2\, dy = \lambda_2\, (2c\, m_p),$$

Similar constraints are valid corresponding to the charge of a single proton.

We have also the following complementing constraints,

1. $$\int_\Omega |\phi_D|^2\, dx\, dy = \lambda_1 (m_D)_T,$$
2. $$\int_\Omega |\phi_T|^2\, dx\, dy = \lambda_1 (m_T)_T,$$
3. $$\int_\Omega |\phi_{H_e}|^2\, dx\, dy = \lambda_2 (m_{H_e})_T,$$
4. $$\int_\Omega |\phi_N|^2\, dx\, dy = \lambda_2 (m_N)_T,$$

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5.

$$\lambda_1 + \lambda_2 = 1.$$

With such results and statements in mind and simplifying the interacting terms, we re-define the functional J now denoting it by J_1, here already including the Lagrange multipliers concerning the constraints, where

$$\begin{aligned}
J_1(\phi, \omega, E, \lambda) \quad = \quad & \frac{\gamma_p^D}{2} \int_\Omega (\nabla \phi_p^D) \cdot (\nabla \phi_p^D)\, dy \\
& + \frac{\gamma_N^D}{2} \int_\Omega (\nabla \phi_N^D) \cdot (\nabla \phi_N^D)\, dx\, dy \\
& \frac{\gamma_p^T}{2} \int_\Omega (\nabla \phi_p^T) \cdot (\nabla \phi_p^T)\, dy \\
& + \frac{\gamma_{N_1}^T}{2} \int_\Omega (\nabla \phi_{N_1}^T) \cdot (\nabla \phi_{N_1}^T)\, dx\, dy \\
& + \frac{\gamma_{N_2}^T}{2} \int_\Omega (\nabla \phi_{N_2}^T) \cdot (\nabla \phi_{N_2}^T)\, dx\, dy \\
& + \frac{\gamma_{2p}^{H_e}}{2} \int_\Omega (\nabla \phi_{2p}^{H_e}) \cdot (\nabla \phi_{2p}^{H_e})\, dy \\
& + \frac{\gamma_{N_1}^{H_e}}{2} \int_\Omega (\nabla \phi_{N_1}^{H_e}) \cdot (\nabla \phi_{N_1}^{H_e})\, dx\, dy \\
& + \frac{\gamma_{N_2}^{H_e}}{2} \int_\Omega (\nabla \phi_{N_2}^{H_e}) \cdot (\nabla \phi_{N_2}^{H_e})\, dx\, dy \\
& + \frac{\gamma_N}{2} \int_\Omega (\nabla \phi_N) \cdot (\nabla \phi_N)\, dx \\
& + \frac{\alpha_D}{2} \int_\Omega |\phi_D|^4\, dx + \frac{\alpha_T}{2} \int_\Omega |\phi_T|^4\, dx \\
& + \frac{\alpha_{H_e}}{2} \int_\Omega |\phi_{H_e}|^4\, dx + \frac{\alpha_N}{2} \int_\Omega |\phi_N|^4\, dx \\
& - \omega^2 \int_\Omega (|\phi_D|^2 + |\phi_T|^2)\, dx \\
& - \omega_1^2 \int_\Omega |\phi_N|^2\, dx + J_{Aux},
\end{aligned} \tag{87}$$

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where the functional J_{Aux} stands for

$$\begin{aligned}
J_{Aux} \quad = \quad & -\int_\Omega (E_N^D)_5(y) \left(\int_\Omega |\phi_N^D(x,y)|^2 \, dx - m_N \right) \, dy \\
& -\int_\Omega (E_{N_1}^T)_6(y) \left(\int_\Omega |\phi_{N_1}^T(x,y)|^2 \, dx - m_N \right) \, dy \\
& -\int_\Omega (E_{N_2}^T)_7(y) \left(\int_\Omega |\phi_{N_2}^T(x,y)|^2 \, dx - m_N \right) \, dy \\
& -\int_\Omega (E_{N_1}^{H_e})_8(y) \left(\int_\Omega |\phi_{N_1}^{H_e}(x,y)|^2 \, dx - m_N \right) \, dy \\
& -\int_\Omega (E_{N_2}^{H_e})_9(y) \left(\int_\Omega |\phi_{N_2}^{H_e}(x,y)|^2 \, dx - m_N \right) \, dy \\
& -(E_D)_2 \left(\int_\Omega |\phi_p^D(y)|^2 \, dy - \lambda_1 c m_p \right) \\
& -(E_T)_3 \left(\int_\Omega |\phi_p^T(y)|^2 \, dy - \lambda_1 c m_p \right) \\
& -(E_{H_e})_3 \left(\int_\Omega |\phi_{2P}^{H_e}(x,y)|^2 \, dy - \lambda_2 \, 2 c m_p \right) \\
& -E_5 \left(\int_\Omega |\phi_D|^2 \, dx \, dy - \lambda_1 (m_D)_T \right) \\
& -E_6 \left(\int_\Omega |\phi_T|^2 \, dx \, dy - \lambda_1 (m_T)_T \right) \\
& -E_7 \left(\int_\Omega |\phi_{H_e}|^2 \, dx \, dy - \lambda_2 (m_{H_e})_T \right) \\
& -E_8 \left(\int_\Omega |\phi_N|^2 \, dx \, dy - \lambda_2 (m_N)_T \right) \\
& -E_9 (\lambda_1 + \lambda_2 - 1). \qquad (88)
\end{aligned}$$

Remark 18.1. *In order to obtain consistent results it is necessary to set*

$$(\alpha_N, \alpha_{H_e}) \gg (\alpha_D, \alpha_T).$$

In such a case, a higher temperature corresponding to a large ω^2, though such a nuclear reaction, will result in a small λ_1 and a higher kinetics energy for the neutron field, corresponding to a large ω_1^2 and λ_2 closer to 1.

19. A more detailed mathematical description of the hydrogen nuclear fusion

In this section we develop in more details another model for the hydrogen nuclear fusion.

Remark 19.1. *Denoting by $i \in \mathbb{C}$ the imaginary unit, in this and in the subsequent sections, for the time-dependent case we generically define the gradient of a scalar function $u(x,t)$ with domain in $\mathbb{R}^4$, denoted by $\nabla u(x,t)$, as*

$$\nabla u(x,t) = (iu_t(x,t), u_{x_1}(x,t), u_{x_2}(x,t), u_{x_3}(x,t)),$$

so that

$$\nabla u \cdot \nabla u = -u_t^2 + \sum_{j=1}^{3} u_{x_j}^2.$$

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

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Here such a set Ω stands for a control volume in which an ionized gas (plasma) flows. Such a gas comprises ionized Deuterium and Tritium atoms intended, through a suitable higher temperature, to chemically react resulting in atoms of Hellion and a field of single energetic Neutrons.

Symbolically such a reaction stands for

$$\text{Deuterium}^{+} \;+\; \text{Tritium}^{+} \rightarrow \text{Helium}^{++} \;+\; \text{Neutron (energetic)}.$$

We recall that the ionized Deuterium atom is comprised by a proton and a neutron and the ionized Tritium atom is comprised by a proton and two neutrons.

Moreover, the ionized Helium atom is comprised by two protons and two neutrons.

As previously mentioned, resulting from such a chemical reaction up surges also an energetic neutron which the higher kinetics energy has a great variety of applications, including its conversion in electric energy.

We highlight the model here presented includes electric and magnetic fields and the corresponding potential ones.

Denoting by t the time on the interval $[0, t_f]$, at this point we define the following density functions:

1. For the Deuterium field

$$|\phi_D(x,y,t)|^2 = |\phi_p^D(y,t)|^2 + |\phi_N^D(x,y,t)|^2 |\phi_p^D(y,t)|^2 \frac{1}{m_p},$$

2. For the Tritium field

$$|\phi_T(x,y,t)|^2 = |\phi_p^T(y,t)|^2 + (|\phi_{N_1}^T(x,y,t)|^2 + |\phi_{N_2}^T(x,y,t)|^2)|\phi_p^T(y,t)|^2 \frac{1}{m_p},$$

3. For the Helium field

$$|\phi_{H_e}(x,y,t)|^2 = |\phi_{2p}^{H_e}(y,t)|^2 + (|\phi_{N_1}^{H_e}(x,y,t)|^2 + |\phi_{N_2}^{H_e}(x,y,t)|^2)|\phi_{2p}^{H_e}(y,t)|^2 \frac{1}{2\, m_p},$$

4. For the Neutron field

$$\phi_N = \phi_N(x,t),$$

5. For the electronic field resulting from the ionization

$$\phi_e = \phi_e(x,y,t).$$

Furthermore, we define also the related densities

1.
$$\rho_D(y,t) = \int_\Omega |\phi_D(x,y,t)|^2 \, dx,$$

2.
$$\rho_T(y,t) = \int_\Omega |\phi_T(x,y,t)|^2 \, dx,$$

$$\rho_{H_e}(y,t) = \int_\Omega |\phi_{H_e}(x,y,t)|^2 \, dx,$$

$$\rho_N(x,t) = |\phi_N(x,t)|^2,$$

$$\rho_e(y,t) = \int_\Omega |\phi_e(x,y,t)|^2 \, dx.$$

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For the chemical reaction in question we consider that one unit of mass of fractional proportion α_D of ionized Deuterium and α_T of ionized Tritium results in one unit of mass of fractional proportion α_{H_e} of ionized Helium and α_N of neutrons.

Symbolic, this stands for

$$1 = \alpha_D + \alpha_T = \alpha_{H_e} + \alpha_N.$$

Concerning the control volume Ω in question and related surface control $\partial\Omega$, we assume such a volume has an initial (fot $t = 0$) amount of ionized Deuterium of $(m_D)_0$ and an initial amount of ionized Tritium of $(m_T)_0$. The initial amount of ionized Helium and single neutrons are supposed to be zero.

On the other hand, about the surface control $\partial\Omega$, we assume there is a part $\Omega_1 \subset \partial\Omega$ for which is allowed the entrance and exit of Deuterium and Tritium ionized atoms.

We assume also there is another part $\partial\Omega_2 \subset \partial\Omega$ such that $\partial\Omega_1 \cap \partial\Omega_2 = \emptyset$ for which is allowed only the exit of ionized Helium atoms and neutrons, but not their entrance.

In $\partial\Omega_2$ is allowed the exit only (not the entrance) of ionized Deuterium and Tritium atoms.

Indeed, we assume the following relations for the masses:

1. $$(m_{H_e,N})_T(t) = m_{H_e,N}(t) + \int_0^t \int_{\partial\Omega_2} (\rho_{H_e}(x,\tau) + \rho_N(x,\tau))\mathbf{u}\cdot\mathbf{n}\, dS\, d\tau,$$
2. $$m_{H_e,N}(t) = m_{H_e}(t) + m_N(t),$$
3. $$m_{H_e}(t) = \int_\Omega \rho_{H_e}(x,t)\, dx,$$
4. $$m_N(t) = \int_\Omega \rho_N(x,t)\, dx,$$
5. $$(m_{H_e})_T(t) = \int_\Omega \rho_{H_e}(x,t)\, dx + \int_0^t \int_{\partial\Omega_2} \rho_{H_e}(x,\tau)\mathbf{u}\cdot\mathbf{n}\, d\Gamma d\tau,$$
6. $$(m_N)_T(t) = \int_\Omega \rho_N(x,t)\, dx + \int_0^t \int_{\partial\Omega_2} \rho_N(x,\tau)\mathbf{u}\cdot\mathbf{n}\, d\Gamma d\tau,$$
7. $$\frac{(m_N)_T(t)}{(m_{H_e})_T(t)} = \frac{\alpha_N}{\alpha_{H_e}},$$

   so that

   $$\alpha_N m_{H_e})_T(t) = \alpha_{H_e}(m_N)_T(t),$$
8. $$(m_D)(t) = (m_D)_0 - \int_0^t \int_{\partial\Omega_1\cup\partial\Omega_2} (\rho_D(x,\tau))\mathbf{u}\cdot\mathbf{n}\, dS\, d\tau - \alpha_D(m_{H_e,N})_T(t),$$
9. $$(m_T)(t) = (m_T)_0 - \int_0^t \int_{\partial\Omega_1\cup\partial\Omega_2} (\rho_T(x,\tau))\mathbf{u}\cdot\mathbf{n}\, dS\, d\tau - \alpha_T(m_{H_e,N})_T(t),$$
10. $$(m_e)_T(t) = m_e(t) + \int_0^t \int_{\partial\Omega_2} (\rho_e(x,\tau))\mathbf{u}\cdot\mathbf{n}\, dS\, d\tau,$$
11. $$m_e(t) = \int_\Omega \rho_e(x,t)\, dx.$$

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12.
$$m_e(t) = \int_\Omega |\phi_p^D(x,t)|^2\, dx \frac{m_e}{m_p} + \int_\Omega |\phi_p^T(x,t)|^2\, dx \frac{m_e}{m_p} + \int_\Omega |\phi_{2p}^{H_e}(x,t)|^2\, dx \frac{m_e}{m_p}.$$

Here **n** denotes the outward normal vectorial fields to the concerning surfaces.

Having clarified such masses relations, we define the functional

$$J(\phi, \rho, \mathbf{r}, \mathbf{u}, \mathbf{E}, \mathbf{A}, \mathbf{B})$$

where

$$J = G(\nabla u) + F(\phi) + E_c(\phi, \mathbf{r}) + F_1 + F_2 + F_3,$$

and where we assume $\gamma_p^D > 0$, $\gamma_p^T > 0$, $\gamma_N^D > 0$, $\gamma_{N_1}^T > 0$, $\gamma_{N_2}^T > 0$, $\gamma_{2p}^{H_e} > 0$, $\gamma_{N_1}^{H_e} > 0$, $\gamma_{N_2}^{H_e} > 0$, $\gamma_N > 0$, $\gamma_e > 0$ and $\alpha_D > 0$, $\alpha_T > 0$, $\alpha_{H_e} > 0$, $\alpha_N > 0$, $\alpha_{DT} > 0$, $\alpha_{H_e\, N} > 0$, $\alpha_{e,e} > 0$, $\alpha_{H_e,e} < 0$ so that

$$\begin{aligned}
G(\nabla\phi) \quad = \quad & \frac{\gamma_p^D}{2} \int_0^{t_f} \int_\Omega (\nabla\phi_p^D) \cdot (\nabla\phi_p^D)\, dy\, dt \\
& + \frac{\gamma_N^D}{2} \int_0^{t_f} \int_\Omega (\nabla\phi_N^D) \cdot (\nabla\phi_N^D)\, dx\, dy\, dt \\
& \frac{\gamma_p^T}{2} \int_0^{t_f} \int_\Omega (\nabla\phi_p^T) \cdot (\nabla\phi_p^T)\, dy\, dt \\
& + \frac{\gamma_{N_1}^T}{2} \int_0^{t_f} \int_\Omega (\nabla\phi_{N_1}^T) \cdot (\nabla\phi_{N_1}^T)\, dx\, dy\, dt \\
& + \frac{\gamma_{N_2}^T}{2} \int_0^{t_f} \int_\Omega (\nabla\phi_{N_2}^T) \cdot (\nabla\phi_{N_2}^T)\, dx\, dy\, dt \\
& + \frac{\gamma_{2p}^{H_e}}{2} \int_0^{t_f} \int_\Omega (\nabla\phi_{2p}^{H_e}) \cdot (\nabla\phi_{2p}^{H_e})\, dy\, dt \\
& + \frac{\gamma_{N_1}^{H_e}}{2} \int_0^{t_f} \int_\Omega (\nabla\phi_{N_1}^{H_e}) \cdot (\nabla\phi_{N_1}^{H_e})\, dx\, dy\, dt \\
& + \frac{\gamma_{N_2}^{H_e}}{2} \int_0^{t_f} \int_\Omega (\nabla\phi_{N_2}^{H_e}) \cdot (\nabla\phi_{N_2}^{H_e})\, dx\, dy\, dt \\
& + \frac{\gamma_N}{2} \int_0^{t_f} \int_\Omega (\nabla\phi_N) \cdot (\nabla\phi_N)\, dx\, dt \\
& + \frac{\gamma_e}{2} \int_0^{t_f} \int_\Omega (\nabla\phi_e) \cdot (\nabla\phi_e)\, dx\, dy\, dt, \qquad (89)
\end{aligned}$$

and

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$$
\begin{aligned}
F(\phi) \;=\; & \frac{\alpha_D}{2}\int_0^{t_f}\int_\Omega \frac{|\phi_D(x-\xi_1,y-\xi_2,t)|^2|\phi_D(\xi_1,\xi_2,t)|^2}{|(x,y)-(\xi_1,\xi_2)|}\,dx\,dy\,d\xi_1\,d\xi_2\,dt \\
& +\frac{\alpha_T}{2}\int_0^{t_f}\int_\Omega \frac{|\phi_T(x-\xi_1,y-\xi_2,t)|^2|\phi_T(\xi_1,\xi_2,t)|^2}{|(x,y)-(\xi_1,\xi_2)|}\,dx\,dy\,d\xi_1\,d\xi_2\,dt \\
& +\frac{\alpha_{DT}}{2}\int_0^{t_f}\int_\Omega \frac{|\phi_D(x-\xi_1,y-\xi_2,t)|^2|\phi_T(\xi_1,\xi_2,t)|^2}{|(x,y)-(\xi_1,\xi_2)|}\,dx\,dy\,d\xi_1\,d\xi_2\,dt \\
& +\frac{\alpha_{H_e}}{2}\int_0^{t_f}\int_\Omega \frac{|\phi_{H_e}(x-\xi_1,y-\xi_2,t)|^2|\phi_{H_e}(\xi_1,\xi_2,t)|^2}{|(x,y)-(\xi_1,\xi_2)|}\,dx\,dy\,d\xi_1\,d\xi_2\,dt \\
& +\frac{\alpha_N}{2}\int_0^{t_f}\int_\Omega \frac{|\phi_N(x-\xi,t)|^2|\phi_N(\xi)|^2}{|x-\xi,t|}\,dx\,d\xi\,dt \\
& +\sum_{j=1}^{2}\frac{\alpha_{H_e\,N}}{2}\int_0^{t_f}\int_\Omega \frac{|\phi_{H_e}(x_1-\xi_1,y-\xi_2,t)|^2|\phi_N(\xi_j,t)|^2}{|(x,y)-(\xi_1,\xi_2)|}\,dx\,dy\,d\xi_1\,d\xi_2\,dt \\
& +\frac{\alpha_{H_e,e}}{2}\int_0^{t_f}\int_\Omega \frac{|\phi_{H_e}(x-\xi_1,y-\xi_2,t)|^2|\phi_e(\xi_1,\xi_2,t)|^2}{|(x,y)-(\xi_1,\xi_2)|}\,dx\,dy\,d\xi_1\,d\xi_2\,dt \\
& +\frac{\alpha_{e,e}}{2}\int_0^{t_f}\int_\Omega \frac{|\phi_e(x-\xi_1,y-\xi_2,t)|^2|\phi_e(\xi_1,\xi_2,t)|^2}{|(x,y)-(\xi_1,\xi_2)|}\,dx\,dy\,d\xi_1\,d\xi_2\,dt
\end{aligned}
\tag{90}
$$

and the internal kinetics energy is expressed by

$$
\begin{aligned}
E_c(\phi,\mathbf{r}) \;=\; & \frac{1}{2}\int_0^{t_f}\int_\Omega |\phi_D|^2\,\frac{\partial \mathbf{r}_D}{\partial t}\cdot\frac{\partial \mathbf{r}_D}{\partial t}\,dx\,dy\,dt \\
& +\frac{1}{2}\int_0^{t_f}\int_\Omega |\phi_T|^2\,\frac{\partial \mathbf{r}_T}{\partial t}\cdot\frac{\partial \mathbf{r}_T}{\partial t}\,dx\,dy\,dt \\
& +\frac{1}{2}\int_0^{t_f}\int_\Omega |\phi_{H_e}|^2\,\frac{\partial \mathbf{r}_{H_e}}{\partial t}\cdot\frac{\partial \mathbf{r}_{H_e}}{\partial t}\,dx\,dy\,dt \\
& +\frac{1}{2}\int_0^{t_f}\int_\Omega |\phi_N|^2\,\frac{\partial \mathbf{r}_N}{\partial t}\cdot\frac{\partial \mathbf{r}_N}{\partial t}\,dx\,dy\,dt \\
& +\frac{1}{2}\int_0^{t_f}\int_\Omega |\phi_e|^2\,\frac{\partial \mathbf{r}_e}{\partial t}\cdot\frac{\partial \mathbf{r}_e}{\partial t}\,dx\,dy\,dt,
\end{aligned}
\tag{91}
$$

Here it is worth highlighting we have approximated the initially discrete set of indices s of particles as a continuous positive real variable s.

Moreover,

$$
F_1 = \frac{1}{4\pi}\int_0^{t_f} \|\operatorname{curl}\mathbf{A}-\mathbf{B}_0\|_2\,dt,
$$

$$
\begin{aligned}
F_2 \;=\; & \int_0^{t_f}\int_\Omega \mathbf{E}_{ind}\cdot K_p|\phi_p^D|^2\left(\mathbf{u}+\frac{\partial \mathbf{r}_D}{\partial t}\right)\,dx\,dy\,dt \\
& +\int_0^{t_f}\int_\Omega \mathbf{E}_{ind}\cdot K_p|\phi_p^T|^2\left(\mathbf{u}+\frac{\partial \mathbf{r}_T}{\partial t}\right)\,dx\,dy\,dt \\
& +\int_0^{t_f}\int_\Omega \mathbf{E}_{ind}\cdot K_p|\phi_{2p}^{H_e}|^2\left(\mathbf{u}+\frac{\partial \mathbf{r}_{H_e}}{\partial t}\right)\,dx\,dy\,dt \\
& +\int_0^{t_f}\int_\Omega \mathbf{E}_{ind}\cdot K_e|\phi_e|^2\left(\mathbf{u}+\frac{\partial \mathbf{r}_e}{\partial t}\right)\,dx\,dy\,dt,
\end{aligned}
\tag{92}
$$

where K_p and K_e are appropriate real constants related to the respective charges.

Here $\mathbf{u} = (u_1, u_2, u_3)$ is the fluid velocity field and

$$
\mathbf{r}_D,\ \mathbf{r}_T,\ \mathbf{r}_{H_e},\ \mathbf{r}_N,\ \mathbf{r}_e
$$

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are fields of displacements for the corresponding atom fields.

Also $\mathbf{A}$ denotes the magnetic potential, $\mathbf{B}_0$ an external magnetic field and $\mathbf{B}$ is the total magnetic field.

Moreover, $\mathbf{E}_{ind}$ is an induced electric field.

Finally,

$$\begin{aligned} F_3 &= \frac{C_D}{2}\int_0^{t_f}\int_\Omega \nabla_{(x,y)}\mathbf{r}_D\cdot\nabla_{(x,y)}\mathbf{r}_D\,dx\,dy\,dt + \frac{C_T}{2}\int_0^{t_f}\int_\Omega \nabla_{(x,y)}\mathbf{r}_T\cdot\nabla_{(x,y)}\mathbf{r}_T\,dx\,dy\,dt \\ & \frac{C_{H_e}}{2}\int_0^{t_f}\int_\Omega \nabla_{(x,y)}\mathbf{r}_{H_e}\cdot\nabla_{(x,y)}\mathbf{r}_{H_e}\,dx\,dy\,dt + \frac{C_N}{2}\int_0^{t_f}\int_\Omega \nabla_{(x,y)}\mathbf{r}_N\cdot\nabla_{(x,y)}\mathbf{r}_N\,dx\,dy\,dt \\ & \frac{C_e}{2}\int_0^{t_f}\int_\Omega \nabla_{(x,y)}\mathbf{r}_e\cdot\nabla_{(x,y)}\mathbf{r}_e\,dx\,dy\,dt, \end{aligned} \tag{93}$$

for appropriate real positive constants C_D C_T, C_{H_e}, C_N, C_e.

Such a functional J is subject to the following constraints:

1. The momentum conservation equation for the fluid motion

$$\rho\left(\frac{\partial u_k}{\partial t} + u_j\frac{\partial u_k}{\partial x_j}\right) = \rho f_k - \frac{\partial P}{\partial x_k} + \tau_{kj,j} + (F_E)_k + (F_M)_k,$$

$\forall k \in \{1,2,3\}$.

Here $\rho = \rho_D + \rho_T + \rho_{H_e} + \rho_N + \rho_e$ is the total density and P is the fluid pressure field.

Furthermore,

$$\tau_{ij} = \mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3}\delta_{ij}\sum_{k=1}^{3}\frac{\partial u_k}{\partial x_k}\right),$$

$\forall i,j \in \{1,2,3\}$,

$$\mathbf{F}_E = \{(F_E)_k\} = \left(K_p(|\phi_p^D|^2 + |\phi_p^T|^2 + |\phi_{2p}^{H_e}|^2) + K_e\int_\Omega |\phi_e|^2\,dx\right)\mathbf{E},$$

and

$$\begin{aligned} \mathbf{F}_M &= \{(F_M)_k\} \\ &= \Bigg(K_p\Bigg(|\phi_p^D|^2\left(\mathbf{u} + \frac{\partial \mathbf{r}_D}{\partial t}\right) \\ & |\phi_p^T|^2\left(\mathbf{u} + \frac{\partial \mathbf{r}_T}{\partial t}\right) \\ & +|\phi_{2p}^{H_e}|^2\left(\mathbf{u} + \frac{\partial \mathbf{r}_{H_e}}{\partial t}\right)\Bigg) \\ & +K_e|\phi_e|^2\left(\mathbf{u} + \frac{\partial \mathbf{r}_e}{\partial t}\right)\Bigg) \times \mathbf{B}. \end{aligned} \tag{94}$$

2. Mass conservation equation:

$$\frac{\partial \rho}{\partial t} + \text{ div }(\rho\mathbf{u}) = 0.$$

3. Energy equation

$$\rho\frac{De}{Dt} + P(\text{ div }\mathbf{u}) = \frac{\partial Q}{\partial t} - \text{ div }\mathbf{q},$$

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where we assume the Fourier law

$$\mathbf{q} = -K\nabla T,$$

where $T = T(x,t)$ is the scalar field of temperature.

Also,

$$\begin{aligned} e &= \frac{\rho}{2}\mathbf{u}\cdot\mathbf{u} + \frac{\rho_D}{2}\frac{\partial \mathbf{r}_D}{\partial t}\cdot\frac{\partial \mathbf{r}_D}{\partial t} \\ &+ \frac{\rho_T}{2}\frac{\partial \mathbf{r}_T}{\partial t}\cdot\frac{\partial \mathbf{r}_T}{\partial t} \\ &+ \frac{\rho_{H_e}}{2}\frac{\partial \mathbf{r}_{H_e}}{\partial t}\cdot\frac{\partial \mathbf{r}_{H_e}}{\partial t} \\ &+ \frac{\rho_N}{2}\frac{\partial \mathbf{r}_N}{\partial t}\cdot\frac{\partial \mathbf{r}_N}{\partial t} \\ &+ \frac{\rho_e}{2}\frac{\partial \mathbf{r}_e}{\partial t}\cdot\frac{\partial \mathbf{r}_e}{\partial t} \end{aligned} \tag{95}$$

and

$$\frac{De}{Dt} = \frac{\partial e}{\partial t} + u_j\frac{\partial e}{\partial x_j}.$$

4.

$$P = F_7(\rho, T),$$

for an appropriate scalar function F_7.

5. Mass relations

(a)

$$m_D(t) = \int_\Omega \rho_D(x,t)\,dx,$$

(b)

$$m_T(t) = \int_\Omega \rho_T(x,t)\,dx,$$

(c)

$$m_{He}(t) = \int_\Omega \rho_{H_e}(x,t)\,dx,$$

(d)

$$m_N(t) = \int_\Omega \rho_N(x,t)\,dx,$$

(e)

$$m_e(t) = \int_\Omega \rho_e(x,t)\,dx,$$

(f)

$$(m_{H_e})_T(t) = \int_\Omega \rho_{H_e}(x,t)\,dx + \int_0^t \int_{\partial\Omega_2} \rho_{H_e}(x,\tau)\mathbf{u}\cdot\mathbf{n}\,d\Gamma d\tau,$$

(g)

$$(m_N)_T(t) = \int_\Omega \rho_N(x,t)\,dx + \int_0^t \int_{\partial\Omega_2} \rho_N(x,\tau)\mathbf{u}\cdot\mathbf{n}\,d\Gamma d\tau,$$

(h)

$$\frac{(m_N)_T(t)}{(m_{H_e})_T(t)} = \frac{\alpha_N}{\alpha_{H_e}},$$

so that

$$\alpha_N m_{H_e})_T(t) = \alpha_{H_e}(m_N)_T(t),$$

where,

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(a)
$$(m_{H_e,N})_T(t) = m_{H_e,N}(t) + \int_0^t \int_{\partial\Omega_2} (\rho_{H_e}(x,\tau))\mathbf{u}\cdot\mathbf{n}\, dS\, d\tau,$$
(b)
$$m_{H_e,N}(t) = m_{H_e}(t) + m_N(t),$$
(c)
$$(m_D)(t) = (m_D)_0 - \int_0^t \int_{\partial\Omega_1\cup\partial\Omega_2} (\rho_D(x,\tau))\mathbf{u}\cdot\mathbf{n}\, dS\, d\tau - \alpha_D(m_{H_e,N})_T(t),$$
(d)
$$(m_T)(t) = (m_T)_0 - \int_0^t \int_{\partial\Omega_1\cup\partial\Omega_2} (\rho_T(x,\tau))\mathbf{u}\cdot\mathbf{n}\, dS\, d\tau - \alpha_T(m_{H_e,N})_T(t),$$
(e)
$$(m_e)_T(t) = m_e(t) + \int_0^t \int_{\partial\Omega_2} (\rho_T(x,\tau))\mathbf{u}\cdot\mathbf{n}\, dS\, d\tau.$$
(f)
$$m_e(t) = \int_\Omega |\phi_p^D(x,t)|^2\, dx \frac{m_e}{m_p} + \int_\Omega |\phi_p^T(x,t)|^2\, dx \frac{m_e}{m_p} + \int_\Omega |\phi_{2p}^{H_e}(x,t)|^2\, dx \frac{m_e}{m_p}.$$

6. Other mass constraints

(a)
$$\int_\Omega |\phi_N^D(x,y,t)|^2\, dx = m_N,$$
(b)
$$\int_\Omega |\phi_{N_1}^T(x,y,t)|^2\, dx = m_N,$$
(c)
$$\int_\Omega |\phi_{N_2}^T(x,y,t)|^2\, dx = m_N,$$
(d)
$$\int_\Omega |\phi_{N_1}^{H_e}(x,y,t)|^2\, dx = m_N,$$
(e)
$$\int_\Omega |\phi_{N_2}^{H_e}(x,y,t)|^2\, dx = m_N.$$

7. For the induced electric field, we must have

$$\begin{aligned}
&\text{curl } \mathbf{E}_{ind} + \frac{1}{c}\text{ curl } \left(\hat{K}_p|\phi_p^D|^2\left(\mathbf{u} + \frac{\partial \mathbf{r}_D}{\partial t}\right)\right.\\
&+\hat{K}_p|\phi_p^T|^2\left(\mathbf{u} + \frac{\partial \mathbf{r}_T}{\partial t}\right)\\
&+\hat{K}_p|\phi_{2p}^{H_e}|^2\left(\mathbf{u} + \frac{\partial \mathbf{r}_{H_e}}{\partial t}\right)\\
&\left.+\ \hat{K}_e\int_\Omega |\phi_e(x,y,t)|^2\left(\mathbf{u}(y,t) + \frac{\partial \mathbf{r}_e(x,y,t)}{\partial t}\, dx\right)\right)\\
&\times(\text{ curl } \mathbf{A} - \mathbf{B}_0) - \frac{1}{c}\frac{\partial}{\partial t}(\text{ curl } \mathbf{A} - \mathbf{B}_0) = \mathbf{0},
\end{aligned} \tag{96}$$

where $\hat{K}_p$ and $\hat{K}_e$ are appropriate real constants related to the respective charges.

8. A Maxwell equation:

$$\text{div } \mathbf{B} = 0,$$

where

$$\mathbf{B} = \mathbf{B}_0 - \text{ curl } \mathbf{A}.$$

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9. Another Maxwell equation:

$$\text{div } \mathbf{E} = 4\pi \left(K_p(|\phi_p^D|^2 + |\phi_p^T|^2 + |\phi_{2p}^{H_e}|^2) + K_e \int_\Omega |\phi_e(x,y,t)|^2 \, dx \right),$$

where the total electric field $\mathbf{E}$ stands for

$$\mathbf{E} = \mathbf{E}_{ind} + \mathbf{E}_\rho,$$

and where generically denoting

$$F(\phi) = \int_\Omega f_5(\phi, x, \xi) \, dx \, d\xi,$$

we have also

$$\mathbf{E}_\rho = \left\{ \int_\Omega \frac{\partial f_5(\phi, x, \xi)}{\partial x_k} \, d\xi \right\}.$$

At this point we generically denote

$$\langle h_1, h_2 \rangle_{L^2} = \int_0^{t_f} \int_\Omega h_1 \, h_2 \, dx \, dy \, dt.$$

Thus, already including the Lagrange multipliers concerning the restrictions indicated, the extended functional J_3 stands for

$$\begin{aligned} & J_3 = J_3(\phi, \mathbf{u}, \mathbf{r}, P, \mathbf{A}, \mathbf{B}, \mathbf{E}, \Lambda, E) \\ = \; & G(\nabla\phi) + F(\phi) + E_c(\phi, \mathbf{r}) + F_1 + F_2 + F_3 \\ & + \left\langle \Lambda_k, \rho \left(\frac{\partial u_k}{\partial t} + u_j \frac{\partial u_k}{\partial x_j} \right) - \rho f_k + \frac{\partial P}{\partial x_k} - \tau_{kj,j} - (F_E)_k - (F_M)_k \right\rangle_{L^2} \\ & + \left\langle \Lambda_4, \; \frac{\partial \rho}{\partial t} + \text{ div } (\rho \mathbf{u}) \right\rangle_{L^2} + J_{Aux_1} + J_{Aux_2} + J_{Aux_3} + J_{Aux_4}, \end{aligned} \tag{97}$$

where,

$$\begin{aligned} J_{Aux_1} \; = \; & \left\langle \Lambda_5, \; \rho \frac{De}{Dt} + P(\text{ div } \mathbf{u}) - \frac{\partial Q}{\partial t} + \text{ div } \mathbf{q} \right\rangle_{L^2} \\ & + \langle \Lambda_6, \; P - F_7(\rho, T) \rangle_{L^2}, \end{aligned} \tag{98}$$

$$\begin{aligned} J_{Aux_2} \; = \; & \left\langle \Lambda_7, m_D(t) - \int_\Omega \rho_D(x,t) \, dx \right\rangle_{L^2} \\ & + \left\langle \Lambda_8, m_T(t) - \int_\Omega \rho_T(x,t) \, dx \right\rangle_{L^2} \\ & \left\langle \Lambda_9, m_{H_e}(t) - \int_\Omega \rho_{H_e}(x,t) \, dx \right\rangle_{L^2} \\ & \left\langle \Lambda_{10}, m_N(t) - \int_\Omega \rho_N(x,t) \, dx \right\rangle_{L^2} \\ & \left\langle \Lambda_{11}, m_e(t) - \int_\Omega \rho_e(x,t) \, dx \right\rangle_{L^2} \\ & \int_0^{t_f} E_12(t)(\alpha_N m_{H_e})_T(t) - \alpha_{H_e}(m_N)_T(t)) \, dt, \end{aligned} \tag{99}$$

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$$
\begin{aligned}
J_{Aux_3} \quad = \quad & -\int_0^{t_f}\int_\Omega (E_N^D)_5(y,t)\left(\int_\Omega |\phi_N^D(x,y,t)|^2\,dx - m_N\right)\,dy\,dt \\
& -\int_0^{t_f}\int_\Omega (E_{N_1}^T)_6(y,t)\left(\int_\Omega |\phi_{N_1}^T(x,y,t)|^2\,dx - m_N\right)\,dy\,dt \\
& -\int_0^{t_f}\int_\Omega (E_{N_2}^T)_7(y,t)\left(\int_\Omega |\phi_{N_2}^T(x,y,t)|^2\,dx - m_N\right)\,dy\,dt \\
& -\int_0^{t_f}\int_\Omega (E_{N_1}^{H_e})_8(y,t)\left(\int_\Omega |\phi_{N_1}^{H_e}(x,y,t)|^2\,dx - m_N\right)\,dy\,dt \\
& -\int_0^{t_f}\int_\Omega (E_{N_2}^{H_e})_9(y,t)\left(\int_\Omega |\phi_{N_2}^{H_e}(x,y,t)|^2\,dx - m_N\right)\,dy\,dt, \qquad (100)
\end{aligned}
$$

$$
\begin{aligned}
J_{Aux_4} \quad = \quad & \langle \Lambda_{12},\ \text{curl}\,\mathbf{E}_{ind} \\
& +\frac{1}{c}\,\text{curl}\,\left(\hat{K}_p|\phi_p^D|^2\left(\mathbf{u}+\frac{\partial \mathbf{r}_D}{\partial t}\right)\right. \\
& +\hat{K}_p|\phi_p^T|^2\left(\mathbf{u}+\frac{\partial \mathbf{r}_T}{\partial t}\right) \\
& +\hat{K}_p|\phi_{2p}^{H_e}|^2\left(\mathbf{u}+\frac{\partial \mathbf{r}_{H_e}}{\partial t}\right) \\
& +\left.\hat{K}_e\int_\Omega |\phi_e(x,y,t)|^2\left(\mathbf{u}(y,t)+\frac{\partial \mathbf{r}_e(x,y,t)}{\partial t}\,dx\right)\right) \\
& \times(\,\text{curl}\,\mathbf{A}-\mathbf{B}_0)-\frac{1}{c}\frac{\partial}{\partial t}(\,\text{curl}\,\mathbf{A}-\mathbf{B}_0)\Big\rangle_{L^2} \\
& +\langle \Lambda_{13},\ \text{div}\,\mathbf{B}\rangle_{L^2} \\
& +\left\langle \Lambda_{14},\ \text{div}\,\mathbf{E}-4\pi\left(K_p(|\phi_p^D|^2+|\phi_p^T|^2+|\phi_{2p}^{H_e}|^2)+K_e\int_\Omega |\phi_e(x,y,t)|^2\,dx\right)\right\rangle_{L^2}. \qquad (101)
\end{aligned}
$$

Here we recall the following definitions and relations:

1. For the Deuterium field

$$|\phi_D(x,y,t)|^2 = |\phi_p^D(y,t)|^2 + |\phi_N^D(x,y,t)|^2|\phi_p^D(y,t)|^2\frac{1}{m_p},$$

2. For the Tritium field

$$|\phi_D(x,y,t)|^2 = |\phi_p^D(y,t)|^2 + (|\phi_{N_1}^D(x,y,t)|^2 + |\phi_{N_2}^D(x,y,t)|^2)|\phi_p^D(y,t)|^2\frac{1}{m_p},$$

3. For the Helium field

$$|\phi_{H_e}(x,y,t)|^2 = |\phi_{2p}^{H_e}(y,t)|^2 + (|\phi_{N_1}^{H_e}(x,y,t)|^2 + |\phi_{N_2}^{H_e}(x,y,t)|^2)|\phi_{2p}^{H_e}(y,t)|^2\frac{1}{2\,m_p},$$

4. For the Neutron field

$$\phi_N = \phi_N(x,t),$$

5. For the electronic field resulting from the ionization

$$\phi_e = \phi_e(x,y,t).$$

1.

$$\rho_D(y,t) = \int_\Omega |\phi_D(x,y,t)|^2\,dx,$$

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2.
$$\rho_T(y,t) = \int_\Omega |\phi_T(x,y,t)|^2\, dx,$$

$$\rho_{H_e}(y,t) = \int_\Omega |\phi_{H_e}(x,y,t)|^2\, dx,$$

$$\rho_N(x,t) = |\phi_N(x,t)|^2,$$

$$\rho_e(y,t) = \int_\Omega |\phi_e(x,y,t)|^2\, dx.$$

Also,

$$\rho = \rho_D + \rho_T + \rho_{H_e} + \rho_N + \rho_e,$$

1.
$$(m_{H_e,N})_T(t) = m_{H_e,N}(t) + \int_0^t \int_{\partial\Omega_2} (\rho_{H_e}(x,\tau) + \rho_N(x,\tau))\mathbf{u}\cdot\mathbf{n}\, dS\, d\tau,$$

2.
$$m_{H_e,N}(t) = m_{H_e}(t) + m_N(t),$$

3.
$$m_{H_e}(t) = \int_\Omega \rho_{H_e}(x,t)\, dx,$$

4.
$$m_N(t) = \int_\Omega \rho_N(x,t)\, dx,$$

5.
$$(m_D)(t) = (m_D)_0 - \int_0^t \int_{\partial\Omega_1\cup\partial\Omega_2} (\rho_D(x,\tau))\mathbf{u}\cdot\mathbf{n}\, dS\, d\tau - \alpha_D (m_{H_e,N})_T(t),$$

6.
$$(m_T)(t) = (m_T)_0 - \int_0^t \int_{\partial\Omega_1\cup\partial\Omega_2} (\rho_T(x,\tau))\mathbf{u}\cdot\mathbf{n}\, dS\, d\tau - \alpha_T (m_{H_e,N})_T(t),$$

7.
$$(m_{H_e})_T(t) = \int_\Omega \rho_{H_e}(x,t)\, dx + \int_0^t \int_{\partial\Omega_2} \rho_{H_e}(x,\tau)\mathbf{u}\cdot\mathbf{n}\, d\Gamma d\tau,$$

8.
$$(m_N)_T(t) = \int_\Omega \rho_N(x,t)\, dx + \int_0^t \int_{\partial\Omega_2} \rho_N(x,\tau)\mathbf{u}\cdot\mathbf{n}\, d\Gamma d\tau,$$

9.
$$\frac{(m_N)_T(t)}{(m_{H_e})_T(t)} = \frac{\alpha_N}{\alpha_{H_e}},$$

so that

$$\alpha_N m_{H_e})_T(t) = \alpha_{H_e}(m_N)_T(t),$$

10.
$$(m_e)_T(t) = m_e(t) - \int_0^t \int_{\partial\Omega_2} (\rho_e(x,\tau))\mathbf{u}\cdot\mathbf{n}\, dS\, d\tau,$$

11.
$$m_e(t) = \int_\Omega \rho_e(x,t)\, dx.$$

12.
$$m_e(t) = \int_\Omega |\phi_p^D(x,t)|^2\, dx \frac{m_e}{m_p} + \int_\Omega |\phi_p^T(x,t)|^2\, dx \frac{m_e}{m_p} + \int_\Omega |\phi_{2p}^{H_e}(x,t)|^2\, dx \frac{m_e}{m_p}.$$

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Finally,

$$\mathbf{E} = \mathbf{E}_{ind} + \mathbf{E}_{\rho},$$

and where generically denoting

$$F(\phi) = \int_{\Omega} f_5(\phi, x, \xi)\, dx\, d\xi,$$

we have also

$$\mathbf{E}_{\rho} = \left\{ \int_{\Omega} \frac{\partial f_5(\phi, x, \xi)}{\partial x_k}\, d\xi \right\}.$$

and,

$$\mathbf{B} = \mathbf{B}_0 - \text{ curl } \mathbf{A}.$$

20. A final mathematical description of the hydrogen nuclear fusion

In this section we develop in even more details another model for the hydrogen nuclear fusion.

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

Here such a set Ω stands for a control volume in which an ionized gas (plasma) flows. Such a gas comprises ionized Deuterium and Tritium atoms intended, through a suitable higher temperature, to chemically react resulting in atoms of Helium and a field of single energetic Neutrons.

Symbolically such a reaction stands for

$$\text{Deuterium}^{+} \ + \ \text{Tritium}^{+} \rightarrow \text{Helium}^{++} \ + \ \text{Neutron (energetic)}.$$

We recall that the ionized Deuterium atom is comprised by a proton and a neutron and the ionized Tritium atom is comprised by a proton and two neutrons.

Moreover, the ionized Helium atom is comprised by two protons and two neutrons.

As previously mentioned, resulting from such a chemical reaction up surges also an energetic neutron which the higher kinetics energy has a great variety of applications, including its conversion in electric energy.

We highlight the model here presented includes electric and magnetic fields and the corresponding potential ones.

Denoting by t the time on the interval $[0, t_f]$, at this point we define the following density functions:

1. For a single Deuterium atom indexed by s:

$$|\phi_D(x, y, t, s)|^2 = |\phi_p^D(y, t, s)|^2 + |\phi_N^D(x, y, t, s)|^2 |\phi_p^D(y, t, s)|^2 \frac{1}{m_p},$$

2. For a single Tritium atom indexed by s:

$$|\phi_T(x, y, t, s)|^2 = |\phi_p^T(y, t, s)|^2 + (|\phi_{N_1}^T(x, y, t, s)|^2 + |\phi_{N_2}^T(x, y, t, s)|^2) |\phi_p^T(y, t, s)|^2 \frac{1}{m_p},$$

3. For a single Helium atom indexed by s:

$$|\phi_{H_e}(x, y, t, s)|^2 = |\phi_{2p}^{H_e}(y, t, s)|^2 + (|\phi_{N_1}^{H_e}(x, y, t, s)|^2 + |\phi_{N_2}^{H_e}(x, y, t, s)|^2) |\phi_{2p}^{H_e}(y, t, s)|^2 \frac{1}{2\, m_p},$$

4. For the Neutron field:

$$\phi_N = \phi_N(x, t, s),$$

5. For the electronic field resulting from the ionization

$$\phi_e = \phi_e(x, y, t, s).$$

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Furthermore, we define also the related densities

1.
$$\rho_D(y,t) = \int_0^{N_D(t)} \int_\Omega |\phi_D(x,y,t,s)|^2 \, dx \, ds,$$

2.
$$\rho_T(y,t) = \int_0^{N_T(t)} \int_\Omega |\phi_T(x,y,t,s)|^2 \, dx \, ds,$$

$$\rho_{H_e}(y,t) = \int_0^{N_{H_e}(t)} \int_\Omega |\phi_{H_e}(x,y,t,s)|^2 \, dx \, ds,$$

$$\rho_N(x,t) = \int_0^{N_N(t)} |\phi_N(x,t,s)|^2 \, ds,$$

$$\rho_e(y,t) = \int_0^{N_e(t)} \int_\Omega |\phi_e(x,y,t,s)|^2 \, dx \, ds.$$

For the chemical reaction in question we consider that one unit of mass of fractional proportion α_D of ionized Deuterium and α_T of ionized Tritium results in one unit of mass of fractional proportion α_{H_e} of ionized Helium and α_N of neutrons.

Symbolically, this stands for

$$1 = \alpha_D + \alpha_T = \alpha_{H_e} + \alpha_N.$$

Concerning the control volume Ω in question and related surface control $\partial\Omega$, we assume such a volume has an initial (fot $t = 0$) amount of ionized Deuterium of $(m_D)_0$ and an initial amount of ionized Tritium of $(m_T)_0$. The initial amount of ionized Helium and single neutrons are supposed to be zero.

On the other hand, about the surface control $\partial\Omega$, we assume there is a part $\Omega_1 \subset \partial\Omega$ for which is allowed the entrance and exit of Deuterium and Tritium ionized atoms.

We assume also there is another part $\partial\Omega_2 \subset \partial\Omega$ such that $\partial\Omega_1 \cap \partial\Omega_2 = \emptyset$ for which is allowed only the exit of ionized Helium atoms and neutrons, but not their entrance.

In $\partial\Omega_2$ is allowed the exit only (not the entrance) of ionized Deuterium and Tritium atoms.

Indeed, we assume the following relations for the masses:

1.
$$(m_{H_e,N})_T(t) = m_{H_e,N}(t) + \int_0^t \int_{\partial\Omega_2} (\rho_{H_e}(x,\tau) + \rho_N(x,\tau))\mathbf{u} \cdot \mathbf{n} \, dS \, d\tau,$$

2.
$$m_{H_e,N}(t) = m_{H_e}(t) + m_N(t),$$

3.
$$m_{H_e}(t) = \int_\Omega \rho_{H_e}(x,t) \, dx,$$

4.
$$m_N(t) = \int_\Omega \rho_N(x,t) \, dx,$$

5.
$$(m_D)(t) = (m_D)_0 - \int_0^t \int_{\partial\Omega_1 \cup \partial\Omega_2} (\rho_D(x,\tau))\mathbf{u} \cdot \mathbf{n} \, dS \, d\tau - \alpha_D (m_{H_e,N})_T(t),$$

6.
$$(m_T)(t) = (m_T)_0 - \int_0^t \int_{\partial\Omega_1 \cup \partial\Omega_2} (\rho_T(x,\tau))\mathbf{u} \cdot \mathbf{n} \, dS \, d\tau - \alpha_T (m_{H_e,N})_T(t),$$

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7.
$$(m_{H_e})_T(t) = \int_\Omega \rho_{H_e}(x,t)\, dx + \int_0^t \int_{\partial\Omega_2} \rho_{H_e}(x,\tau)\mathbf{u}\cdot\mathbf{n}\, d\Gamma d\tau,$$

8.
$$(m_N)_T(t) = \int_\Omega \rho_N(x,t)\, dx + \int_0^t \int_{\partial\Omega_2} \rho_N(x,\tau)\mathbf{u}\cdot\mathbf{n}\, d\Gamma d\tau,$$

9.
$$\frac{(m_N)_T(t)}{(m_{H_e})_T(t)} = \frac{\alpha_N}{\alpha_{H_e}},$$

so that
$$\alpha_N m_{H_e})_T(t) = \alpha_{H_e}(m_N)_T(t),$$

10.
$$(m_e)_T(t) = m_e(t) + \int_0^t \int_{\partial\Omega_2} (\rho_e(x,\tau))\mathbf{u}\cdot\mathbf{n}\, dS\, d\tau,$$

11.
$$m_e(t) = \int_\Omega \rho_e(x,t)\, dx.$$

12.
$$\begin{aligned} m_e(t) &= \int_0^{N_D(t)} \int_\Omega |\phi_p^D(y,t,s)|^2\, dy\, ds \frac{m_e}{m_p} + \int_0^{N_T(t)} \int_\Omega |\phi_p^T(y,t,s)|^2\, dy\, ds \frac{m_e}{m_p} \\ &+ \int_0^{N_p(t)} \int_\Omega |\phi_{2p}^{H_e}(y,t,s)|^2\, dy\, ds \frac{m_e}{m_p}. \end{aligned} \tag{102}$$

Here $\mathbf{n}$ denotes the outward normal vectorial fields to the concerning surfaces.

Having clarified such masses relations, denoting by $N_D(t)$ $N_T(t)$, $N_{H_e}(t)$, $N_N(t)$, $N_e(t)$ the respective indexed number of particles at time t, we define the functional

$$J(\phi, \rho, \mathbf{r}, \mathbf{u}, \mathbf{E}, \mathbf{A}, \mathbf{B}, \{N_D, N_T, N_{H_e}, N_N, N_e\})$$

where

$$J = G(\nabla u) + F(\phi) + E_c(\phi, \mathbf{r}) + F_1 + F_2 + F_3 + F_4,$$

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and where we assume $\gamma_p^D > 0$, $\gamma_p^T > 0$, $\gamma_N^D > 0$, $\gamma_{N_1}^T > 0$, $\gamma_{N_2}^T > 0$, $\gamma_{2p}^{H_e} > 0$, $\gamma_{N_1}^{H_e} > 0$, $\gamma_{N_2}^{H_e} > 0$, $\gamma_N > 0$, $\gamma_e > 0$ and $\alpha_D > 0$, $\alpha_T > 0$, $\alpha_{H_e} > 0$, $\alpha_N > 0$, $\alpha_{DT} > 0$, $\alpha_{H_e\,N} > 0$, $\alpha_{e,e} > 0$, $\alpha_{H_e,e} < 0$ so that

$$
\begin{aligned}
G(\nabla\phi) \;=\; & \frac{\gamma_p^D}{2}\int_0^{t_f}\int_0^{N_D(t)}\int_\Omega (\nabla\phi_p^D)\cdot(\nabla\phi_p^D)\,dy\,ds\,dt \\
& +\frac{\gamma_N^D}{2}\int_0^{t_f}\int_0^{N_D(t)}\int_\Omega (\nabla\phi_N^D)\cdot(\nabla\phi_N^D)\,dx\,dy\,ds\,dt \\
& \frac{\gamma_p^T}{2}\int_0^{t_f}\int_0^{N_T(t)}\int_\Omega (\nabla\phi_p^T)\cdot(\nabla\phi_p^T)\,dy\,ds\,dt \\
& +\frac{\gamma_{N_1}^T}{2}\int_0^{t_f}\int_0^{N_T(t)}\int_\Omega (\nabla\phi_{N_1}^T)\cdot(\nabla\phi_{N_1}^T)\,dx\,dy\,ds\,dt \\
& +\frac{\gamma_{N_2}^T}{2}\int_0^{t_f}\int_0^{N_T(t)}\int_\Omega (\nabla\phi_{N_2}^T)\cdot(\nabla\phi_{N_2}^T)\,dx\,dy\,ds\,dt \\
& +\frac{\gamma_{2p}^{H_e}}{2}\int_0^{t_f}\int_0^{N_{H_e}(t)}\int_\Omega (\nabla\phi_{2p}^{H_e})\cdot(\nabla\phi_{2p}^{H_e})\,dy\,ds\,dt \\
& +\frac{\gamma_{N_1}^{H_e}}{2}\int_0^{t_f}\int_0^{N_{H_e}(t)}\int_\Omega (\nabla\phi_{N_1}^{H_e})\cdot(\nabla\phi_{N_1}^{H_e})\,dx\,dy\,ds\,dt \\
& +\frac{\gamma_{N_2}^{H_e}}{2}\int_0^{t_f}\int_0^{N_{H_e}(t)}\int_\Omega (\nabla\phi_{N_2}^{H_e})\cdot(\nabla\phi_{N_2}^{H_e})\,dx\,dy\,ds\,dt \\
& +\frac{\gamma_N}{2}\int_0^{t_f}\int_0^{N_N(t)}\int_\Omega (\nabla\phi_N)\cdot(\nabla\phi_N)\,dx\,ds\,dt \\
& +\frac{\gamma_e}{2}\int_0^{t_f}\int_0^{N_e(t)}\int_\Omega (\nabla\phi_e)\cdot(\nabla\phi_e)\,dx\,dy\,ds\,dt, \qquad (103)
\end{aligned}
$$

and

$$
\begin{aligned}
& F(\phi) = \\
& \frac{\alpha_D}{2}\int_0^{t_f}\int_0^{N_D(t)}\int_0^{N_D(t)}\int_\Omega \frac{|\phi_D(x-\xi_1,y-\xi_2,t,s-s_1)|^2|\phi_D(\xi_1,\xi_2,t,s_1)|^2}{|(x,y)-(\xi_1,\xi_2)|}\,dx\,dy\,d\xi_1\,d\xi_2\,ds\,ds_1\,dt \\
& +\frac{\alpha_T}{2}\int_0^{t_f}\int_0^{N_T(t)}\int_0^{N_T(t)}\int_\Omega \frac{|\phi_T(x-\xi_1,y-\xi_2,t,s-s_1)|^2|\phi_T(\xi_1,\xi_2,t,s_1)|^2}{|(x,y)-(\xi_1,\xi_2)|}\,dx\,dy\,d\xi_1\,d\xi_2\,ds\,ds_1\,dt \\
& +\frac{\alpha_{DT}}{2}\int_0^{t_f}\int_0^{N_D(t)}\int_0^{N_T(t)}\int_\Omega \frac{|\phi_D(x-\xi_1,y-\xi_2,t,s-s_1)|^2|\phi_T(\xi_1,\xi_2,t,s_1)|^2}{|(x,y)-(\xi_1,\xi_2)|}\,dx\,dy\,d\xi_1\,d\xi_2\,dt \\
& +\frac{\alpha_{H_e}}{2}\int_0^{t_f}\int_0^{N_{H_e}(t)}\int_0^{N_{H_e}(t)}\int_\Omega \frac{|\phi_{H_e}(x-\xi_1,y-\xi_2,t,s-s_1)|^2|\phi_{H_e}(\xi_1,\xi_2,t)|^2}{|(x,y)-(\xi_1,\xi_2,s_1)|}\,dx\,dy\,d\xi_1\,d\xi_2\,ds\,ds_1\,dt \\
& +\frac{\alpha_N}{2}\int_0^{t_f}\int_0^{N_N(t)}\int_0^{N_N(t)}\int_\Omega \frac{|\phi_N(x-\xi,t,s-s_1)|^2|\phi_N(\xi,t,s_1)|^2}{|x-\xi|}\,dx\,d\xi\,ds\,ds_1\,dt \\
& +\sum_{j=1}^{2}\frac{\alpha_{H_e\,N}}{2}\int_0^{t_f}\int_0^{N_{H_e}(t)}\int_0^{N_D(t)}\int_\Omega \frac{|\phi_{H_e}(x_1-\xi_1,y-\xi_2,t)|^2|\phi_N(\xi_j,t)|^2}{|(x,y)-(\xi_1,\xi_2)|}\,dx\,dy\,d\xi_1\,d\xi_2\,ds\,ds_1\,dt \\
& +\frac{\alpha_{H_e,e}}{2}\int_0^{t_f}\int_0^{N_{H_e}(t)}\int_0^{N_e(t)}\int_\Omega \frac{|\phi_{H_e}(x-\xi_1,y-\xi_2,t,s-s_1)|^2|\phi_e(\xi_1,\xi_2,t,s_1)|^2}{|(x,y)-(\xi_1,\xi_2)|}\,dx\,dy\,d\xi_1\,d\xi_2\,ds\,ds_1\,dt \\
& +\frac{\alpha_{e,e}}{2}\int_0^{t_f}\int_0^{N_e(t)}\int_0^{N_e(t)}\int_\Omega \frac{|\phi_e(x-\xi_1,y-\xi_2,t,s-s_1)|^2|\phi_e(\xi_1,\xi_2,t,s_1)|^2}{|(x,y)-(\xi_1,\xi_2)|}\,dx\,dy\,d\xi_1\,d\xi_2\,ds\,ds_1\,dt \qquad (104)
\end{aligned}
$$

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and the internal kinetics energy is expressed by

$$\begin{aligned} E_c(\phi,\mathbf{r}) &= \frac{1}{2}\int_0^{t_f}\int_0^{N_D(t)}\int_\Omega |\phi_D|^2 \frac{\partial \mathbf{r}_D}{\partial t}\cdot\frac{\partial \mathbf{r}_D}{\partial t}\, dx\, dy\, ds\, dt \\ &+\frac{1}{2}\int_0^{t_f}\int_0^{N_T(t)}\int_\Omega |\phi_T|^2 \frac{\partial \mathbf{r}_T}{\partial t}\cdot\frac{\partial \mathbf{r}_T}{\partial t}\, dx\, dy\, ds\, dt \\ &+\frac{1}{2}\int_0^{t_f}\int_0^{N_{H_e}(t)}\int_\Omega |\phi_{H_e}|^2 \frac{\partial \mathbf{r}_{H_e}}{\partial t}\cdot\frac{\partial \mathbf{r}_{H_e}}{\partial t}\, dx\, dy\, ds\, dt \\ &+\frac{1}{2}\int_0^{t_f}\int_0^{N_N(t)}\int_\Omega |\phi_N|^2 \frac{\partial \mathbf{r}_N}{\partial t}\cdot\frac{\partial \mathbf{r}_N}{\partial t}\, dx\, dy\, ds\, dt \\ &+\frac{1}{2}\int_0^{t_f}\int_0^{N_e(t)}\int_\Omega |\phi_e|^2 \frac{\partial \mathbf{r}_e}{\partial t}\cdot\frac{\partial \mathbf{r}_e}{\partial t}\, dx\, dy\, ds\, dt, \end{aligned} \tag{105}$$

Moreover,

$$F_1 = \frac{1}{4\pi}\int_0^{t_f} \|\operatorname{curl}\mathbf{A}-\mathbf{B}_0\|_2\, dt,$$

$$\begin{aligned} F_2 &= \int_0^{t_f}\int_0^{N_D(t)}\int_\Omega \mathbf{E}_{ind}\cdot K_p|\phi_p^D|^2\left(\mathbf{u}+\frac{\partial \mathbf{r}_D}{\partial t}\right) dx\, dy\, ds\, dt \\ &+\int_0^{t_f}\int_0^{N_T(t)}\int_\Omega \mathbf{E}_{ind}\cdot K_p|\phi_p^T|^2\left(\mathbf{u}+\frac{\partial \mathbf{r}_T}{\partial t}\right) dx\, dy\, ds\, dt \\ &+\int_0^{t_f}\int_0^{N_{H_e}(t)}\int_\Omega \mathbf{E}_{ind}\cdot K_p|\phi_{2p}^{H_e}|^2\left(\mathbf{u}+\frac{\partial \mathbf{r}_{H_e}}{\partial t}\right) dx\, dy\, ds\, dt \\ &+\int_0^{t_f}\int_0^{N_e(t)}\int_\Omega \mathbf{E}_{ind}\cdot K_e|\phi_e|^2\left(\mathbf{u}+\frac{\partial \mathbf{r}_e}{\partial t}\right) dx\, dy\, ds\, dt, \end{aligned} \tag{106}$$

where K_p and K_e are appropriate real constants related to the respective charges.

Here $\mathbf{u} = (u_1, u_2, u_3)$ is the fluid velocity field and

$$\mathbf{r}_D,\ \mathbf{r}_T,\ \mathbf{r}_{H_e},\ \mathbf{r}_N,\ \mathbf{r}_e$$

are fields of displacements for the corresponding particle fields.

Also $\mathbf{A}$ denotes the magnetic potential, $\mathbf{B}_0$ an external magnetic field and $\mathbf{B}$ is the total magnetic field.

Moreover, $\mathbf{E}_{ind}$ is an induced electric field.

Also,

$$\begin{aligned} F_3 &= \frac{C_D}{2}\int_0^{t_f}\int_0^{N_D(t)}\int_\Omega \nabla_{(x,y)}\mathbf{r}_D\cdot\nabla_{(x,y)}\mathbf{r}_D\, dx\, dy\, ds\, dt \\ &+\frac{C_T}{2}\int_0^{t_f}\int_0^{N_T(t)}\int_\Omega \nabla_{(x,y)}\mathbf{r}_T\cdot\nabla_{(x,y)}\mathbf{r}_T\, dx\, dy\, ds\, dt \\ &+\frac{C_{H_e}}{2}\int_0^{t_f}\int_0^{N_{H_e}(t)}\int_\Omega \nabla_{(x,y)}\mathbf{r}_{H_e}\cdot\nabla_{(x,y)}\mathbf{r}_{H_e}\, dx\, dy\, ds\, dt \\ &+\frac{C_N}{2}\int_0^{t_f}\int_0^{N_N(t)}\int_\Omega \nabla_{(x,y)}\mathbf{r}_N\cdot\nabla_{(x,y)}\mathbf{r}_N\, dx\, dy\, ds\, dt \\ &\frac{C_e}{2}\int_0^{t_f}\int_0^{N_e(t)}\int_\Omega \nabla_{(x,y)}\mathbf{r}_e\cdot\nabla_{(x,y)}\mathbf{r}_e\, dx\, dy\, ds\, dt, \end{aligned} \tag{107}$$

for appropriate real positive constants C_D C_T, C_{H_e}, C_N, C_e.

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Finally,

$$\begin{aligned} F_4 &= \frac{\varepsilon_D}{2}\int_0^{t_f}\left(\frac{\partial N_D(t)}{\partial t}\right)^2 dt + \frac{\varepsilon_T}{2}\int_0^{t_f}\left(\frac{\partial N_D(t)}{\partial t}\right)^2 dt \\ &+\frac{\varepsilon_N}{2}\int_0^{t_f}\left(\frac{\partial N_N(t)}{\partial t}\right)^2 dt + \frac{\varepsilon_{H_e}}{2}\int_0^{t_f}\left(\frac{\partial N_{H_e}(t)}{\partial t}\right)^2 dt \\ &+\frac{\varepsilon_e}{2}\int_0^{t_f}\left(\frac{\partial N_e(t)}{\partial t}\right)^2 dt, \end{aligned} \tag{108}$$

where ε_D, ε_T, ε_N, ε_{H_e}, ε_e are small real positive constants.

Such a functional J is subject to the following constraints:

1. The momentum conservation equation for the fluid motion

$$\rho\left(\frac{\partial u_k}{\partial t} + u_j\frac{\partial u_k}{\partial x_j}\right) = \rho f_k - \frac{\partial P}{\partial x_k} + \tau_{kj,j} + (F_E)_k + (F_M)_k,$$

$\forall k \in \{1,2,3\}$.

Here $\rho = \rho_D + \rho_T + \rho_{H_e} + \rho_N + \rho_e$ is the total density and P is the fluid pressure field.

Furthermore,

$$\tau_{ij} = \mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3}\delta_{ij}\sum_{k=1}^{3}\frac{\partial u_k}{\partial x_k}\right),$$

$\forall i,j \in \{1,2,3\}$,

$$\mathbf{F}_E = \{(F_E)_k\} = \left(K_p\left(\int_0^{N_D(t)}|\phi_p^D|^2\,ds + \int_0^{N_T(t)}|\phi_p^T|^2\,ds + \int_0^{N_{H_e}(t)}|\phi_{2p}^{H_e}|^2\,ds\right) + K_e\int_0^{N_e(t)}|\phi_e|^2\,ds\right)\mathbf{E},$$

and

$$\begin{aligned} \mathbf{F}_M &= \{(F_M)_k\} \\ &= \left(K_p\left(\int_0^{N_D(t)}|\phi_p^D|^2\left(\mathbf{u} + \frac{\partial \mathbf{r}_D}{\partial t}\right)ds\right.\right. \\ &\quad \int_0^{N_T(t)}|\phi_p^T|^2\left(\mathbf{u} + \frac{\partial \mathbf{r}_T}{\partial t}\right)ds \\ &\quad \left.+\int_0^{N_{H_e}(t)}|\phi_{2p}^{H_e}|^2\left(\mathbf{u} + \frac{\partial \mathbf{r}_{H_e}}{\partial t}\right)ds\right) \\ &\quad \left.+K_e\int_0^{N_e(t)}|\phi_e|^2\left(\mathbf{u} + \frac{\partial \mathbf{r}_e}{\partial t}\right)ds\right)\times\mathbf{B}. \end{aligned} \tag{109}$$

2. Mass conservation equation:

$$\frac{\partial \rho}{\partial t} + \operatorname{div}(\rho\mathbf{u}) = 0.$$

3. Energy equation

$$\rho\frac{De}{Dt} + P(\operatorname{div}\mathbf{u}) = \frac{\partial Q}{\partial t} - \operatorname{div}\mathbf{q},$$

where we assume the Fourier law

$$\mathbf{q} = -K\nabla T,$$

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where $T = T(x,t)$ is the scalar field of temperature.

Also,

$$\begin{aligned} e &= \frac{\rho}{2}\mathbf{u}\cdot\mathbf{u} + \frac{\rho_D}{2}\frac{\partial \mathbf{r}_D}{\partial t}\cdot\frac{\partial \mathbf{r}_D}{\partial t} \\ &+ \frac{\rho_T}{2}\frac{\partial \mathbf{r}_T}{\partial t}\cdot\frac{\partial \mathbf{r}_T}{\partial t} \\ &+ \frac{\rho_{H_e}}{2}\frac{\partial \mathbf{r}_{H_e}}{\partial t}\cdot\frac{\partial \mathbf{r}_{H_e}}{\partial t} \\ &+ \frac{\rho_N}{2}\frac{\partial \mathbf{r}_N}{\partial t}\cdot\frac{\partial \mathbf{r}_N}{\partial t} \\ &+ \frac{\rho_e}{2}\frac{\partial \mathbf{r}_e}{\partial t}\cdot\frac{\partial \mathbf{r}_e}{\partial t} \end{aligned} \tag{110}$$

and

$$\frac{De}{Dt} = \frac{\partial e}{\partial t} + u_j\frac{\partial e}{\partial x_j}.$$

4.
$$P = F_7(\rho, T),$$

for an appropriate scalar function F_7.

5. Mass relations

(a)
$$m_D(t) = \int_\Omega \rho_D(x,t)\,dx,$$

(b)
$$m_T(t) = \int_\Omega \rho_T(x,t)\,dx,$$

(c)
$$m_{He}(t) = \int_\Omega \rho_{H_e}(x,t)\,dx,$$

(d)
$$m_N(t) = \int_\Omega \rho_N(x,t)\,dx,$$

(e)
$$m_e(t) = \int_\Omega \rho_e(x,t)\,dx,$$

where,

(a)
$$(m_{H_e,N})_T(t) = m_{H_e,N}(t) + \int_0^t \int_{\partial\Omega_2} (\rho_{H_e}(x,\tau))\mathbf{u}\cdot\mathbf{n}\,dS\,d\tau,$$

(b)
$$m_{H_e,N}(t) = m_{H_e}(t) + m_N(t),$$

(c)
$$(m_D)(t) = (m_D)_0 - \int_0^t \int_{\partial\Omega_1\cup\partial\Omega_2} (\rho_D(x,\tau))\mathbf{u}\cdot\mathbf{n}\,dS\,d\tau - \alpha_D(m_{H_e,N})_T(t),$$

(d)
$$(m_T)(t) = (m_T)_0 - \int_0^t \int_{\partial\Omega_1\cup\partial\Omega_2} (\rho_T(x,\tau))\mathbf{u}\cdot\mathbf{n}\,dS\,d\tau - \alpha_T(m_{H_e,N})_T(t),$$

(e)
$$(m_{H_e})_T(t) = \int_\Omega \rho_{H_e}(x,t)\,dx + \int_0^t \int_{\partial\Omega_2} \rho_{H_e}(x,\tau)\mathbf{u}\cdot\mathbf{n}\,d\Gamma d\tau,$$

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(f)

$$(m_N)_T(t) = \int_\Omega \rho_N(x,t)\, dx + \int_0^t \int_{\partial\Omega_2} \rho_N(x,\tau)\mathbf{u}\cdot\mathbf{n}\, d\Gamma d\tau,$$

(g)

$$\frac{(m_N)_T(t)}{(m_{H_e})_T(t)} = \frac{\alpha_N}{\alpha_{H_e}},$$

so that

$$\alpha_N m_{H_e})_T(t) = \alpha_{H_e}(m_N)_T(t),$$

(h)

$$(m_e)_T(t) = m_e(t) + \int_0^t \int_{\partial\Omega_2} (\rho_T(x,\tau))\mathbf{u}\cdot\mathbf{n}\, dS\, d\tau.$$

(i)

$$\begin{aligned} m_e(t) &= \int_0^{N_D(t)} \int_\Omega |\phi_p^D(y,t,s)|^2\, dy\, dy\, ds \frac{m_e}{m_p} + \int_0^{N_T(t)} \int_\Omega |\phi_p^T(y,t,s)|^2\, dy\, ds \frac{m_e}{m_p} \\ &+ \int_0^{N_p(t)} \int_\Omega |\phi_{2p}^{H_e}(y,t,s)|^2\, dy\, ds \frac{m_e}{m_p}. \end{aligned} \tag{111}$$

6. Other mass constraints

(a)

$$\int_\Omega |\phi_N^D(x,y,t,s)|^2\, dx = m_N,$$

(b)

$$\int_\Omega |\phi_{N_1}^T(x,y,t,s)|^2\, dx = m_N,$$

(c)

$$\int_\Omega |\phi_{N_2}^T(x,y,t,s)|^2\, dx = m_N,$$

(d)

$$\int_\Omega |\phi_{N_1}^{H_e}(x,y,t,s)|^2\, dx = m_N,$$

(e)

$$\int_\Omega |\phi_{N_2}^{H_e}(x,y,t,s)|^2\, dx = m_N,$$

(f)

$$\int_\Omega |\phi_p^D(x,t,s)|^2\, dx = m_p,$$

(g)

$$\int_\Omega |\phi_p^T(x,t,s)|^2\, dx = m_p,$$

(h)

$$\int_\Omega |\phi_{2p}^{H_e}(x,t,s)|^2\, dx = 2\, m_p,$$

7.

$$m_D(t) = m_p\, N_D(t) + m_N\, N_D(t)$$

$$m_T(t) = m_p\, N_T(t) + m_N\, N_T(t),$$

$$m_{H_e}(t) = 2m_p\, N_{H_e}(t) + 2m_N\, N_{H_e}(t),$$

$$m_e(t) = m_e\, N_D(t) + m_e\, N_T(t) + 2\, m_e\, N_{H_e}(t).$$

8. For the induced electric field, we must have

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$$
\begin{aligned}
&\text{curl } \mathbf{E}_{ind} + \frac{1}{c} \text{ curl } \left(\hat{K}_p \int_0^{N_D(t)} |\phi_p^D|^2 \left(\mathbf{u} + \frac{\partial \mathbf{r}_D}{\partial t} \right) \, ds \right. \\
&+ \hat{K}_p \int_0^{N_T(t)} |\phi_p^T|^2 \left(\mathbf{u} + \frac{\partial \mathbf{r}_T}{\partial t} \right) \, ds \\
&+ \hat{K}_p \int_0^{N_{H_e}(t)} |\phi_{2p}^{H_e}|^2 \left(\mathbf{u} + \frac{\partial \mathbf{r}_{H_e}}{\partial t} \right) \, ds \\
&\left. + \hat{K}_e \int_0^{N_e(t)} \int_\Omega |\phi_e(x,y,t,s)|^2 \left(\mathbf{u}(y,t) + \frac{\partial \mathbf{r}_e(x,y,t)}{\partial t} \, dx \right) \, ds \right) \\
&\times (\text{ curl } \mathbf{A} - \mathbf{B}_0) - \frac{1}{c} \frac{\partial}{\partial t} (\text{ curl } \mathbf{A} - \mathbf{B}_0) = \mathbf{0}, \qquad (112)
\end{aligned}
$$

where $\hat{K}_p$ and $\hat{K}_e$ are appropriate real constants related to the respective charges.

9. A Maxwell equation:

$$\text{div } \mathbf{B} = 0,$$

where

$$\mathbf{B} = \mathbf{B}_0 - \text{ curl } \mathbf{A}.$$

10. Another Maxwell equation:

$$
\begin{aligned}
\text{div } \mathbf{E} \quad = \quad & 4\pi \left(K_p \left(\int_0^{N_D(t)} |\phi_p^D|^2 \, ds + \int_0^{N_T(t)} |\phi_p^T|^2 \, ds + \int_0^{N_{H_e}(t)} |\phi_{2p}^{H_e}|^2 \, ds \right) \right. \\
& \left. + K_e \int_0^{N_e(t)} \int_\Omega |\phi_e(x,y,t,s)|^2 \, dx \, ds \right), \qquad (113)
\end{aligned}
$$

where the total electric field $\mathbf{E}$ stands for

$$\mathbf{E} = \mathbf{E}_{ind} + \mathbf{E}_\rho,$$

and where generically denoting

$$F(\phi) = \int_\Omega f_5(\phi, x, t\xi, s) \, dx \, d\xi \, ds,$$

we have also

$$\mathbf{E}_\rho = \left\{ \int_\Omega \frac{\partial f_5(\phi, x, t, \xi, s)}{\partial x_k} \, d\xi \, ds \right\}.$$

At this point we generically denote

$$\langle h_1, h_2 \rangle_{L^2} = \int_0^{t_f} \int_\Omega h_1 \, h_2 \, dx \, dy \, dt.$$

Thus, already including the Lagrange multipliers concerning the restrictions indicated, the extended functional J_3 stands for

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$$
\begin{aligned}
& J_3 = J_3(\phi, \mathbf{u}, \mathbf{r}, P, \mathbf{A}, \mathbf{B}, \mathbf{E}, \Lambda, E, \{N_D, N_T, N_{H_e}, N_N, N_e\}) \\
= \; & G(\nabla\phi) + F(\phi) + E_c(\phi, \mathbf{r}) + F_1 + F_2 + F_3 + F_4 \\
& + \left\langle \Lambda_k, \rho \left(\frac{\partial u_k}{\partial t} + u_j \frac{\partial u_k}{\partial x_j} \right) - \rho f_k + \frac{\partial P}{\partial x_k} - \tau_{kj,j} - (F_E)_k - (F_M)_k \right\rangle_{L^2} \\
& + \left\langle \Lambda_4, \; \frac{\partial \rho}{\partial t} + \text{ div } (\rho \mathbf{u}) \right\rangle_{L^2} + J_{Aux_1} + J_{Aux_2} + J_{Aux_3} + J_{Aux_4} + J_{Aux_5},
\end{aligned} \tag{114}
$$

where,

$$
\begin{aligned}
J_{Aux_1} \; = \; & \left\langle \Lambda_5, \; \rho \frac{De}{Dt} + P(\text{ div } \mathbf{u}) - \frac{\partial Q}{\partial t} + \text{ div } \mathbf{q} \right\rangle_{L^2} \\
& + \langle \Lambda_6, \; P - F_7(\rho, T) \rangle_{L^2},
\end{aligned} \tag{115}
$$

$$
\begin{aligned}
J_{Aux_2} \; = \; & \left\langle \Lambda_7, m_D(t) - \int_\Omega \rho_D(x,t) \, dx \right\rangle_{L^2} \\
& + \left\langle \Lambda_8, m_T(t) - \int_\Omega \rho_T(x,t) \, dx \right\rangle_{L^2} \\
& \left\langle \Lambda_9, m_{H_e}(t) - \int_\Omega \rho_{H_e}(x,t) \, dx \right\rangle_{L^2} \\
& \left\langle \Lambda_{10}, m_N(t) - \int_\Omega \rho_N(x,t) \, dx \right\rangle_{L^2} \\
& \left\langle \Lambda_{11}, m_e(t) - \int_\Omega \rho_e(x,t) \, dx \right\rangle_{L^2} \\
& \int_0^{t_f} E_{12}(t)(\alpha_N m_{H_e})_T(t) - \alpha_{H_e}(m_N)_T(t)) \, dt,
\end{aligned} \tag{116}
$$

$$
\begin{aligned}
J_{Aux_3} \; = \; & - \int_0^{t_f} \int_\Omega (E_N^D)_5(y,t,s) \left(\int_\Omega |\phi_N^D(x,y,t,s)|^2 \, dx - m_N \right) \, dy \, dt \\
& - \int_0^{t_f} \int_\Omega (E_{N_1}^T)_6(y,t,s) \left(\int_\Omega |\phi_{N_1}^T(x,y,t,s)|^2 \, dx - m_N \right) \, dy \, dt \\
& - \int_0^{t_f} \int_\Omega (E_{N_2}^T)_7(y,t,s) \left(\int_\Omega |\phi_{N_2}^T(x,y,t,s)|^2 \, dx - m_N \right) \, dy \, dt \\
& - \int_0^{t_f} \int_\Omega (E_{N_1}^{H_e})_8(y,t,s) \left(\int_\Omega |\phi_{N_1}^{H_e}(x,y,t,s)|^2 \, dx - m_N \right) \, dy \, dt \\
& - \int_0^{t_f} \int_\Omega (E_{N_2}^{H_e})_9(y,t,s) \left(\int_\Omega |\phi_{N_2}^{H_e}(x,y,t,s)|^2 \, dx - m_N \right) \, dy \, dt, \\
& - \int_0^{t_f} \int_\Omega (E_p^D)(t,s) \left(\int_\Omega |\phi_p^D(y,t,s)|^2 \, dy - m_p \right) \, ds \, dt, \\
& - \int_0^{t_f} \int_\Omega (E_p^T)(t,s) \left(\int_\Omega |\phi_p^T(y,t,s)|^2 \, dy - m_p \right) \, ds \, dt, \\
& - \int_0^{t_f} \int_\Omega (E_{2p}^{H_e})(t,s) \left(\int_\Omega |\phi_{2p}^{H_e}(y,t,s)|^2 \, dy - 2m_p \right) \, ds \, dt,
\end{aligned} \tag{117}
$$

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$$
\begin{aligned}
J_{Aux_4} \;=\; & \langle \Lambda_{12},\ \text{curl}\ \mathbf{E}_{ind} \\
& + \frac{1}{c}\ \text{curl}\ \left(\hat{K}_p \int_0^{N_D(t)} |\phi_p^D|^2 \left(\mathbf{u} + \frac{\partial \mathbf{r}_D}{\partial t} \right)\ ds \right. \\
& + \hat{K}_p \int_0^{N_T(t)} |\phi_p^T|^2 \left(\mathbf{u} + \frac{\partial \mathbf{r}_T}{\partial t} \right)\ ds \\
& + \hat{K}_p \int_0^{N_{H_e}(t)} |\phi_{2p}^{H_e}|^2 \left(\mathbf{u} + \frac{\partial \mathbf{r}_{H_e}}{\partial t} \right)\ ds \\
& \left. + \hat{K}_e \int_0^{N_e(t)} \int_\Omega |\phi_e(x,y,t,s)|^2 \left(\mathbf{u}(y,t) + \frac{\partial \mathbf{r}_e(x,y,t,s)}{\partial t}\ dx \right)\ ds \right) \\
& \times (\ \text{curl}\ \mathbf{A} - \mathbf{B}_0) - \frac{1}{c}\frac{\partial}{\partial t}(\ \text{curl}\ \mathbf{A} - \mathbf{B}_0) \Big\rangle_{L^2} \\
& + \langle \Lambda_{13},\ \text{div}\ \mathbf{B} \rangle_{L^2} \\
& + \Big\langle \Lambda_{14},\ \text{div}\ \mathbf{E} - 4\pi \left(K_p \left(\int_0^{N_D(t)} |\phi_p^D|^2\ ds + \int_0^{N_T(t)} |\phi_p^T|^2\ ds + \int_0^{N_{H_e}(t)} |\phi_{2p}^{H_e}|^2\ ds \right) \right. \\
& \left. + K_e \int_\Omega |\phi_e|^2\ dx\ ds \right) \Big\rangle_{L^2}. \qquad (118)
\end{aligned}
$$

$$
\begin{aligned}
J_{Aux_5} \;=\; & \langle \Lambda_{15},\ m_D(t) - (m_p\ N_D(t) + m_N\ N_D(t)) \rangle_{L^2} \\
& + \langle \Lambda_{16},\ m_T(t) - (m_p\ N_T(t) + m_N\ N_T(t)) \rangle_{L^2} \\
& + \langle \Lambda_{17},\ m_{H_e}(t) - (2m_p\ N_{H_e}(t) + 2m_N\ N_{H_e}(t)) \rangle_{L^2} \\
& + \langle \Lambda_{18},\ m_e(t) - (m_e\ N_D(t) + m_e\ N_T(t) + 2\ m_e\ N_{H_e}(t)) \rangle_{L^2}. \qquad (119)
\end{aligned}
$$

Here we recall the following definitions and relations:

1. For the Deuterium field

$$|\phi_D(x,y,t,s)|^2 = |\phi_p^D(y,t,s)|^2 + |\phi_N^D(x,y,t,s)|^2 |\phi_p^D(y,t,s)|^2 \frac{1}{m_p},$$

2. For the Tritium field

$$|\phi_T(x,y,t,s)|^2 = |\phi_p^T(y,t,s)|^2 + (|\phi_{N_1}^T(x,y,t,s)|^2 + |\phi_{N_2}^T(x,y,t,s)|^2) |\phi_p^D(y,t,s)|^2 \frac{1}{m_p},$$

3. For the Helium field

$$|\phi_{H_e}(x,y,t,s)|^2 = |\phi_{2p}^{H_e}(y,t,s)|^2 + (|\phi_{N_1}^{H_e}(x,y,t,s)|^2 + |\phi_{N_2}^{H_e}(x,y,t,s)|^2) |\phi_{2p}^{H_e}(y,t,s)|^2 \frac{1}{2\ m_p},$$

4. For the Neutron field

$$\phi_N = \phi_N(x,t,s),$$

5. For the electronic field resulting from the ionization

$$\phi_e = \phi_e(x,y,t,s).$$

1.

$$\rho_D(y,t) = \int_0^{N_D(t)} \int_\Omega |\phi_D(x,y,t,s)|^2\ dx\ ds,$$

2.

$$\rho_T(y,t) = \int_0^{N_T(t)} \int_\Omega |\phi_T(x,y,t,s)|^2\ dx\ ds,$$

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$$\rho_{H_e}(y,t) = \int_0^{N_{H_e}(t)} \int_\Omega |\phi_{H_e}(x,y,t,s)|^2 \, dx \, ds,$$

$$\rho_N(x,t) = \int_0^{N_N(t)} |\phi_N(x,t,s)|^2 \, ds,$$

$$\rho_e(y,t) = \int_0^{N_e(t)} \int_\Omega |\phi_e(x,y,t,s)|^2 \, dx \, ds.$$

Also,

$$\rho = \rho_D + \rho_T + \rho_{H_e} + \rho_N + \rho_e,$$

1.
$$(m_{H_e,N})_T(t) = m_{H_e,N}(t) + \int_0^t \int_{\partial\Omega_2} (\rho_{H_e}(x,\tau) + \rho_N(x,\tau))\mathbf{u}\cdot\mathbf{n} \, dS \, d\tau,$$

2.
$$m_{H_e,N}(t) = m_{H_e}(t) + m_N(t),$$

3.
$$m_{H_e}(t) = \int_\Omega \rho_{H_e}(x,t) \, dx,$$

4.
$$m_N(t) = \int_\Omega \rho_N(x,t) \, dx,$$

5.
$$(m_D)(t) = (m_D)_0 - \int_0^t \int_{\partial\Omega_1\cup\partial\Omega_2} (\rho_D(x,\tau))\mathbf{u}\cdot\mathbf{n} \, dS \, d\tau - \alpha_D (m_{H_e,N})_T(t),$$

6.
$$(m_T)(t) = (m_T)_0 - \int_0^t \int_{\partial\Omega_1\cup\partial\Omega_2} (\rho_T(x,\tau))\mathbf{u}\cdot\mathbf{n} \, dS \, d\tau - \alpha_T (m_{H_e,N})_T(t),$$

7.
$$(m_{H_e})_T(t) = \int_\Omega \rho_{H_e}(x,t) \, dx + \int_0^t \int_{\partial\Omega_2} \rho_{H_e}(x,\tau)\mathbf{u}\cdot\mathbf{n} \, d\Gamma d\tau,$$

8.
$$(m_N)_T(t) = \int_\Omega \rho_N(x,t) \, dx + \int_0^t \int_{\partial\Omega_2} \rho_N(x,\tau)\mathbf{u}\cdot\mathbf{n} \, d\Gamma d\tau,$$

9.
$$\frac{(m_N)_T(t)}{(m_{H_e})_T(t)} = \frac{\alpha_N}{\alpha_{H_e}},$$

so that

$$\alpha_N (m_{H_e})_T(t) = \alpha_{H_e} (m_N)_T(t),$$

10.
$$(m_e)_T(t) = m_e(t) - \int_0^t \int_{\partial\Omega_2} (\rho_e(x,\tau))\mathbf{u}\cdot\mathbf{n} \, d\Gamma \, d\tau,$$

11.
$$m_e(t) = \int_\Omega \rho_e(x,t) \, dx.$$

12.
$$\begin{aligned} m_e(t) \quad = \quad & \int_0^{N_D(t)} \int_\Omega |\phi_p^D(y,t,s)|^2 \, dy \, dy \, ds \frac{m_e}{m_p} + \int_0^{N_T(t)} \int_\Omega |\phi_p^T(y,t,s)|^2 \, dy \, ds \frac{m_e}{m_p} \\ & + \int_0^{N_p(t)} \int_\Omega |\phi_{2p}^{H_e}(y,t,s)|^2 \, dy \, ds \frac{m_e}{m_p}. \end{aligned} \tag{120}$$

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Finally,

$$\mathbf{E} = \mathbf{E}_{ind} + \mathbf{E}_{\rho},$$

and where generically denoting

$$F(\phi) = \int_{\Omega} f_5(\phi, x, t, \xi, s)\, dx\, d\xi\, ds,$$

we have also

$$\mathbf{E}_{\rho} = \left\{ \int_{\Omega} \frac{\partial f_5(\phi, x, t, \xi, s)}{\partial x_k}\, d\xi\, ds \right\}.$$

and,

$$\mathbf{B} = \mathbf{B}_0 - \text{ curl } \mathbf{A}.$$

21. A qualitative modeling for a general phase transition process

In this section we develop a general qualitative modeling for a phase transition process.

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

Such a set Ω is supposed to a be a fixed volume in which an amount of mass of a substance A with a density function u will develop phase a transition for another phase with corresponding density function v. The total mass m_T is suppose to be kept constant throughout such a process.

We model such transition in phase through a functional $J : V \times V \to \mathbb{R}$ where

$$\begin{aligned} J(u,v) \quad = \quad & \frac{\gamma_1}{2} \int_{\Omega} \nabla u \cdot \nabla u\, dx + \frac{\alpha_1}{2} \int_{\Omega} u^4\, dx \\ & \frac{\gamma_2}{2} \int_{\Omega} \nabla v \cdot \nabla v\, dx + \frac{\alpha_2}{2} \int_{\Omega} v^4\, dx \\ & -\frac{1}{2} \int_{\Omega} \omega^2 (u^2 + v^2)\, dx - \frac{E}{2} \left(\int_{\Omega} (u^2 + v^2)\, dx - m_T \right). \end{aligned} \tag{121}$$

Here $\gamma_1 > 0,\ \gamma_2 > 0,\ \alpha_1 > 0,\ \alpha_2 > 0$ and $V = W^{1,2}(\Omega)$.

The phases corresponding to u and v are connected through a Lagrange multiplier E, which represents the chemical potential of the chemical process in question.

We assume the temperature is directly proportional to the internal kinetics E_C energy where

$$E_C = \frac{1}{2} \int_{\Omega} u^2 \frac{\partial \mathbf{r}_u}{\partial t} \cdot \frac{\partial \mathbf{r}_u}{\partial t}\, dx.$$

For a internal vibrational motion, we assume approximately

$$\mathbf{r}_u \approx e^{i\omega t} \mathbf{w}_5(x),$$

for an appropriate frequency ω and vectorial function $\mathbf{w}_5$.

Thus, the temperature $T = T(x,t)$ is indeed proportional to ω^2, that is, symbolically, we may write

$$T \propto E_1 \propto \omega^2.$$

Therefore, we start with the system with a phase corresponding to $u \approx 1$ and $v \approx 0$ at $\omega = 1$. Gradually increasing the temperature to a corresponding $\omega = 15$, we obtain a transition to a phase corresponding to $u \approx 0$ and $v \approx 1$.

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At this point, we also define the index normalized corresponding densities

$$\phi_u = \frac{u^2}{u^2 + v^2}$$

and

$$\phi_v = \frac{v^2}{u^2 + v^2}.$$

Finally, we have obtained some numerical results for the following parameters: $\Omega = [0, 1] \subset \mathbb{R}$, $\gamma_1 = \gamma_2 = 1$, $\alpha = 0.1$, $\alpha_2 = 10^3$.

1. We start with $\omega = 1$ corresponding to $\phi_u \approx 1$ and $\phi_v \approx 0$ in Ω.

   For the corresponding solutions ϕ_u and ϕ_v, please see Figures 15 and 16, respectively.
2. We end the process with $\omega = 15$ corresponding to $\phi_u \approx 0$ and $\phi_v \approx 1$ in Ω.

   For the corresponding solutions ϕ_u and ϕ_v, please see Figures 17 and 18, respectively.

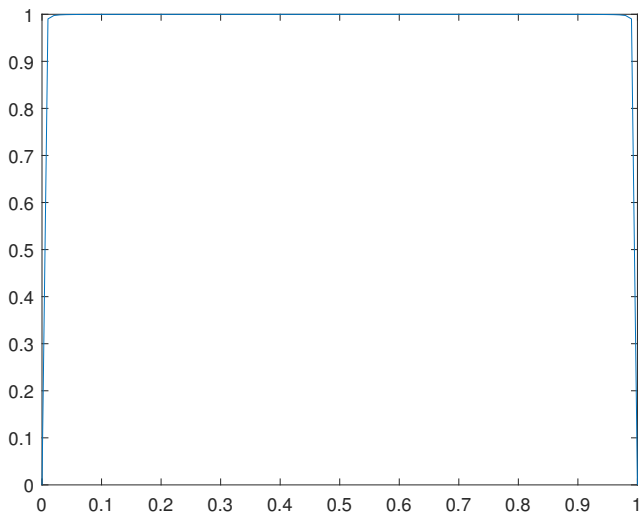

Figure 15. Solution $\phi_u(x)$ for $\omega = 1$.

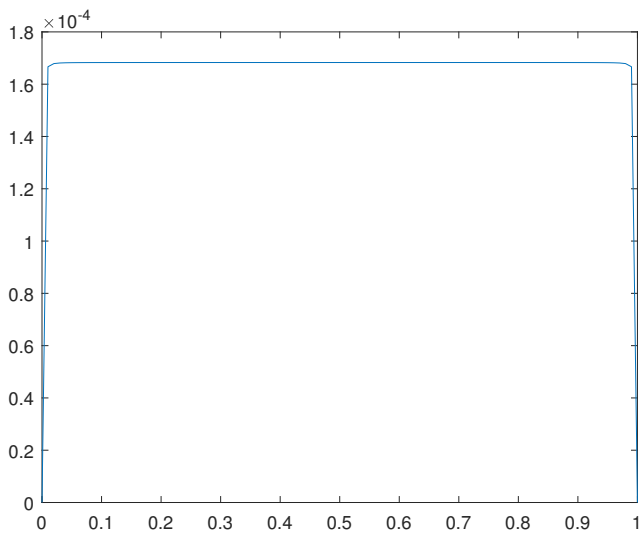

Figure 16. Solution $\phi_v(x)$ for $\omega = 1$.

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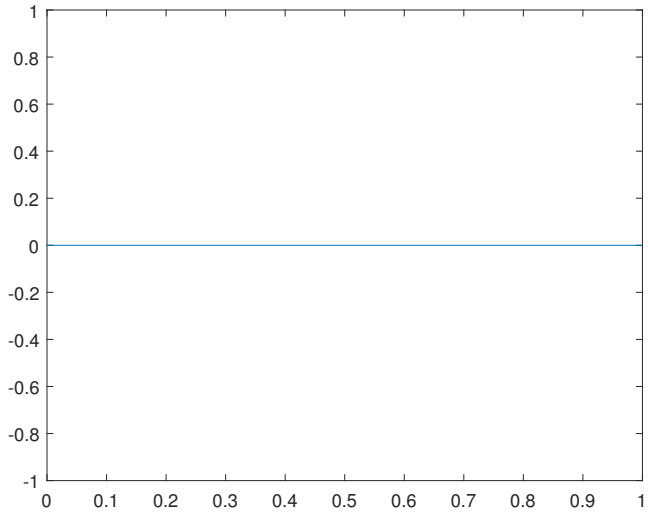

Figure 17. Solution $\phi_u(x)$ for $\omega = 15$.

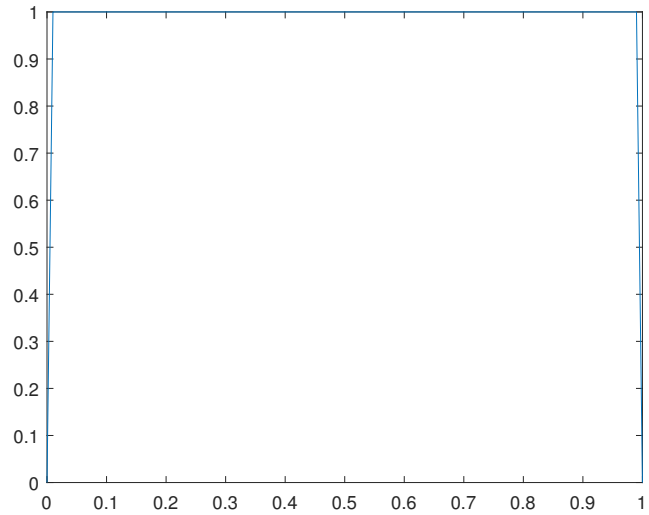

Figure 18. Solution $\phi_v(x)$ for $\omega = 15$.

22. A mathematical description of a hydrogen molecule in a quantum mechanics context

In this section we develop a mathematical description for a hydrogen molecule.

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

Observe that a single hydrogen molecule comprises two hydrogen atoms physically linked through their electrons.

We recall that each hydrogen atom comprises one proton, one neutron and one electron.

Since the electric charge interaction effects are much higher than those related to the respective masses, in a first analysis we neglect the single neutron densities.

Denoting $(x, y, z) \in \Omega \times \Omega \times \Omega$ and time $t \in [0, t_f]$, generically, for a particle p_{jkl} at the atom A_{kl} in the molecule M_l, we define the following general density:

$$|\phi_{(p_{jkl})_T}(x, y, z, t)|^2 = \frac{|\phi_{p_{jkl}}(x, y, z, t)|^2 |\phi_{A_{kl}}(y, z, t)|^2 |\phi_{M_l}(z, t)|^2}{m_{A_{jk}} m_{M_l}}.$$

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Here we have the particle density $|\phi_{p_{jkl}}(x,y,z,t)|^2$ in the atom A_{kl} with density $|\phi_{A_{kl}}(y,z,t)|^2$, at the molecule M_l with a global density $|\phi_{M_l}(z,t)|^2$.

Here we have also denoted, $m_{p_{jkl}}$ the particle mass, $m_{A_{kl}}$ the mass of atom A_{kl} and m_{M_l} the mass of molecule M_l, so that we set the following constraints:

1. $$\int_\Omega |\phi_{p_{jkl}}(x,y,z,t)|^2\, dx = m_{p_{jkl}},$$
2. $$\int_\Omega |\phi_{A_{kl}}(y,z,t)|^2\, dy = m_{A_{kl}},$$
3. $$\int_\Omega |\phi_{M_l}(z,t)|^2\, dz = m_{M_l}.$$

At this point we denote for the atoms A_1 e A_2 of a hydrogen molecule:

1. $m_{e_j} = m_e$: mass of electron e_j in the atom A_j, where $j \in \{1,2\}$.
2. $m_{p_j} = m_p$: mass of proton p_j in the atom A_j, where $j \in \{1,2\}$.

Therefore, considering the respective indexed densities for the particles in question, we define the total hydrogen molecule density, denoted by $|\phi_{H_2}(x,y,z,t)|^2$ as

$$\begin{aligned} |\phi_{H_2}(x,y,z,t)|^2 \quad = \quad & \frac{|\phi_{p_1}(x,y,z,t)|^2|\phi_{A_1}(y,z,t)|^2|\phi_M(z,t)|^2}{m_{A_1}m_M} \\ & + \frac{|\phi_{e_1}(x,y,z,t)|^2|\phi_{A_1}(y,z,t)|^2|\phi_M(z,t)|^2}{m_{A_1}m_M} \\ & + \frac{|\phi_{p_2}(x,y,z,t)|^2|\phi_{A_2}(y,z,t)|^2|\phi_M(z,t)|^2}{m_{A_2}m_M} \\ & + \frac{|\phi_{e_2}(x,y,z,t)|^2|\phi_{A_2}(y,z,t)|^2|\phi_M(z,t)|^2}{m_{A_2}m_M}. \end{aligned} \tag{122}$$

Such system is subject to the following constraints:

1. From the proton p_1 in the atom A_1:
$$\int_\Omega |\phi_{p_1}(x,y,z,t)|^2\, dx = m_p,$$
2. For the proton p_2 in the atom A_2:
$$\int_\Omega |\phi_{p_2}(x,y,z,t)|^2\, dx = m_p,$$
3. For the atom A_1:
$$\int_\Omega |\phi_{A_1}(y,z,t)|^2\, dy = m_{A_1},$$
4. For the atom A_2:
$$\int_\Omega |\phi_{A_2}(y,z,t)|^2\, dy = m_{A_2},$$
5. For the electrons e_1 and e_2, concerning the physical electronic link between the atoms:
$$\int_\Omega |\phi_{e_1}(x,y,z,t)|^2\, dx + \int_\Omega |\phi_{e_2}(x,y,z,t)|^2\, dx = 2m_e.$$

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6. For the total molecular density:

$$\int_\Omega |\phi_M(z,t)|^2\, dz = m_M.$$

Therefore, already including the Lagrange multipliers, the corresponding variational formulation for such a system stands for $J : V \to \mathbb{R}$, where

$$J(\phi, E) = G(\nabla\phi) + F(\phi) + J_{Aux}(\phi, E).$$

Here we denote

$$|(\phi_{p_j})_T|^2 = \frac{|\phi_{p_j}(x,y,z,t)|^2 |\phi_{A_j}(y,z,t)|^2 |\phi_M(z,t)|^2}{m_{A_j} m_M},$$

$$|(\phi_{e_j})_T|^2 = \frac{|\phi_{e_j}(x,y,z,t)|^2 |\phi_{A_j}(y,z,t)|^2 |\phi_M(z,t)|^2}{m_{A_j} m_M}, \ \forall j \in \{1,2\}$$

we assume $\gamma_{(p_j)} > 0,\ \gamma_{e_j} > 0,\ \gamma_{A_j} > 0,\ \gamma_M > 0,\ \alpha_{(p_j)_T} > 0,\ \alpha_{(e_j)_T} > 0\ \alpha_{(p_j\, e_k)_T} < 0,\ \forall j,k \in \{1,2\}$,

$$\begin{aligned} G(\nabla\phi) \quad = \quad & \frac{\gamma_{p_j}}{2} \int_0^{t_f} \int_\Omega (\nabla\phi_{p_j}) \cdot (\nabla\phi_{p_j})\, dx\, dy\, dz\, dt \\ & + \frac{\gamma_{e_j}}{2} \int_0^{t_f} \int_\Omega (\nabla\phi_{e_j}) \cdot (\nabla\phi_{e_j})\, dx\, dy\, dz\, dt \\ & \frac{\gamma_{A_j}}{2} \int_\Omega (\nabla\phi_{A_j}) \cdot (\nabla\phi_{A_j})\, dy\, dz\, dt \\ & + \frac{\gamma_M}{2} \int_0^{t_f} \int_\Omega (\nabla\phi_M) \cdot (\nabla\phi_M)\, dz\, dt \end{aligned} \tag{123}$$

and

$$\begin{aligned} & F(\phi) = \\ & \frac{\alpha_{(p_j)_T}}{2} \int_0^{t_f} \int_\Omega \frac{|\phi_{(p_j)_T}(x-\xi_1, y-\xi_2, z-\xi_3, t)|^2 |\phi_{(p_j)_T}(\xi_1,\xi_2,\xi_3,t)|^2}{|(x,y,z) - (\xi_1,\xi_2,\xi_3)|}\, dx\, dy\, dz; d\xi_1\, d\xi_2\, d\xi_3\, dt \\ & + \frac{\alpha_{(e_j)_T}}{2} \int_0^{t_f} \int_\Omega \frac{|\phi_{(e_j)_T}(x-\xi_1, y-\xi_2, z-\xi_3, t)|^2 |\phi_{(e_j)_T}(\xi_1,\xi_2,\xi_3,t)|^2}{|(x,y,z) - (\xi_1,\xi_2,\xi_3)|}\, dx\, dy\, dz\, d\xi_1\, d\xi_2\, d\xi_3\, dt \\ & + \frac{\alpha_{(p_j\, e_k)_T}}{2} \int_0^{t_f} \int_\Omega \frac{|\phi_{(p_j)_T}(x-\xi_1, y-\xi_2, z-\xi_3, t)|^2 |\phi_{(e_k)_T}(\xi_1,\xi_2,\xi_3,t)|^2}{|(x,y,z) - (\xi_1,\xi_2,\xi_3)|}\, dx\, dy\, dz\, d\xi_1\, d\xi_2\, d\xi_3\, dt \end{aligned}$$

Finally,

$$\begin{aligned} J_{Aux}(\phi, E) \quad = \quad & \int_0^{t_f} \int_\Omega (E_p)_j(y,z,t) \left(\int_\Omega |\phi_{p_j}(x,y,z,t)|^2\, dx - m_p \right) dy\, dz\, dt \\ & \int_0^{t_f} \int_\Omega (E_e)(y,z,t) \left(\int_\Omega (|\phi_{e_1}(x,y,z,t)|^2 + |\phi_{e_2}(x,y,z,t)|^2)\, dx - 2m_e \right) dy\, dz\, dt \\ & \int_0^{t_f} \int_\Omega (E_A)_j(z,t) \left(\int_\Omega |\phi_{A_j}(y,z,t)|^2\, dy - m_{A_j} \right) dz\, dt \\ & \int_0^{t_f} (E_M)(t) \left(\int_\Omega |\phi_M(z,t)|^2\, dz - m_M \right) dt. \end{aligned} \tag{124}$$

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Remark 22.1. *We highlight the two electrons which link the atoms are at same level of energy E_e. Morever, each atom has its energy level E_{A_j} and the molecule as a whole has also its energy level E_M.*

23. A mathematical model for the water hydrolysis

In this section we develop a modeling for a chemical reaction known as the water hydrolysis.

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

In such a volume Ω containing a total mass m_T of water initially at the temperature 25 C with pressure 1 atm, we intend to model the following reaction

$$H_2O \rightleftharpoons OH^- + H^+$$

which as previously mentioned is the well known water hydrolysis.

We highlight H_2O stand for a water molecule which subject to an appropriate electric potential is decomposed into a ionized OH^- molecule and ionized H^+ atom.

It is also well known that the water symbol H_2O corresponds to a molecule with two hydrogen (H) atoms and one oxygen (O) atom.

Moreover, the oxygen atom O has 8 protons, 8 neutrons and 8 electrons whereas the hydrogen atom H has one proton, one neutron and one electron.

Remark 23.1. *Here we have assumed that a unit mass of H_2O reacts into a fractional mass α_B of OH^- and a fractional mass α_C of H^+.*

Symbolically, we have:

$$1 = \alpha_B + \alpha_C.$$

To clarify the notation we set the conventions:

1. H_2O molecule generically corresponds to wave function ϕ_1.
2. OH^- molecule corresponds to wave function ϕ_2.
3. H^+ hydrogen atom corresponds to wave function ϕ_3.

At this point we define the following densities:

1. For the H_2O water density (for charges), denoted by $|\phi_1|^2$, we have

$$\begin{aligned}
|\phi_1(x,y,z,t)|^2 \quad = \quad & K_p \sum_{j=1}^{2} |(\phi_1^H)_{p_j}(x,y,z,t)|^2 \frac{|(\phi_1^H)_{A_j}(y,z,t)|^2 |(\phi_1)_M(z,t)|^2}{(m)_{A_j}^H \ (m_1)_M} \\
& + K_e \sum_{j=1}^{2} |(\phi_1^H)_{e_j}(x,y,z,t)|^2 \frac{|(\phi_1^H)_{A_j}(y,z,t)|^2 |(\phi_1)_M(z,t)|^2}{(m_1)_{A_j}^H \ (m_1)_M} \\
& + K_p \sum_{j=1}^{8} |(\phi_1^O)_{p_j}(x,y,z,t)|^2 \frac{|(\phi_1^O)_A(y,z,t)|^2 |(\phi_1)_M(z,t)|^2}{(m)_A^O \ (m_1)_M} \\
& + K_e \sum_{j=1}^{8} |(\phi_1^O)_{e_j}(x,y,z,t)|^2 \frac{|(\phi_1^O)_A(y,z,t)|^2 |(\phi_1)_M(z,t)|^2}{(m)_A^O \ (m_1)_M}
\end{aligned} \tag{125}$$

where $(m_1)_M$ is the mass of a single water molecule and generically $|(\phi_1^H)_{p_j}(x,y,z,t)|^2$ refers to the hydrogen proton p_j at the hydrogen atom A_j concerning the H_2O molecular density and so on.

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2. For the OH^- density, denoted by $|\phi_2|^2$, we have

$$\begin{aligned}
|\phi_2(x,y,z,t)|^2 &= K_p|(\phi_2^H)_p(x,y,z,t)|^2\frac{|(\phi_2^H)_A(y,z,t)|^2|(\phi_2)_M(z,t)|^2}{(m)_A^H\ (m_2)_M}\\
&+K_e|(\phi_2^H)_{e_1}(x,y,z,t)|^2\frac{|(\phi_2^H)_A(y,z,t)|^2|(\phi_2)_M(z,t)|^2}{(m)_A^H\ (m_2)_M}\\
&+K_e|(\phi_2^{OH^-})_{e_2}(x,z,t)|^2\frac{|(\phi_2)_M(z,t)|^2}{(m_2)_M}\\
&+K_p\sum_{j=1}^{8}|(\phi_2^O)_{p_j}(x,y,z,t)|^2\frac{|(\phi_2^O)_A(y,z,t)|^2|(\phi_2)_M(z,t)|^2}{(m)_A^O\ (m_2)_M}\\
&+K_e\sum_{j=1}^{8}|(\phi_2^O)_{e_j}(x,y,z,t)|^2\frac{|(\phi_2^O)_A(y,z,t)|^2|(\phi_2)_M(z,t)|^2}{(m)_A^O\ (m_2)_M},
\end{aligned} \tag{126}$$

where $(m_2)_M$ is the mass of a single molecule of OH^-.

3. For the ionized hydrogen atom have

$$|\phi_3(x,y,t)|^2 = K_p|(\phi_3^H)_p(x,y,t)|^2\frac{|(\phi_3^H)_A(y,t)|^2}{(m_3)_A}.$$

where we have denoted $(m_3)_A$ is the mass of a single atom of H^+.

Here $K_p > 0$ and $K_e < 0$ are appropriate real constants concerning a proton and an electron charge, respectively.

The system is subject to the following constraints:

1. $$\int_\Omega |(\phi_1^H)_{p_j}(x,y,z,t)|^2\,dx = m_p,\ \forall j \in \{1,2\},$$
2. $$\int_\Omega |(\phi_1^H)_{e_j}(x,y,z,t)|^2\,dx = m_e,\ \forall j \in \{1,2\},$$
3. $$\int_\Omega |(\phi_1^O)_{p_j}(x,y,z,t)|^2\,dx = m_p,\ \forall j \in \{1,8\},$$
4. $$\int_\Omega |(\phi_1^O)_{e_j}(x,y,z,t)|^2\,dx = m_e,\ \forall j \in \{1,8\},$$
5. $$\int_\Omega |(\phi_2^H)_p(x,y,z,t)|^2\,dx = m_p,$$
6. $$\int_\Omega |(\phi_2^H)_{e_1}(x,y,z,t)|^2\,dx = m_e,$$
7. $$\int_\Omega |(\phi_2^H)_{e_2}(x,y,z,t)|^2\,dx = m_e,$$
8. $$\int_\Omega |(\phi_2^O)_{p_j}(x,y,z,t)|^2\,dx = m_p,\ \forall j \in \{1,8\},$$
9. $$\int_\Omega |(\phi_2^O)_{e_j}(x,y,z,t)|^2\,dx = m_e,\ \forall j \in \{1,8\},$$
10. $$\int_\Omega |(\phi_3^H)_p(x,z,t)|^2\,dx = m_p,$$

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11.
$$\int_\Omega |(\phi_1^H)_{A_j}(y,z,t)|^2\, dy = m_A^H, \forall j \in \{1,2\},$$

12.
$$\int_\Omega |(\phi_1^O)_A(y,z,t)|^2\, dy = m_A^O,$$

13.
$$\int_\Omega |(\phi_2^H)_A(y,z,t)|^2\, dy = m_A^H,$$

14.
$$\int_\Omega |(\phi_2^O)_A(y,z,t)|^2\, dy = m_A^O,$$

15.
$$\int_\Omega |(\phi_3^H)_A(y,z,t)|^2\, dy = m_A^H,$$

16.
$$\int_\Omega (|(\phi_1)_M(z,t)|^2 + |(\phi_2)_M(z,t)|^2 + |(\phi_3)_M(z,t)|^2)\, dz = m_T,$$

17.
$$\int_\Omega (\alpha_C |(\phi_2)_M(z,t)|^2 - \alpha_B |(\phi_3)_M(z,t)|^2)\, dz = 0.$$

Already including the Lagrange multipliers for the constraints, the variational formulation for such system. denoted by the functional $J(\phi, E)$ stands for

$$J(\phi, E) = G(\nabla\phi) + F(\phi) + F_1(\phi) - J_{Aux}(\phi, E),$$

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where

$$
\begin{aligned}
G(\nabla\phi) \quad = \quad & \frac{\gamma_p}{2}\sum_{j=1}^{2}\int_0^{t_f}\int_\Omega \nabla(\phi_1^H)_{p_j}\cdot\nabla(\phi_1^H)_{p_j}\,dx\,dy\,dz\,dt \\
& +\frac{\gamma_e}{2}\sum_{j=1}^{2}\int_0^{t_f}\int_\Omega \nabla(\phi_1^H)_{e_j}\cdot\nabla(\phi_1^H)_{e_j}\,dx\,dy\,dz\,dt \\
& +\frac{\gamma_p}{2}\sum_{j=8}^{2}\int_0^{t_f}\int_\Omega \nabla(\phi_1^O)_{p_j}\cdot\nabla(\phi_1^O)_{p_j}\,dx\,dy\,dz\,dt \\
& +\frac{\gamma_e}{2}\sum_{j=1}^{2}\int_0^{t_f}\int_\Omega \nabla(\phi_1^O)_{e_j}\cdot\nabla(\phi_1^O)_{e_j}\,dx\,dy\,dz\,dt \\
& +\frac{\gamma_p}{2}\int_0^{t_f}\int_\Omega \nabla(\phi_2^H)_{p}\cdot\nabla(\phi_2^H)_{p}\,dx\,dy\,dz\,dt \\
& +\frac{\gamma_e}{2}\int_0^{t_f}\int_\Omega \nabla(\phi_2^H)_{e_1}\cdot\nabla(\phi_2^H)_{e_1}\,dx\,dy\,dz\,dt \\
& +\frac{\gamma_e}{2}\sum_{j=1}^{2}\int_0^{t_f}\int_\Omega \nabla(\phi_2^{OH^-})_{e_2}\cdot\nabla(\phi_1^{OH^-})_{e_2}\,dx\,dz\,dt \\
& +\frac{\gamma_p}{2}\sum_{j=8}^{2}\int_0^{t_f}\int_\Omega \nabla(\phi_2^O)_{p_j}\cdot\nabla(\phi_2^O)_{p_j}\,dx\,dy\,dz\,dt \\
& +\frac{\gamma_e}{2}\sum_{j=1}^{2}\int_0^{t_f}\int_\Omega \nabla(\phi_2^O)_{e_j}\cdot\nabla(\phi_2^O)_{e_j}\,dx\,dy\,dz\,dt \\
& +\frac{\gamma_p}{2}\sum_{j=1}^{2}\int_0^{t_f}\int_\Omega \nabla(\phi_2^H)_{p}\cdot\nabla(\phi_2^O)_{p}\,dx\,dy\,dt \\
& +\frac{\gamma_{A^H}}{2}\sum_{j=1}^{2}\int_0^{t_f}\int_\Omega \nabla(\phi_1^H)_{A_j}\cdot\nabla(\phi_1^H)_{A_j}\,dy\,dz\,dt \\
& +\frac{\gamma_{A^O}}{2}\int_0^{t_f}\int_\Omega \nabla(\phi_1^O)_{A}\cdot\nabla(\phi_1^O)_{A}\,dy\,dz\,dt \\
& +\frac{\gamma_{A^H}}{2}\int_0^{t_f}\int_\Omega \nabla(\phi_2^H)_{A}\cdot\nabla(\phi_2^H)_{A}\,dy\,dz\,dt \\
& +\frac{\gamma_{A^O}}{2}\int_0^{t_f}\int_\Omega \nabla(\phi_2^O)_{A}\cdot\nabla(\phi_2^O)_{A}\,dy\,dz\,dt \\
& +\frac{\gamma_{M_1}}{2}\int_0^{t_f}\int_\Omega \nabla(\phi_1)_{M}\cdot\nabla(\phi_1)_{M}\,dz\,dt \\
& +\frac{\gamma_{M_2}}{2}\int_0^{t_f}\int_\Omega \nabla(\phi_2)_{M}\cdot\nabla(\phi_2)_{M}\,dz\,dt \\
& \frac{\gamma_{A_3}}{2}\int_0^{t_f}\int_\Omega \nabla(\phi_3)_{A}\cdot\nabla(\phi_3)_{A}\,dy\,dt.
\end{aligned}
$$

Here $\gamma_p > 0$, $\gamma_e > 0$, $\gamma_A^H > 0$,, $\gamma_A^O > 0$, $\gamma_{M_1} > 0$, $\gamma_{M_2} > 0$, $\gamma_{A_3} > 0$.

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Moreover,

$$
\begin{aligned}
& F(\phi) \\
= \; & \frac{\alpha_1}{2}\int_0^{t_f}\int_\Omega \frac{|\phi_1(x-\xi_1,y-\xi_2,z-\xi_3,t)|^2|\phi_1(\xi_1,\xi_2,\xi_3,t)|^2}{|(x,y,z)-(\xi_1,\xi_2,\xi_3)|}\,dx\,dy\,dz\,dx_1\,dx_2\,dx_3\,dt \\
& +\frac{\alpha_2}{2}\int_0^{t_f}\int_\Omega \frac{|\phi_2(x-\xi_1,y-\xi_2,z-\xi_3,t)|^2|\phi_2(\xi_1,\xi_2,\xi_3,t)|^2}{|(x,y,z)-(\xi_1,\xi_2,\xi_3)|}\,dx\,dy\,dz\,dx_1\,dx_2\,dx_3\,dt \\
& +\frac{\alpha_3}{2}\int_0^{t_f}\int_\Omega \frac{|\phi_3(x-\xi_1,z-\xi_3,t)|^2|\phi_3(\xi_1,\xi_3,t)|^2}{|(x,y,z)-(\xi_1,\xi_2,\xi_3)|}\,dx\,dy\,dz\,dx_1\,dx_3\,dt \\
& +\frac{\alpha_{23}}{2}\int_0^{t_f}\int_\Omega \frac{|\phi_2(x-\xi_1,y-\xi_2,z-\xi_3,t)|^2|\phi_3(\xi_1,\xi_3,t)|^2}{|(x,y,z)-(\xi_1,\xi_2,\xi_3)|}\,dx\,dy\,dz\,dx_1\,dx_2\,dx_3\,dt
\end{aligned}
$$

where $\alpha_1 > 0$, $\alpha_2 > 0$, $\alpha_3 > 0$ and $\alpha_{23} > 0$.

Furthermore,

$$
F_1(\phi) \;=\; \int_0^{t_f}\int_\Omega V(x,y,z,t)(|\phi_1|^2+|\phi_2|^2+|\phi_3|^2)\,dx\,dy\,dz\,dt, \tag{127}
$$

where $V = V(x,y,z,t)$ is an electric potential originated from an external electric field $\mathbf{E}$ applied on Ω.

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Finally,

$$
\begin{aligned}
& J_{Aux}(\phi, E) \\
= & \sum_{j=1}^{2} \int_0^{t_f} \int_\Omega (E_1)^H_{p_j}(y,z,t) \left(\int_\Omega |(\phi_1^H)_{p_j}(x,y,z,t)|^2 \, dx - m_p \right) dy \, dz \, dt \\
& + \sum_{j=1}^{2} \int_0^{t_f} \int_\Omega (E_1)^H_{e_j}(y,z,t) \left(\int_\Omega |(\phi_1^H)_{e_j}(x,y,z,t)|^2 \, dx - m_e \right) dy \, dz \, dt \\
& + \sum_{j=8}^{2} \int_0^{t_f} \int_\Omega (E_1)^O_{p_j}(y,z,t) \left(\int_\Omega |(\phi_1^O)_{p_j}(x,y,z,t)|^2 \, dx - m_p \right) dy \, dz \, dt \\
& + \sum_{j=8}^{2} \int_0^{t_f} \int_\Omega (E_1)^O_{e_j}(y,z,t) \left(\int_\Omega |(\phi_1^O)_{e_j}(x,y,z,t)|^2 \, dx - m_e \right) dy \, dz \, dt \\
& + \int_0^{t_f} \int_\Omega (E_2)^H_{p}(y,z,t) \left(\int_\Omega |(\phi_2^H)_{p}(x,y,z,t)|^2 \, dx - m_p \right) dy \, dz \, dt \\
& + \sum_{j=8}^{2} \int_0^{t_f} \int_\Omega (E_2)^O_{p_j}(y,z,t) \left(\int_\Omega |(\phi_2^O)_{p_j}(x,y,z,t)|^2 \, dx - m_p \right) dy \, dz \, dt \\
& + \sum_{j=8}^{2} \int_0^{t_f} \int_\Omega (E_2)^O_{e_j}(y,z,t) \left(\int_\Omega |(\phi_2^O)_{e_j}(x,y,z,t)|^2 \, dx - m_e \right) dy \, dz \, dt \\
& + \int_0^{t_f} \int_\Omega (E_3)^H_{p}(y,t) \left(\int_\Omega |(\phi_3^H)_{p}(x,y,t)|^2 \, dx - m_p \right) dy \, dt \\
& + \sum_{j=1}^{2} \int_0^{t_f} \int_\Omega (E_4)^H_{A_j}(z,t) \left(\int_\Omega (|(\phi_1)^H_{A_j}(y,z,t)|^2 \, dy - m^H_{A_j} \right) dz \, dt \\
& + \int_0^{t_f} \int_\Omega \int_\Omega (E_4)^O_{A}(z,t) \left(\int_\Omega (|(\phi_1)^O_{A}(y,z,t)|^2 \, dy - m^O_{A} \right) dz \, dt \\
& + \int_0^{t_f} \int_\Omega (E_5)^H_{A}(z,t) \left(\int_\Omega (|(\phi_2)^H_{A}(y,z,t)|^2 \, dy - m^H_{A} \right) dz \, dt \\
& + \int_0^{t_f} \int_\Omega (E_5)^O_{A}(z,t) \left(\int_\Omega (|(\phi_2)^O_{A}(y,z,t)|^2 \, dy - m^O_{A} \right) dz \, dt \\
& \int_0^{t_f} (E_6)^H_{A}(t) \left(\int_\Omega (|(\phi_3)^H_{A}(y,t)|^2 \, dy - m^H_{A} \right) dt \\
& + \int_0^{t_f} (E_7)(t) \left(\int_\Omega (|(\phi_1)_M(z,t)|^2 + |(\phi_2)_M(z,t)|^2 + |(\phi_3)_M(z,t)|^2) \, dz - m_T \right) dt \\
& + \int_0^{t_f} (E_8)(t) \left(\int_\Omega (\alpha_C |(\phi_2)_M(z,t)|^2 - \alpha_B |(\phi_3)_M(z,t)|^2) \, dz \right) dt. \qquad (128)
\end{aligned}
$$

24. A mathematical model for the Austenite and Martensite phase transition

In this section we consider a phase transition of a solid solution of $\gamma - Fe$ ($\gamma - iron$) and carbon with a $0.75/100$ proportion of carbon, known as austenite, initially at a temperature above and close to $723\ C$ and rapidly cooled to a temperature of about $25\ C$, developing a phase transition which generates a solid solution of $\alpha - Fe$ ($\alpha - iron$) and carbon known as martensite.

Let $\Omega \subset \mathbb{R}^3$ be an open, bounded and connected set with a regular boundary denoted by $\partial\Omega$ which contains an amount of austenite at $723\ C$ and which, as previously mentioned, is rapidly cooled to a temperature $25\ C$ on a time interval $[0, t_f]$, resulting a phase known as martensite.

We recall the $\gamma - Fe$ of austenite phase presents a multi-faced cubic crystalline structure in a micro-structure with carbon atoms.

On the other hand, $\alpha - F_e$ structure of the martensite phase has a CCC cubic centralized crystalline structure in a micro-structure with carbon atoms.

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At this point, we also recall that the F_e (iron) atom has 26 protons, 26 electrons and 30 neutrons. On the other hand a $Carbon_{12}$ atom has 6 protons and this same number of electrons and neutrons. Here we define the density function ϕ_1, representing the Austenite phase, where:

$$\begin{aligned}
|\phi_1(x,y,z,t)|^2 &= \sum_{j=1}^{26} |\phi_{p_j}^{\gamma-F_e}(x,y,z,t)|^2 |\phi_A^{\gamma-F_e}(y,z,t)|^2 |\phi_1^{\gamma}(z,t)|^2 \frac{1}{(m_A^{\gamma})^2} \\
&+ \sum_{j=1}^{26} |\phi_{e_j}^{\gamma-F_e}(x,y,z,t)|^2 |\phi_A^{\gamma-F_e}(y,z,t)|^2 |\phi_1^{\gamma}(z,t)|^2 \frac{1}{(m_A^{\gamma})^2} \\
&+ \sum_{j=1}^{30} |\phi_{N_j}^{\gamma-F_e}(x,y,z,t)|^2 |\phi_A^{\gamma-F_e}(y,z,t)|^2 |\phi_1^{\gamma}(z,t)|^2 \frac{1}{(m_A^{\gamma})^2} \\
&+ \sum_{j=1}^{6} |(\phi_1^{C})_{p_j}(x,y,z,t)|^2 |(\phi_1^{C})_A(y,z,t)|^2 |\phi_1^{C}(z,t)|^2 \frac{1}{(m_A^{C})^2} \\
&+ \sum_{j=1}^{6} |(\phi_1^{C})_{e_j}(x,y,z,t)|^2 |(\phi_1^{C})_A(y,z,t)|^2 |\phi_1^{C}(z,t)|^2 \frac{1}{(m_A^{C})^2} \\
&+ \sum_{j=1}^{6} |(\phi_1^{C})_{N_j}(x,y,z,t)|^2 |(\phi_1^{C})_A(y,z,t)|^2 |\phi_1^{C}(z,t)|^2 \frac{1}{(m_A^{C})^2}. \qquad (129)
\end{aligned}$$

Similarly, we define the density function for the Martensite phase, which is denoted by ϕ_2, where:

$$\begin{aligned}
|\phi_2(x,y,z,t)|^2 &= \sum_{j=1}^{26} |\phi_{p_j}^{\alpha-F_e}(x,y,z,t)|^2 |\phi_A^{\gamma-F_e}(y,z,t)|^2 |\phi_1^{\alpha}(z,t)|^2 \frac{1}{(m_A^{\alpha})^2} \\
&+ \sum_{j=1}^{26} |\phi_{e_j}^{\alpha-F_e}(x,y,z,t)|^2 |\phi_A^{\alpha-F_e}(y,z,t)|^2 |\phi_1^{\gamma}(z,t)|^2 \frac{1}{(m_A^{\alpha})^2} \\
&+ \sum_{j=1}^{30} |\phi_{N_j}^{\alpha-F_e}(x,y,z,t)|^2 |\phi_A^{\alpha-F_e}(y,z,t)|^2 |\phi_1^{\alpha}(z,t)|^2 \frac{1}{(m_A^{\alpha})^2} \\
&+ \sum_{j=1}^{6} |(\phi_1^{C})_{p_j}(x,y,z,t)|^2 |(\phi_1^{C})_A(y,z,t)|^2 |\phi_1^{C}(z,t)|^2 \frac{1}{(m_A^{C})^2} \\
&+ \sum_{j=1}^{6} |(\phi_2^{C})_{e_j}(x,y,z,t)|^2 |(\phi_2^{C})_A(y,z,t)|^2 |\phi_2^{C}(z,t)|^2 \frac{1}{(m_A^{C})^2} \\
&+ \sum_{j=1}^{6} |(\phi_2^{C})_{N_j}(x,y,z,t)|^2 |(\phi_2^{C})_A(y,z,t)|^2 |\phi_2^{C}(z,t)|^2 \frac{1}{(m_A^{C})^2}. \qquad (130)
\end{aligned}$$

For the $CFC\ \gamma - F_e\ (\gamma - iron)$ corresponding to the Austenite phase, such density functions are subject to the following constraints:

Defining

$$C_\gamma = \{(\varepsilon_1,0,0),\ (0,\varepsilon_2,0),\ (0,0,\varepsilon_3),\ :\ \varepsilon_j \in \{+1,-1\},\ \forall j \in \{1,2,3\}\},$$

$$(C_\gamma)_1 = \{(\varepsilon_1,\varepsilon_2,\varepsilon_3),\ :\ \varepsilon_j \in \{+1,-1\},\ \forall j \in \{1,2,3\}\},$$

and

$$(C_\gamma)_2 = \{(\varepsilon_1,\varepsilon_2,0),\ (\varepsilon_1,0,\varepsilon_3),(0,\varepsilon_2,\varepsilon_3),\ :\ \varepsilon_j \in \{+1,-1\},\ \forall j \in \{1,2,3\}\},$$

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we must have

$$\phi_A^{\gamma-F_e}(y, z_1+\varepsilon_1\delta_z, z_2+\varepsilon_2\delta_z, z_3+\varepsilon_3\delta_z, t) = \phi_A^{\gamma-F_e}(y, z_1+\tilde{\varepsilon}_1\delta_z, z_2+\tilde{\varepsilon}_2\delta_z, z_3+\tilde{\varepsilon}_3\delta_z, t),$$

$\forall \varepsilon, \tilde{\varepsilon} \in C_\gamma$, where $\delta_z \in \mathbb{R}^+$ is a small real parameter related to $\gamma - F_e$ crystalline structure dimensions.

We must have also,

$$\phi_A^{\gamma-F_e}(y, z_1+\varepsilon_1\delta_z, z_2+\varepsilon_2\delta_z, z_3+\varepsilon_3\delta_z, t) = \phi_A^{\gamma-F_e}(y, z_1+\tilde{\varepsilon}_1\delta_z, z_2+\tilde{\varepsilon}_2\delta_z, z_3+\tilde{\varepsilon}_3\delta_z, t),$$

$\forall \varepsilon, \tilde{\varepsilon} \in (C_\gamma)_1$ and,

$$(\phi_1^C)_A(y, z_1+\varepsilon_1\delta_z, z_2+\varepsilon_2\delta_z, z_3+\varepsilon_3\delta_z, t) = (\phi_1^C)_A(y, z_1+\tilde{\varepsilon}_1\delta_z, z_2+\tilde{\varepsilon}_2\delta_z, z_3+\tilde{\varepsilon}_3\delta_z, t),$$

$\forall \varepsilon, \tilde{\varepsilon} \in (C_\gamma)_2$.

For the CCC $\alpha - F_e$ $(\alpha - iron)$ corresponding to the Austenite phase, such density functions are subject to the following constraints:

Defining

$$C_\alpha = \{(\varepsilon_1, \varepsilon_2, \varepsilon_3), : \varepsilon_j \in \{+1, -1\}, \forall j \in \{1, 2, 3\}\},$$

$$(C_\alpha)_1 = \{(\varepsilon_1, \varepsilon_2, \varepsilon_3), : \varepsilon_1, \varepsilon_2 \in \{+1, -1\} \text{ and } \varepsilon_3 = 0\},$$

$$(C_\alpha)_2 = \{(\varepsilon_1, \varepsilon_2, \varepsilon_3), : \varepsilon_1 = \varepsilon_2 = 0 \text{ and } \varepsilon_3 \in \{+1, -1\}\},$$

we must have

$$\phi_A^{\alpha-F_e}(y, z_1+\varepsilon_1\hat{\delta}_z, z_2+\varepsilon_2\hat{\delta}_z, z_3+\varepsilon_3\hat{\delta}_z, t) = \phi_A^{\alpha-F_e}(y, z_1+\tilde{\varepsilon}_1\hat{\delta}_z, z_2+\tilde{\varepsilon}_2\hat{\delta}_z, z_3+\tilde{\varepsilon}_3\hat{\delta}_z, t),$$

$\forall \varepsilon, \tilde{\varepsilon} \in C_\alpha$, where $\hat{\delta}_z \in \mathbb{R}^+$ is a small real parameter related to $\alpha - F_e$ crystalline structure dimensions.

We must have also,

$$(\phi_2^C)_A(y, z_1+\varepsilon_1\hat{\delta}_z, z_2+\varepsilon_2\hat{\delta}_z, z_3+\varepsilon_3\hat{\delta}_z, t) = (\phi_2^C)_A(y, z_1+\tilde{\varepsilon}_1\hat{\delta}_z, z_2+\tilde{\varepsilon}_2\hat{\delta}_z, z_3+\tilde{\varepsilon}_3\hat{\delta}_z, t),$$

$\forall \varepsilon, \tilde{\varepsilon} \in (C_\alpha)_1 \cup (C_\alpha)_2$.

The other constraints for the densities are given by:

1. For the Austenite phase:

   (a)
   $$\int_\Omega |\phi_{p_j}^{\gamma-F_e}(x, y, z, t)|^2 \, dx = m_p, \ \forall j \in \{1, 26\},$$

   (b)
   $$\int_\Omega |\phi_{e_j}^{\gamma-F_e}(x, y, z, t)|^2 \, dx = m_e, \ \forall j \in \{1, 26\},$$

   (c)
   $$\int_\Omega |\phi_{N_j}^{\gamma-F_e}(x, y, z, t)|^2 \, dx = m_N, \ \forall j \in \{1, 30\},$$

   (d)
   $$\int_\Omega |\phi_A^{\gamma-F_e}(x, y, z, t)|^2 \, dx = m_A^\gamma,$$

   (e)
   $$\int_\Omega |(\phi_1^C)_{p_j}(x, y, z, t)|^2 \, dx = m_p, \ \forall j \in \{1, 6\},$$

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(f)
$$\int_\Omega |(\phi_1^C)_{e_j}(x,y,z,t)|^2\, dx = m_e,\ \forall j \in \{1,6\},$$
(g)
$$\int_\Omega |(\phi_1^C)_{N_j}(x,y,z,t)|^2\, dx = m_N,\ \forall j \in \{1,6\},$$
(h)
$$\int_\Omega |(\phi_1^C)_A(x,y,z,t)|^2\, dx = m_A^C,$$

2. For the Martensite phase:

(a)
$$\int_\Omega |\phi_{p_j}^{\alpha-F_e}(x,y,z,t)|^2\, dx = m_p,\ \forall j \in \{1,26\},$$
(b)
$$\int_\Omega |\phi_{e_j}^{\alpha-F_e}(x,y,z,t)|^2\, dx = m_e,\ \forall j \in \{1,26\},$$
(c)
$$\int_\Omega |\phi_{N_j}^{\alpha-F_e}(x,y,z,t)|^2\, dx = m_N,\ \forall j \in \{1,30\},$$
(d)
$$\int_\Omega |\phi_A^{\alpha-F_e}(x,y,z,t)|^2\, dx = m_A^\alpha,$$
(e)
$$\int_\Omega |(\phi_2^C)_{p_j}(x,y,z,t)|^2\, dx = m_p,\ \forall j \in \{1,6\},$$
(f)
$$\int_\Omega |(\phi_2^C)_{e_j}(x,y,z,t)|^2\, dx = m_e,\ \forall j \in \{1,6\},$$
(g)
$$\int_\Omega |(\phi_2^C)_{N_j}(x,y,z,t)|^2\, dx = m_N,\ \forall j \in \{1,6\},$$
(h)
$$\int_\Omega |(\phi_2^C)_A(x,y,z,t)|^2\, dx = m_A^C.$$

3. For the total F_e (iron) mass,
$$\int_\Omega |\phi_1^\gamma(z,t)|^2\, dz + \int_\Omega |\phi_2^\gamma(z,t)|^2\, dz = (m_{F_e})_T,$$

4. For the total Carbon mass
$$\int_\Omega |\phi_1^C(z,t)|^2\, dz + \int_\Omega |\phi_2^C(z,t)|^2\, dz = (m_C)_T.$$

At this point we define the functional J which models such a pahse transition in question, where
$$J(\phi, E) = G(\nabla\phi) + F(\phi) + F_1(\phi) + J_{Aux}(\phi, E)$$
where

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$$
\begin{aligned}
G(\nabla\phi) \quad = \quad & \sum_{j=1}^{26} \frac{\hat{\gamma}_p^{\gamma-F_e}}{2} \int_0^{t_f} \int_\Omega \nabla\phi_{p_j}^{\gamma-F_e} \cdot \nabla\phi_{p_j}^{\gamma-F_e}\, dx\, dy\, dz\, dt \\
& + \sum_{j=1}^{26} \frac{\hat{\gamma}_e^{\gamma-F_e}}{2} \int_0^{t_f} \int_\Omega \nabla\phi_{e_j}^{\gamma-F_e} \cdot \nabla\phi_{e_j}^{\gamma-F_e}\, dx\, dy\, dz\, dt \\
& + \sum_{j=1}^{30} \frac{\hat{\gamma}_N^{\gamma-F_e}}{2} \int_0^{t_f} \int_\Omega \nabla\phi_{N_j}^{\gamma-F_e} \cdot \nabla\phi_{N_j}^{\gamma-F_e}\, dx\, dy\, dz\, dt \\
& + \sum_{j=1}^{26} \frac{\hat{\gamma}_p^{\alpha-F_e}}{2} \int_0^{t_f} \int_\Omega \nabla\phi_{p_j}^{\alpha-F_e} \cdot \nabla\phi_{p_j}^{\alpha-F_e}\, dx\, dy\, dz\, dt \\
& + \sum_{j=1}^{26} \frac{\hat{\gamma}_e^{\alpha-F_e}}{2} \int_0^{t_f} \int_\Omega \nabla\phi_{e_j}^{\alpha-F_e} \cdot \nabla\phi_{e_j}^{\gamma-F_e}\, dx\, dy\, dz\, dt \\
& + \sum_{j=1}^{30} \frac{\hat{\gamma}_N^{\alpha-F_e}}{2} \int_0^{t_f} \int_\Omega \nabla\phi_{N_j}^{\alpha-F_e} \cdot \nabla\phi_{N_j}^{\alpha-F_e}\, dx\, dy\, dz\, dt \\
& + \frac{\hat{\gamma}_A^{\gamma}}{2} \int_0^{t_f} \int_\Omega (\nabla\phi_A^{\gamma-F_e}(y,z,t) \cdot \nabla\phi_A^{\gamma-F_e}(y,z,t))\, dy\, dz\, dt \\
& + \frac{\hat{\gamma}_A^{\alpha}}{2} \int_0^{t_f} \int_\Omega (\nabla\phi_A^{\alpha-F_e}(y,z,t) \cdot \nabla\phi_A^{\alpha-F_e}(y,z,t))\, dy\, dz\, dt \\
& + \sum_{j=1}^{6} \frac{\hat{\gamma}_p^{C}}{2} \int_0^{t_f} \int_\Omega \nabla(\phi_1^C)_{p_j} \cdot \nabla(\phi_1^C)_{p_j}\, dx\, dy\, dz\, dt \\
& + \sum_{j=1}^{6} \frac{\hat{\gamma}_e^{C}}{2} \int_0^{t_f} \int_\Omega \nabla(\phi_1^C)_{e_j} \cdot \nabla(\phi_1^C)_{e_j}\, dx\, dy\, dz\, dt \\
& + \sum_{j=1}^{6} \frac{\hat{\gamma}_N^{C}}{2} \int_0^{t_f} \int_\Omega \nabla(\phi_1^C)_{N_j} \cdot \nabla(\phi_1^C)_{N_j}\, dx\, dy\, dz\, dt \\
& + \sum_{j=1}^{6} \frac{\hat{\gamma}_p^{C}}{2} \int_0^{t_f} \int_\Omega \nabla(\phi_2^C)_{p_j} \cdot \nabla(\phi_2^C)_{p_j}\, dx\, dy\, dz\, dt \\
& + \sum_{j=1}^{6} \frac{\hat{\gamma}_e^{C}}{2} \int_0^{t_f} \int_\Omega \nabla(\phi_2^C)_{e_j} \cdot \nabla(\phi_2^C)_{e_j}\, dx\, dy\, dz\, dt \\
& + \sum_{j=1}^{6} \frac{\hat{\gamma}_N^{C}}{2} \int_0^{t_f} \int_\Omega \nabla(\phi_2^C)_{N_j} \cdot \nabla(\phi_2^C)_{N_j}\, dx\, dy\, dz\, dt \\
& + \frac{\hat{\gamma}_A^{C}}{2} \int_0^{t_f} \int_\Omega (\nabla(\phi_1^C)_A \cdot \nabla(\phi_1^C)_A)\, dy\, dz\, dt + \frac{\hat{\gamma}_A^{C}}{2} \int_0^{t_f} \int_\Omega (\nabla(\phi_2^C)_A \cdot \nabla(\phi_2^C)_A)\, dy\, dz\, dt \\
& + \frac{\hat{\gamma}_T^{\gamma}}{2} \int_0^{t_f} \int_\Omega (\nabla(\phi_1^\gamma) \cdot \nabla(\phi_1^\gamma))\, dz\, dt + \frac{\hat{\gamma}_T^{\gamma}}{2} \int_0^{t_f} \int_\Omega (\nabla(\phi_1^\alpha) \cdot \nabla(\phi_1^\alpha))\, dz\, dt \\
& + \frac{\hat{\gamma}_T^{C}}{2} \int_0^{t_f} \int_\Omega (\nabla(\phi_1^C) \cdot \nabla(\phi_1^C))\, dz\, dt + \frac{\hat{\gamma}_T^{\gamma}}{2} \int_0^{t_f} \int_\Omega (\nabla(\phi_2^C) \cdot \nabla(\phi_2^C))\, dz\, dt \qquad (131)
\end{aligned}
$$

Also,

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$$
\begin{aligned}
& F(\phi) \\
= \; & \frac{\hat{\alpha}_1}{2} \int_0^{t_f} \int_\Omega \frac{|\phi_1(x-\xi_1, y-\xi_2, z-\xi_3, t)|^2 |\phi_1(\xi_1, \xi_2, \xi_3, t)|^2}{|(x,y,z)-(\xi_1,\xi_2,\xi_3)|} \, dx \, dy \, dz \, d\xi_1 \, d\xi_2 \, d\xi_3 \, dt \\
& + \frac{\hat{\alpha}_2}{2} \int_0^{t_f} \int_\Omega \frac{|\phi_2(x-\xi_1, y-\xi_2, z-\xi_3, t)|^2 |\phi_2(\xi_1, \xi_2, \xi_3, t)|^2}{|(x,y,z)-(\xi_1,\xi_2,\xi_3)|} \, dx \, dy \, dz \, d\xi_1 \, d\xi_2 \, d\xi_3 \, dt,
\end{aligned}
$$

$$
F_1(\phi) = -\int_0^{t_f} \int_\Omega w^2(z,t)(|\phi_1(z,t)|^2 + \phi_2(z,t)|^2) \, dz \, dt,
$$

Finally, $J_{Aux} = J_{Aux_1} + J_{Aux_2} + J_{Aux_3} + J_{Aux_4} + J_{Aux_5}$, where

$$
\begin{aligned}
J_{Aux_1} = \; & \sum_{j=1}^{26} \int_0^{t_f} \int_\Omega E_{p_j}^{\gamma-F_e}(y,z,t) \left(\int_\Omega |\phi_{p_j}^{\gamma-F_e}(x,y,z,t)|^2 \, dx - m_p \right) \, dy \, dz \, dt \\
& + \sum_{j=1}^{26} \int_0^{t_f} \int_\Omega E_{e_j}^{\gamma-F_e}(y,z,t) \left(\int_\Omega |\phi_{e_j}^{\gamma-F_e}(x,y,z,t)|^2 \, dx - m_e \right) \, dy \, dz \, dt \\
& + \sum_{j=1}^{30} \int_0^{t_f} \int_\Omega E_{N_j}^{\gamma-F_e}(y,z,t) \left(\int_\Omega |\phi_{N_j}^{\gamma-F_e}(x,y,z,t)|^2 \, dx - m_N \right) \, dy \, dz \, dt \\
& \sum_{j=1}^{26} \int_0^{t_f} \int_\Omega E_{p_j}^{\alpha-F_e}(y,z,t) \left(\int_\Omega |\phi_{p_j}^{\alpha-F_e}(x,y,z,t)|^2 \, dx - m_p \right) \, dy \, dz \, dt \\
& + \sum_{j=1}^{26} \int_0^{t_f} \int_\Omega E_{e_j}^{\alpha-F_e}(y,z,t) \left(\int_\Omega |\phi_{e_j}^{\alpha-F_e}(x,y,z,t)|^2 \, dx - m_e \right) \, dy \, dz \, dt \\
& + \sum_{j=1}^{30} \int_0^{t_f} \int_\Omega E_{N_j}^{\alpha-F_e}(y,z,t) \left(\int_\Omega |\phi_{N_j}^{\alpha-F_e}(x,y,z,t)|^2 \, dx - m_N \right) \, dy \, dz \, dt \\
& + \int_0^{t_f} \int_\Omega E_A^{\gamma-F_e}(y,t) \left(\int_\Omega |\phi_A^{\gamma-F_e}(y,z,t)|^2 \, dy - m_A^\gamma \right) \, dz \, dt \\
& + \int_0^{t_f} \int_\Omega E_A^{\alpha-F_e}(y,t) \left(\int_\Omega |\phi_A^{\alpha-F_e}(y,z,t)|^2 \, dy - m_A^\alpha \right) \, dz \, dt
\end{aligned} \tag{132}
$$

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$$
\begin{aligned}
J_{Aux_2} \;=\; & \sum_{j=1}^{26} \int_0^{t_f} \int_\Omega (E_1^C)_{p_j}(y,z,t) \left(\int_\Omega |(\phi_1^C)_{p_j}(x,y,z,t)|^2 \, dx - m_p \right) dy \, dz \, dt \\
& \sum_{j=1}^{26} \int_0^{t_f} \int_\Omega (E_1^C)_{e_j}(y,z,t) \left(\int_\Omega |(\phi_1^C)_{e_j}(x,y,z,t)|^2 \, dx - m_e \right) dy \, dz \, dt \\
& \sum_{j=1}^{26} \int_0^{t_f} \int_\Omega (E_1^C)_{N_j}(y,z,t) \left(\int_\Omega |(\phi_1^C)_{N_j}(x,y,z,t)|^2 \, dx - m_N \right) dy \, dz \, dt \\
& \sum_{j=1}^{26} \int_0^{t_f} \int_\Omega (E_2^C)_{p_j}(y,z,t) \left(\int_\Omega |(\phi_2^C)_{p_j}(x,y,z,t)|^2 \, dx - m_p \right) dy \, dz \, dt \\
& \sum_{j=1}^{26} \int_0^{t_f} \int_\Omega (E_2^C)_{e_j}(y,z,t) \left(\int_\Omega |(\phi_2^C)_{e_j}(x,y,z,t)|^2 \, dx - m_e \right) dy \, dz \, dt \\
& \sum_{j=1}^{26} \int_0^{t_f} \int_\Omega (E_2^C)_{N_j}(y,z,t) \left(\int_\Omega |(\phi_2^C)_{N_j}(x,y,z,t)|^2 \, dx - m_N \right) dy \, dz \, dt \\
& \int_0^{t_f} \int_\Omega (E_1^C)_A(y,t) \left(\int_\Omega |(\phi_1^C)_A(y,z,t)|^2 \, dy - m_A^C \right) dz \, dt \\
& + \int_0^{t_f} \int_\Omega (E_2^C)_A(y,t) \left(\int_\Omega |(\phi_2^C)_A(y,z,t)|^2 \, dy - m_A^C \right) dz \, dt
\end{aligned} \tag{133}
$$

and,

$$
\begin{aligned}
J_{Aux_3} \;=\; & \int_0^{t_f} E_3^{\gamma,\alpha}(t) \left(\int_\Omega (|\phi_1^\gamma(z,t)|^2 + |\phi_2^\alpha(z,t)|^2) \, dz - (m_{F_e})_T \right) dt \\
& + \int_0^{t_f} E_3^C(t) \left(\int_\Omega (|\phi_1^C(z,t)|^2 + |\phi_2^C(z,t)|^2) \, dz - (m_C)_T \right) dt.
\end{aligned} \tag{134}
$$

$$
\begin{aligned}
& J_{Aux_4} \\
= \; & + \sum_{\varepsilon,\, \tilde{\varepsilon} \in C_\gamma} \int_0^{t_f} \int_\Omega E_4^{\varepsilon,\, \tilde{\varepsilon}}(y,z,t) (\phi_A^{\gamma-F_e}(y, z_1 + \varepsilon_1 \delta_z, z_2 + \varepsilon_2 \delta_z, z_3 + \varepsilon_3 \delta_z, t) \\
& - \phi_A^{\gamma-F_e}(y, z_1 + \tilde{\varepsilon}_1 \delta_z, z_2 + \tilde{\varepsilon}_2 \delta_z, z_3 + \tilde{\varepsilon}_3 \delta_z, t)) \, dy \, dz \, dt \\
& \sum_{\varepsilon,\, \tilde{\varepsilon} \in (C_\gamma)_1} \int_0^{t_f} \int_\Omega E_5^{\varepsilon,\, \tilde{\varepsilon}}(y,z,t) \phi_A^{\gamma-F_e}(y, z_1 + \varepsilon_1 \delta_z, z_2 + \varepsilon_2 \delta_z, z_3 + \varepsilon_3 \delta_z, t) \\
& - \phi_A^{\gamma-F_e}(y, z_1 + \tilde{\varepsilon}_1 \delta_z, z_2 + \tilde{\varepsilon}_2 \delta_z, z_3 + \tilde{\varepsilon}_3 \delta_z, t)) \, dy \, dz \, dt \\
& + \sum_{\varepsilon,\, \tilde{\varepsilon} \in (C_\gamma)_2} \int_0^{t_f} \int_\Omega E_6^{\varepsilon,\, \tilde{\varepsilon}}(y,z,t) (\phi_1^C)_A(y, z_1 + \varepsilon_1 \delta_z, z_2 + \varepsilon_2 \delta_z, z_3 + \varepsilon_3 \delta_z, t) \\
& - (\phi_1^C)_A(y, z_1 + \tilde{\varepsilon}_1 \delta_z, z_2 + \tilde{\varepsilon}_2 \delta_z, z_3 + \tilde{\varepsilon}_3 \delta_z, t)) \, dy \, dz \, dt \\
& + \sum_{\varepsilon,\, \tilde{\varepsilon} \in (C_\alpha)} \int_0^{t_f} \int_\Omega E_7^{\varepsilon,\, \tilde{\varepsilon}}(y,z,t) (\phi_A^{\alpha-F_e}(y, z_1 + \varepsilon_1 \hat{\delta}_z, z_2 + \varepsilon_2 \hat{\delta}_z, z_3 + \varepsilon_3 \hat{\delta}_z, t) \\
& - \phi_A^{\alpha-F_e}(y, z_1 + \tilde{\varepsilon}_1 \hat{\delta}_z, z_2 + \tilde{\varepsilon}_2 \hat{\delta}_z, z_3 + \tilde{\varepsilon}_3 \hat{\delta}_z, t)) \, dy \, dz \, dt \\
& + \sum_{\varepsilon,\, \tilde{\varepsilon} \in (C_\alpha)_1 \cup (C_\alpha)_2} \int_0^{t_f} \int_\Omega E_8^{\varepsilon,\, \tilde{\varepsilon}}(y,z,t) ((\phi_2^C)_A(y, z_1 + \varepsilon_1 \hat{\delta}_z, z_2 + \varepsilon_2 \hat{\delta}_z, z_3 + \varepsilon_3 \hat{\delta}_z, t) \\
& - (\phi_2^C)_A(y, z_1 + \tilde{\varepsilon}_1 \hat{\delta}_z, z_2 + \tilde{\varepsilon}_2 \hat{\delta}_z, z_3 + \tilde{\varepsilon}_3 \hat{\delta}_z, t)) \, dy \, dz \, dt.
\end{aligned} \tag{135}
$$

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Finally, for a field of displacements $u = (u_1, u_2, u_3)$ resulting from the action of a external load field $f = (f_1, f_2, f_3)$ and temperature variations, we define

$$\begin{aligned} & J_{Aux_5} \\ = \; & \frac{1}{2}\int_0^{t_f}\int_\Omega \Big(\Lambda_1(x,t)H^1_{ijkl}((e_{ij}(u)-e^1_{ij}(w))(e_{kl}(u)-e^1_{kl}(w))) \\ & + \Lambda_2(z,t)H^2_{ijkl}((e_{ij}(u)-e^2_{ij}(w))(e_{kl}(u)-e^2_{kl}(w)))\Big)\, dx\, dt \\ & -\frac{1}{2}\int_0^{t_f}\int_\Omega \rho(x,t)u_t(x,t)\cdot u_t(x,t)\, dx\, dt \\ & -\langle u_i, f_i\rangle_{L^2}, \end{aligned} \tag{136}$$

where

$$e_{ij}(u) = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right),$$

$$\rho_1(z,t) = \int_\Omega |\phi_1(x,y,z,t)|^2\, dx\, dy,$$

$$\rho_2(z,t) = \int_\Omega |\phi_2(x,y,z,t)|^2\, dx\, dy,$$

$$\rho(z,t) = \rho_1(z,t) + \rho_2(z,t),$$

and

$$\Lambda_1(z,t) = \frac{\rho_1(z,t)}{\rho_1(z,t)+\rho_2(z,t)},$$

$$\Lambda_2(z,t) = \frac{\rho_2(z,t)}{\rho_1(z,t)+\rho_2(z,t)}.$$

Remark 24.1. *The system temperature is supposed to be directly proportional to $w(z,t)^2$, which in this model is a known function obtained experimentally. Finally, the strain tensors $\{e^1_{ij}(w)\}$ and $\{e^2_{ij}(w)\}$ refer to austenite and martensite phases, respectively. Such tensors also depend on the temperature and must be also obtained experimentally.*

25. A note on classical free fields through a variational perspective

This section is strongly based on the first chapter of the book [20], by N.N. Bogoliubov and D.V. Shirkov.

Therefore, the credit for this section is of these mentioned authors. This section is a kind of review of such a book chapter indicated. In fact, what we have done is simply to open more and clarify some calculations, specially about the first variation of the functional L, in order to improve their understanding.

Let $\Omega = \hat{\Omega} \times [0,T] \subset \mathbb{R}^4$ where $\hat{\Omega} \subset \mathbb{R}^3$ is a bounded, open and connected set with a regular boundary denoted by $\partial\hat{\Omega}$.

Consider the Lagrangian density $L : \mathbb{R}^N \times \mathbb{R}^{N\times n} \to \mathbb{R}$ and an action $A : V \to \mathbb{R}$ where

$$A(u) = \int_\Omega L(u, \nabla u)\, dx,$$

$V = W^{1,2}_0(\Omega;\mathbb{R}^N)$.

We denote

$$\nabla u = \left\{\frac{\partial u_i}{\partial x_j}\right\}$$

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and

$$\frac{\partial u_i}{\partial x_j} = (u_i)_{x_j}.$$

Assume $u \in V$ is such that

$$\delta L(u, \nabla u) = \mathbf{0},$$

so that

$$\frac{\partial L(u, \nabla u)}{\partial u_i} - \sum_{k=1}^{n} \frac{d}{dx_k} \left(\frac{\partial L(u, \nabla u)}{\partial (u_i)_{x_k}} \right) = 0, \text{ in } \Omega, \ \forall i \in \{1, \cdots, N\}.$$

We define a change of variables

$$(x')_k = x_k + \delta x_k,$$

where $x_k = (x_0, x_1, x_2, x_3)$ and $x_0 = t$ (here t denotes time).

Also

$$g_{jk} = 0, \text{ if } j \neq k, \ g_{00} = -1 \text{ and } g_{11} = g_{22} = g_{33} = 1, \{g^{jk}\} = \{g_{jk}\}^{-1},$$

$$\delta x_k = \sum_{j=1}^{N} X_j^k \varepsilon \, w^j,$$

where $|\varepsilon| \ll 1$ denotes a small real parameter.

We define also

$$u_i'(x') = u_i(x) + \delta u_i(x),$$

where

$$\delta u_i(x) = \sum_{j=1}^{N} \psi_{ij} \varepsilon \, w^j,$$

and

$$\overline{\delta u_i} = u_i'(x) - u_i(x).$$

Observe that

$$\begin{aligned} \delta u_i(x) &= u_i'(x) - u_i(x) \\ &= u_i'(x') - u_i'(x) + u_i'(x) - u_i(x), \end{aligned} \tag{137}$$

so that

$$\begin{aligned} \overline{\delta u_i(x)} &= u_i'(x) - u_i(x) \\ &= \delta u_i(x) - (u_i'(x') - u_i'(x)) \\ &\quad \sum_{j=1}^{N} \psi_{ij} \varepsilon \, w^j - \sum_{k=1}^{n} \frac{\partial u_i'(\tilde{x}^i)}{dx_k} \delta x_k \\ &= \sum_{j=1}^{N} \psi_{ij} \varepsilon \, w^j - \sum_{k=1}^{n} \frac{\partial u_i(x)}{dx_k} \delta x_k + \mathcal{O}(\varepsilon^2). \end{aligned} \tag{138}$$

Summarizing, we have got

$$\overline{\delta u_i(x)} = \varepsilon \left(\sum_{j=1}^{N} \left(\psi_{ij} w^j - \sum_{k=1}^{n} \frac{\partial u_i(x)}{dx_k} X_j^K w^j \right) \right) + \mathcal{O}(\varepsilon^2).$$

Define now

$$\tilde{A}(u, \varphi_1, \varphi_2, \varepsilon) = \int_\Omega L[u(x + \varepsilon \varphi_2(x)) + \varepsilon \varphi_1(x)] \ \det J(x) \, dx.$$

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where we have generically denoted

$$L[u] \equiv L(u, \nabla u),$$

$$L[u(x+\varepsilon\varphi_2(x))+\varepsilon\varphi_1(x)] \equiv L(u(x+\varepsilon\varphi_2(x))+\varepsilon\varphi_1(x), \nabla u(x+\varepsilon\varphi_2(x))+\varepsilon\nabla\varphi_1(x)),$$

and

$$\begin{aligned} J(x) &= \left\{\frac{\partial x'_j}{\partial x_k}\right\} \\ &= \left\{\frac{\partial(x_j+\varepsilon(\varphi_2)_j(x))}{\partial x_k}\right\} \\ &= \left\{\delta_{jk}+\varepsilon\frac{\partial(\varphi_2)_j(x)}{\partial x_k}\right\}. \end{aligned} \tag{139}$$

From such a last definition we have

$$\det J(x) = 1+\varepsilon\sum_{k=1}^{n}\frac{\partial(\varphi_2)_k(x)}{\partial x_k}+\mathcal{O}(\varepsilon^2).$$

so that

$$\frac{\partial \det J(x)}{\partial\varepsilon}|_{\varepsilon=0} = \sum_{k=1}^{n}\frac{\partial(\varphi_2)_k(x)}{\partial x_k},$$

At this point we define

$$\delta A(u,\varphi_1,\varphi_2) = \frac{d}{d\varepsilon}\left(\tilde{A}(u,\varphi_1,\varphi_2,\varepsilon)\right)|_{\varepsilon=0},$$

so that

$$\begin{aligned} \delta A(u,\varphi_1,\varphi_2) &= \int_\Omega\Bigg(\sum_{i=1}^{N}\Bigg(\frac{\partial L(u,\nabla u)}{\partial u_i}(\varphi_1)_i \\ &\quad+\sum_{k=1}^{n}\left(\frac{\partial L(u,\nabla u)}{\partial(u_i)_{x_k}}((\varphi_1)_i)_{x_k}\right) \\ &\quad+\sum_{k=1}^{n}\frac{\delta L[u]}{\delta u_i}\frac{\partial u_i}{\partial x_k}(\varphi_2)_k\Bigg)+\sum_{k=1}^{n}L[u]\frac{\partial(\varphi_2)_k}{\partial x_k}\Bigg)\,dx. \end{aligned} \tag{140}$$

From this and

$$\frac{\partial L(u,\nabla u)}{\partial u_i}-\frac{d}{dx_k}\left(\frac{\partial L(u,\nabla u)}{\partial u_{x_k}}\right) = 0, \text{ in } \Omega, \ \forall i\in\{1,\cdots,N\},$$

we obtain

$$\begin{aligned} \delta A(u,\varphi_1,\varphi_2) &= \sum_{i=1}^{N}\sum_{k=1}^{n}\left(\int_\Omega\frac{d}{dx_k}\left(\frac{\partial L[u]}{\partial(u_i)_{x_k}}(\varphi_1)_k\right)\right)dx \\ &\quad+\sum_{k=1}^{n}\int_\Omega\frac{d(L[u](\varphi_2)_k)}{dx_k}\,dx. \end{aligned} \tag{141}$$

In particular, for

$$(\varphi_2)_k = \sum_{j=1}^{N}X_j^k w^j$$

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and

$$(\varphi_1)_i = \sum_{j=1}^{N} \left(\psi_{ij} w^j - \sum_{k=1}^{n} \frac{\partial u_i}{\partial x_k} X_j^k w^j \right),$$

we obtain

$$\begin{aligned} & \delta A(u, \varphi_1, \varphi_2) \\ = & \sum_{i=1}^{N} \sum_{k=1}^{n} \int_\Omega \left(\frac{d}{dx_k} \left(\frac{\partial L[u]}{\partial (u_i)_k} \left(\sum_{j=1}^{N} \left(\psi_{ij} - \sum_{l=1}^{n} \frac{\partial u_i(x)}{\partial x_l} X_j^l w^j \right) \right) \right) \right) dx \\ & + \sum_{k=1}^{n} \int_\Omega \frac{\partial L[u] X_j^k w^j}{dx_k} dx \\ = & \sum_{j=1}^{N} \left(\sum_{k=1}^{n} \left(\int_\Omega \frac{d}{dx_k} \left(\sum_{i=1}^{N} \frac{\partial L[u]}{\partial (u_i)_k} \left(\sum_{j=1}^{N} \left(\psi_{ij} - \sum_{l=1}^{n} \frac{\partial u_i(x)}{\partial x_l} X_j^l w^j \right) \right) \right. \right. \right. \\ & \left. \left. \left. + L[u] X_j^k w^j \right) dx \right) \right). \end{aligned} \tag{142}$$

Moreover, we define

$$\theta_k^j = \sum_{i=1}^{N} \left(\frac{\partial L[u]}{\partial (u_i)_{x_k}} \left(-\psi_{ij} + \sum_{l=1}^{n} \frac{\partial u_i}{\partial x_l} X_j^l \right) \right) - L(u) X_j^k$$

so that

$$\delta A(u, \varphi_1, \varphi_2) = - \int_\Omega \sum_{j=1}^{N} \sum_{k=1}^{n} \frac{d(\theta_j^k w^j)}{dx_k} dx,$$

$\forall \{w^j\} \in C_c^\infty(\Omega; \mathbb{R}^N)$.

In particular, for

$$\psi_{ij} = 0$$

and

$$X_j^k = \delta_j^k$$

we obtain the Energy-Momentum tensor T_k^j, where

$$T_k^j \equiv \theta_k^j = \sum_{i=1}^{N} \sum_{l=1}^{n} \left(\frac{\partial L[u]}{\partial (u_i)_{x_k}} \frac{\partial u_i}{\partial x_l} \delta_j^l \right) - L[u] \delta_j^k.$$

25.1. *The Angular-Momentum tensor*

In this subsection we define the following change of variables

$$x'_k = x_k + \sum_{m \neq k} g^{mm} x_m \varepsilon \, w^{km},$$

where

$$w^{km} = -w^{mk}.$$

With such relations in mind, we set

$$\begin{aligned} \delta x_k &= x'_k - x_k \\ &= \varepsilon \sum_{l=1}^{n} \sum_{m<l} w^{ml} (g^{ll} x_l g_m^k - g^{mm} x_m g_l^k). \end{aligned} \tag{143}$$

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We define also,

$$u'_i(x') = u_i(x) + \delta u_i(x)$$

where

$$\delta u_i(x) = \sum_{l=1}^{n} \sum_{j,p<l} A^j_{i(pl)} u_j(x) \varepsilon\, w^{pl}.$$

Moreover, we define

$$\psi_{i(mn)} = \sum_{j=1}^{n} A^j_{i(mn)},$$

where

$$A^j_{i(pl)} = g_{ip}\delta^j_l - g^l_i \delta^j_p.$$

Hence,

$$\psi_{i(mn)} = \sum_{j=1}^{n} A^j_{i(mn)} u_j(x) = g_{in} u_m(x) - g_{jm} u_n(x).$$

For the general variation, we define again

$$\tilde{A}(u, \varphi_1, \varphi_2, \varepsilon) = \int_\Omega L[u(x + \varepsilon\varphi_2(x)) + \varepsilon\varphi_1(x)] \ \det J(x)\ dx.$$

where we have generically denoted

$$L[u] \equiv L(u, \nabla u),$$

$$L[u(x + \varepsilon\varphi_2(x)) + \varepsilon\varphi_1(x)] \equiv L(u(x + \varepsilon\varphi_2(x)) + \varepsilon\varphi_1(x), \nabla u(x + \varepsilon\varphi_2(x)) + \varepsilon\nabla\varphi_1(x)),$$

$$\begin{aligned} J(x) &= \left\{ \frac{\partial x'_j}{\partial x_k} \right\} \\ &= \left\{ \frac{\partial (x_j + \varepsilon(\varphi_2)_j(x))}{\partial x_k} \right\} \\ &= \left\{ \delta_{jk} + \varepsilon \frac{\partial (\varphi_2)_j(x)}{\partial x_k} \right\}. \end{aligned} \tag{144}$$

and

$$\delta A(u, \varphi_1, \varphi_2) = \frac{d}{d\varepsilon} \left(\tilde{A}(u, \varphi_1, \varphi_2, \varepsilon) \right) |_{\varepsilon=0},$$

Moreover, we set

$$(\varphi_2)^{ml}_k = w^{ml}(g^{ll} x_l \delta^k_m - g^{mm} x_m \delta^k_l),$$

and

$$\overline{\delta u_i} = u'_i(x) - u_i(x).$$

Thus,

$$\begin{aligned} \delta u_i(x) &= u'_i(x) - u_i(x) \\ &= u'_i(x') - u'_i(x) + u'_i(x) - u_i(x), \end{aligned} \tag{145}$$

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so that

$$\begin{aligned}
& \overline{\delta u_i(x)} = u_i'(x) - u_i(x) \\
= \; & \delta u_i(x) - (u_i'(x') - u_i'(x)) \\
& \delta u_i(x) - \sum_{k=1}^{n} \frac{\partial u_i(x)}{dx_k} \delta x_k + \mathcal{O}(\varepsilon^2) \\
= \; & \delta u_i(x) - \sum_{l=1}^{n} \sum_{m<l} \sum_{k=1}^{n} \frac{\partial u_i(x)}{\partial x_k} \varepsilon w^{ml} (g^{ll} x_l \delta_m^k - g^{mm} x_m \delta_l^k) + \mathcal{O}(\varepsilon^2) \\
= \; & \varepsilon \left(\sum_{l=1}^{n} \sum_{j,k<l} A_{i(kl)}^{j} u_j(x) w^{kl} - \sum_{l=1}^{n} \sum_{m<l} \sum_{k=1}^{n} \frac{\partial u_i(x)}{\partial x_k} w^{ml} (g^{ll} x_l \delta_m^k - g^{mm} x_m \delta_l^k) \right) + \mathcal{O}(\varepsilon^2),
\end{aligned}$$

With such results in mind, we define

$$\begin{aligned}
(\varphi_1)_i^{ml} \; = \; & \sum_{j,k<l} A_{i(kl)}^{j} u_j(x) w^{ml} \\
& - \sum_{k=1}^{n} \left(\frac{\partial u_i(x)}{\partial x_k} w^{ml} (g^{ll} x_l \delta_m^k - g^{mm} x_m \delta_l^k) \right).
\end{aligned} \tag{146}$$

Similarly as in the previous section, we may obtain

$$\begin{aligned}
& \delta A(u, \varphi_1, \varphi_2) \\
= \; & \frac{d\tilde{A}(u, \varphi_1, \varphi_2, \varepsilon)}{d\varepsilon}|_{\varepsilon=0} \\
= \; & \sum_{l=1}^{n} \sum_{j,m<l} \sum_{k=1}^{n} \sum_{i=1}^{N} \int_\Omega \frac{d}{dx_k} \left(\frac{\partial L[u]}{\partial (u_i)_{x_k}} (A_{i(l,m)^j} u_j(x) + \frac{\partial u_i}{\partial x_p} g^{mm} x_m \delta_l^p - \frac{\partial u_i}{\partial x_p} g^{ll} x_l \delta_m^p) w^{ml} \right) dx \\
& + \sum_{k=1}^{n} \sum_{l=1}^{n} \sum_{j,m<l} \sum_{i=1}^{N} \int_\Omega \frac{d}{dx_k} \left(L[u] (g^{ll} x_l \delta_m^k - g^{mm} x_m \delta_l^k) w^{ml} \right) dx
\end{aligned} \tag{147}$$

Thus,

$$\delta A(u, \varphi_1, \varphi_2) = - \sum_{k=1}^{n} \sum_{m<l} \int_\Omega \frac{d}{dx_k} \left(M_{ml}^k w^{ml} \right) dx,$$

where

$$\begin{aligned}
M_{ml}^k \; = \; & \sum_{i=1}^{N} \sum_{j<l} \frac{\partial L[u]}{\partial (u_i)_{x_k}} \left(A_{ilm}^{j} u_j - \frac{\partial u_i}{\partial x_l} g^{mm} x_m + \frac{\partial u_i}{\partial x_m} g^{ll} x_l \right) \\
& + L[u] (g^{ll} x_l \delta_m^k + g^{mm} x_m \delta_l^k),
\end{aligned} \tag{148}$$

so that

$$\begin{aligned}
M_{lm}^k \; = \; & (g^{mm} x_m T_l^k - g^{ll} x_l T_m^k) \\
& - \sum_{i=1}^{n} \sum_{j<l} \frac{\partial L[u]}{\partial (u_i)_{x_k}} A_{i(lm)}^{j} u_j(x) \\
= \; & L_{ml}^k + S_{ml}^k,
\end{aligned} \tag{149}$$

where

$$L_{ml}^k = (g^{mm} x_m T_l^k - g^{ll} x_l T_m^k)$$

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and

$$S^k_{ml} = -\sum_{i=1}^{N}\sum_{j<l}\frac{\partial L[u]}{\partial (u_i)_{x_k}} A^j_{i(lm)} u_j(x).$$

The tensor $\{L^k_{ml}\}$ is said to be the Orbital angular momentum tensor and $\{S^k_{ml}\}$ is said to be Spin one.

25.2. A note on the solution of the Klein-Gordon equation

For $\Omega = \mathbb{R}^4$, $\Omega_1 = \mathbb{R}^3$ and denoting as usual by $i \in \mathbb{C}$ the imaginary unit, consider the Klein-Gordon equation in distributional sense

$$-\frac{\partial^2 u}{\partial t^2} + \sum_{j=1}^{3}\frac{\partial^2 u}{\partial x_j^2} - m^2 u = 0, \text{ in } \Omega,$$

where $u \in V = W^{1,2}(\Omega)$.

Defining the Fourier transform of u, by

$$\phi(p) = \frac{1}{(2\pi)^{3/2}}\int_\Omega e^{-ip\cdot x} u(x)\, dx,$$

in the momenta space, the last equation is equivalent to

$$\left(p_0^2 - \sum_{j=1}^{3} p_j^2 - m^2\right)\phi(p) = 0, \text{ in } \Omega,$$

where we have denoted $p = (p_0, p_1, p_2, p_3) \in \mathbb{R}^4$, and $x = (x_0, x_1, x_2, x_3) \in \mathbb{R}\ 4$

Observe that a general solution for this last equation is given by the wave function

$$\hat{\phi}(p) = \delta\left(p_0^2 - \sum_{j=1}^{3} p_j^2 - m^2\right)\phi(p),$$

where $\phi \in W^{1,2}(\Omega)$.

Indeed,

$$\begin{aligned}\left(p_0^2 - \sum_{j=1}^{3} p_j^2 - m^2\right)\hat{\phi}(p) &= \left(p_0^2 - \sum_{j=1}^{3} p_j^2 - m^2\right)\delta\left(p_0^2 - \sum_{j=1}^{3} p_j^2 - m^2\right)\phi(p) \\ &= 0, \text{ in } \Omega. \end{aligned} \tag{150}$$

Here, we recall that generically for the Dirac delta function $\delta(t)$, we have

$$\delta(t) = \begin{cases} 0, & \text{if } t \neq 0, \\ +\infty, & \text{if } t = 0. \end{cases} \tag{151}$$

Observe that, for the scalar case in the previous section, we have

$$2T^{00} = \sum_{j=0}^{3}\left(\frac{\partial u}{\partial x_j}\right)^2 + m^2 u.$$

Also, from

$$-\frac{\partial^2 u}{\partial t^2} + \sum_{j=1}^{3}\frac{\partial^2 u}{\partial x_j^2} - m^2 u = 0, \text{ in } \Omega,$$

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we get

$$\int_\Omega \left(\frac{\partial u}{\partial t}\right)^2 dx - \sum_{j=1}^{3} \int_\Omega \left(\frac{\partial u}{\partial x_j}\right)^2 dx - m^2 \int_\Omega u^2 \, dx = 0,$$

so that

$$\int_\Omega \left(\frac{\partial u}{\partial t}\right)^2 dx = \sum_{j=1}^{3} \int_\Omega \left(\frac{\partial u}{\partial x_j}\right)^2 dx + m^2 \int_\Omega u^2 \, dx.$$

From such results, we may infer that

$$\begin{aligned} \int_\Omega T^{00} \, dx &= \int_\Omega \left(\frac{\partial u}{\partial t}\right)^2 dx \\ &= \left\| \frac{\partial u}{\partial t} \right\|_{L^2}^2 \\ &= \sum_{j=1}^{3} \int_\Omega \left(\frac{\partial u}{\partial x_j}\right)^2 dx + m^2 \int_\Omega u^2 \, dx. \end{aligned} \tag{152}$$

On the other hand,

$$\begin{aligned} & \sum_{j=1}^{3} \int_\Omega \left(\frac{\partial u}{\partial x_j}\right)^2 dx \\ = & \frac{1}{(2\pi)^3} \sum_{j=1}^{3} \int_\Omega \left(\int_\Omega i \, p_j \, \hat{\phi}(p) \, e^{ip\cdot x} dp \right) \left(\int_\Omega i \, p'_j \hat{\phi}(p') \, e^{ip'\cdot x} \, dp' \right) dx \\ = & \frac{1}{(2\pi)^3} \sum_{j=1}^{3} \int_\Omega \int_\Omega \left(-p_j \, p'_j \, \hat{\phi}(p) \, \hat{\phi}(p') \int_\Omega e^{i(p+p')\cdot x} \, dx \right) dp \, dp' \\ = & \frac{1}{(2\pi)^{3/2}} \sum_{j=1}^{3} \int_\Omega \int_\Omega \left(-p_j \, p'_j \, \hat{\phi}(p) \, \hat{\phi}(p') \, \delta(p+p') \right) dp \, dp' \\ = & \frac{1}{(2\pi)^{3/2}} \sum_{j=1}^{3} \int_\Omega \left(p_j^2 \, \hat{\phi}(p) \, \hat{\phi}(-p) \right) dp. \end{aligned} \tag{153}$$

Thus, denoting $\hat{p} = (p_1, p_2, p_3)$, $d\hat{p} = dp_1 \, dp_2 \, dp_3$, and

$$p_0(\hat{p}) = \sqrt{\sum_{j=1}^{3} p_j^2 + m^2},$$

we may infer that

$$\begin{aligned} \int_\Omega T^{00} \, dx &= \frac{1}{(2\pi)^{3/2}} \int_\Omega \left(\sum_{j=1}^{3} p_j^2 + m^2 \right) \hat{\phi}(p) \, \hat{\phi}(-p)) \, dp \\ &= \frac{1}{(2\pi)^{3/2}} \int_\Omega \left(\sum_{j=1}^{3} p_j^2 + m^2 \right) \delta \left(p_0^2 - \sum_{j=1}^{3} p_j^2 - m^2 \right) \phi(p) \, \phi(-p)) \, dp \\ &= \frac{1}{(2\pi)^{3/2}} \int_{\Omega_1} \left(p_0(\hat{p})^2 \, \phi(p_0(\hat{p}), \hat{p}) \, \phi(-p_0(\hat{p}), -\hat{p}) \right) d\hat{p}. \end{aligned} \tag{154}$$

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Summarizing we have got

$$\begin{aligned}\int_\Omega T^{00}\,dx &= \frac{1}{(2\pi)^{3/2}}\int_{\Omega_1}\left(p_0(\hat{p})^2\,\phi(p_0(\hat{p}),\hat{p})\,\phi(-p_0(\hat{p}),-\hat{p})\right)\,d\hat{p}\\ &= \left\|\frac{\partial u}{\partial t}\right\|_{L^2}^2,\end{aligned}\tag{155}$$

so that

$$\int_\Omega T^{00}\,dx = \left\|\frac{\partial u}{\partial t}\right\|_{L^2}^2$$

may be expressed as a kind of average expectance of p_0^2 related to the function $\phi(p)$.

25.3. A note on the Dirac equation

In this subsection we denote

$$\Delta^2 = \sum_{j=0}^{3} g^{jj} L_j\,L_j,$$

where

$$L_j = i\,g^{jj}\frac{\partial}{\partial x_j},\ \forall j\in\{0,1,2,3\}.$$

We recall that the relativistic Klein-Gordon equation may be written as

$$(\Delta^2 - m^2)u = 0,\ \text{in}\ \Omega = \mathbb{R}^4.$$

Moreover, for 4×4 matrices γ^k indicated in the subsequent lines, we may obtain

$$\{D_{ij}\}u = \left[-i\left(\sum_{j=0}^{3}\gamma^j\frac{\partial}{\partial x_j}\right) - m\right]\left[-i\left(\sum_{j=0}^{3}\gamma^j\frac{\partial}{\partial x_j}\right) + m\right]u,$$

where

$$D_{ii} = \Delta^2 - m^2$$

and

$$D_{ij} = 0,\ \text{if}\ i\neq j,\ \forall i,j\in\{0,1,2,3\}.$$

Here

$$u = (u_0,u_1,u_2,u_3)^T \in V = W^{1,2}(\Omega;\mathbb{C}^4).$$

In such a case the fundamental Dirac equation stands for

$$\left[i\left(\sum_{j=0}^{3}\gamma^j\frac{\partial}{\partial x_j}\right) - m\right]u = \mathbf{0}\in\mathbb{R}^4,\ \text{in}\ \Omega.$$

Summarizing, if $(u_0,u_1,u_2,u_3)^T\in V$ is a solution of this last Dirac equation, then u_0,u_1,u_2,u_3 are four solutions of the Klein-Gordon equation.

In the momentum configuration space, through the Fourier transform proprieties, the Dirac equation stands for

$$(\hat{p}+m)\hat{u}(p) = \mathbf{0},\ \text{in}\ \mathbb{R}^4,$$

where

$$\hat{p} = \sum_{j=0}^{3} g^{jj}p_j\gamma^j.$$

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Observe that

$$\tilde{u}(p) = \delta(\hat{p} + m)u(p)$$

corresponds to a general solution of the Dirac equation.

Indeed,

$$(\hat{p} + m)\tilde{u}(p) = (\hat{p} + m)\delta(\hat{p} + m)u(p) = \mathbf{0} \in \mathbb{R}^4, \text{ in } \Omega.$$

On the other hand

$$\hat{u}(p) = \delta\left(p_0^2 - \sum_{j=1}^{3} p_j^2 - m^2\right) u(p)$$

correspond to four solutions of the Klein-Gordon equation.

At this point, we assume such a $\hat{u}(p)$ corresponds to a solution of the Dirac equation as well.

Furthermore, here we recall that (please see the first chapter of the book [20], by N.N. Bogoliubov and D.V. Shirkov for details):

$$\gamma^0 = \left\{ \begin{array}{cccc} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{array} \right\}, \tag{156}$$

$$\gamma^1 = \left\{ \begin{array}{cccc} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{array} \right\}, \tag{157}$$

$$\gamma^2 = \left\{ \begin{array}{cccc} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & i & 0 & 0 \\ -i & 0 & 0 & 0 \end{array} \right\}, \tag{158}$$

$$\gamma^3 = \left\{ \begin{array}{cccc} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{array} \right\} \tag{159}$$

and

$$\gamma^5 = \left\{ \begin{array}{cccc} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & -i \\ -i & 0 & 0 & 0 \\ 0 & -i & 0 & 0 \end{array} \right\} \tag{160}$$

where we also denote

$$\alpha_j = \gamma^0\gamma^j, \ \forall j \in \{1,2,3\},$$

$$\sigma_j = i\gamma^5\gamma^0\gamma^j, \ \forall j \in \{1,2,3\},$$

and

$$\beta = \gamma^0.$$

On the other hand, a variational formulation for the Dirac equation corresponds to the functional $A : V \to \mathbb{R}$ where

$$A(u) = \frac{1}{2}\int_\Omega L(u, \nabla u)\, dx,$$

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where

$$L(u,\nabla u) = i\sum_{j=0}^{3}\left(u^*\gamma^j\frac{\partial u}{\partial x_j} - \frac{\partial u^*}{\partial x_j}\gamma^j u\right) - m^2u^*u,$$

where here

$$u = (u_0,u_1,u_2,u_3)^T \in W^{1,2}(\Omega;\mathbb{C}^4).$$

From such statements and definitions, similarly as in the previous sections (please see [20] for details), we may obtain

$$T^{kl} = \frac{i}{2}g^{ll}\left(u^*\gamma^k\frac{\partial u}{\partial x_l} - \frac{\partial u^*}{\partial x_l}\gamma^k u\right),$$

and

$$S^{k,lm} = -\left(\frac{\partial L(u,\nabla u)}{\partial u_{x_k}}A^{u,lm}u - u^*A^{u^*,lm}\frac{\partial L(u,\nabla u)}{\partial u_{x_k}}\right),$$

where

$$A^{u,lm} = \frac{i}{2}\sigma^{ml},$$

$$A^{u^*,lm} = \frac{i}{2}\sigma^{lm},$$

and where

$$\sigma^{lm} = \frac{\gamma^l\gamma^k - \gamma^k\gamma^l}{2},$$

so that

$$S^{k,lm} = \frac{1}{4}u^*\left(\gamma^k\sigma^{lm} - \sigma^{lm}\gamma^k\right)u.$$

Thus,

$$\begin{aligned}
&\int_\Omega S^{k,lm}\,dx\\
&= \frac{1}{4}\int_\Omega\left(u^*\left(\gamma^k\sigma^{lm} - \sigma^{lm}\gamma^k\right)u\right)\,dx\\
&= \frac{1}{4}\frac{1}{(2\pi)^3}\int_\Omega\left(\int_\Omega\int_\Omega\left(\hat{u}(p)e^{ip\cdot x}(\gamma^k\sigma^{lm} - \sigma^{lm}\gamma^k)\hat{u}(p')e^{ip'\cdot x}\right)\,dp\,dp'\right)\,dx\\
&= \frac{1}{4}\frac{1}{(2\pi)^{3/2}}\int_\Omega\int_\Omega\left(\hat{u}(p)(\gamma^k\sigma^{lm} - \sigma^{lm}\gamma^k)\delta(p+p')\hat{u}(p')\right)\,dp\,dp'\\
&= \frac{1}{4}\frac{1}{(2\pi)^{3/2}}\int_\Omega\left(\hat{u}(p)(\gamma^k\sigma^{lm} - \sigma^{lm}\gamma^k)\hat{u}(-p)\right)\,dp\\
&= \frac{1}{4}\frac{1}{(2\pi)^{3/2}}\int_\Omega\left(u(p)(\gamma^k\sigma^{lm} - \sigma^{lm}\gamma^k)\delta\left(p_0^2 - \sum_{j=1}^{3}p_j^2 - m^2\right)u(-p)\right)\,dp\\
&= \frac{1}{4}\frac{1}{(2\pi)^{3/2}}\int_{\Omega_1}\left(u(p_0(\hat{p}),\hat{p})(\gamma^k\sigma^{lm} - \sigma^{lm}\gamma^k)u(-p_0(\hat{p}),-\hat{p})\right)\,d\hat{p},
\end{aligned}\tag{161}$$

where

$$p_0(\hat{p}) = \sqrt{\sum_{j=1}^{3}p_j^2 + m^2}.$$

Summarizing, we have got

$$\int_\Omega S^{k,lm}\,dx = \frac{1}{4(2\pi)^{3/2}}\int_{\Omega_1}\left(u(p_0(\hat{p}),\hat{p})(\gamma^k\sigma^{lm} - \sigma^{lm}\gamma^k)u(-p_0(\hat{p}),-\hat{p})\right)\,d\hat{p},$$

where $\Omega_1 = \mathbb{R}^3$, $\hat{p} = (p_1,p_2,p_3)$ and $d\hat{p} = dp_1\,dp_2\,dp_3$.

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26. A note on quantum field operators

This section is strongly based on the chapter 3, page 53 of the book [21], by G.B. Folland.

Therefore, here we have done a kind of review of these pages of such a book chapter indicated. In fact, we have simply opened more and clarified some calculations, in order to improve their understanding.

Let $\Omega = \hat{\Omega} \times [0, T] \subset \mathbb{R}^4$ where $\hat{\Omega} \subset \mathbb{R}^3$ is a open, bounded and connected set with a regular boundary denoted $\partial\hat{\Omega}$.

Define $V = W^{1,2}(\Omega)$ and

$$V_0 = W_0^{1,2}(\Omega).$$

Consider an operator $H : V_1 = V_0 \cap W^{2,2}(\Omega) \to Y$ where in a distributional sense,

$$H(u) = -\frac{\partial^2 u}{\partial t^2} + \nabla^2 u - m^2 u,$$

and where

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

Suppose there exists operators $B_1 : Y \to Y$ and $B_2 : Y \to Y$ such that

$$B_1 B_2(u) = H(u) + \frac{1}{2}u$$

and

$$B_2 B_1(u) = H(u) - \frac{1}{2}u, \ \forall u \in V_1.$$

Assume also $\phi_0 \in V_1$ is such that

$$\|\phi_0\|_{L^2} = 1,$$

and $B_1\phi_0 = 0$.

Now define

$$\phi_k = \frac{B_2^k(\phi_0)}{\sqrt{k!}}, \ \forall k \in \mathbb{N}.$$

Observe that

$$[B_1 B_2] = B_1 B_2 - B_2 B_1 = I_d.$$

We shall prove by induction that

$$[B_1, B_2^k] = k B_2^{k-1}, \ \forall k \in \mathbb{N}. \tag{162}$$

Indeed, for $k = 1$

$$[B_1, B_2] = I_d = 1 B_2^0,$$

so that (162) holds for $k = 1$.

Suppose now (162) holds for $k \in \mathbb{N}$, so that

$$[B_1, B_2^k] = k B_2^{k-1}.$$

In order to complete the induction, it suffices to prove that (162) holds for $k + 1$.

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Observe that

$$\begin{aligned}
[B_1, B_2^{k+1}] &= (B_1 B_2^{k+1} - B_2^{k+1} B_1) \\
&= (B_1 B_2^k) B_2 - B_2^{k+1} B_1 \\
&= (B_2^k B_1 + k B_2^{k-1}) B_2 - B_2^{k+1} B_1 \\
&= B_2^k (B_1 B_2) + k B_2^k - B_2^{k+1} B_1 \\
&= B_2^k (B_2 B_1 + I_d) + k B_2 - B_2^{k+1} B_1 \\
&= B_2^{k+1} B_1 + B_2^k + k B_2^k - B_2^{k+1} B_1 \\
&= (k+1) B_2^k. \qquad (163)
\end{aligned}$$

Thus, the induction is complete, so that

$$[B_1, B_2^k] = k B_2^{k-1}, \ \forall k \in \mathbb{N}.$$

Moreover, we recall that

$$B_1 \phi_0 = 0,$$

so that

$$\begin{aligned}
B_1 \phi_k &= B_1 \left(\frac{B_2^k \phi_0}{\sqrt{k!}} \right) \\
&= \frac{(B_2^k B_1 + k B_2^{k-1}) \phi_0}{\sqrt{k!}} \\
&= \frac{k \phi_{k-1} \sqrt{(k-1)!}}{\sqrt{k!}} \\
&= \frac{k \phi_{k-1}}{\sqrt{k}} \\
&= \sqrt{k} \phi_{k-1}, \ \forall k \in \mathbb{N}. \qquad (164)
\end{aligned}$$

Summarizing, we have got

$$B_1 \phi_k = \sqrt{k} \phi_{k-1}, \ \forall k \in \mathbb{N}.$$

Now, we shall prove that

$$B_2 \phi_k = \sqrt{k+1} \phi_{k+1}, \ \forall k \in \mathbb{N}.$$

Observe that

$$\begin{aligned}
B_2^{k+1} \phi_0 &= \phi_{k+1} (\sqrt{(k+1)!} \\
&= B_2 (B_2^k \phi_0) \\
&= (B_2 \phi_k) \sqrt{k!}. \qquad (165)
\end{aligned}$$

Summarizing, we have got

$$(B_2 \phi_k) \sqrt{k!} = \phi_{k+1} (\sqrt{(k+1)!},$$

so that

$$(B_2 \phi_k) = \sqrt{k+1} \phi_{k+1}, \ \forall k \in \mathbb{N}.$$

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Finally, from such results, we may infer that

$$\begin{aligned} B_1B_2\phi_k &= B_1(\sqrt{k+1}\phi_{k+1}) \\ &= \sqrt{k+1}B_1\phi_{k+1} \\ &= \sqrt{k+1}\sqrt{k+1}\phi_k \\ &= (k+1)\phi_k,\ \forall k \in \mathbb{N}. \end{aligned} \tag{166}$$

Similarly,

$$\begin{aligned} B_2B_1\phi_k &= B_2(\sqrt{k}\phi_{k-1}) \\ &= \sqrt{k}B_2\phi_{k-1} \\ &= \sqrt{k}\sqrt{k}\phi_k \\ &= k\phi_k. \end{aligned} \tag{167}$$

Therefore we have got

$$H\,\phi_k = B_1B_2\phi_k - \frac{1}{2}\phi_k = (k+1)\phi_k - \frac{1}{2}\phi_k = \left(k+\frac{1}{2}\right)\phi_k,$$

that is

$$H\phi_k = \left(k+\frac{1}{2}\right)\phi_k,\ \forall k \in \mathbb{N}.$$

Thus, for each $k \in \mathbb{N}$, $k+\frac{1}{2}$ is an eigenvalue of H with corresponding eigenvector ϕ_k.

26.1. An application concerning the harmonic oscillator operator in quantum mechanics

In this section we have the aim of representing the relativistic Klein-Gordon equation through the creation and annihilation operations related to the harmonic oscillator in quantum mechanics.

Consider first the one-dimensional Hamiltonian, corresponding to the harmonic oscillator, namely

$$H = -\frac{\hbar}{2m}\frac{d^2}{dx^2} + K\frac{x^2}{2},$$

which through an appropriate re-scale results into the following related Hamiltonian H_0, where

$$H_0 = \frac{1}{2}\left(-\frac{d^2}{dx^2} + x^2\right).$$

Define now the operators

$$B_1 = A = \frac{1}{\sqrt{2}}\left(x + \frac{d}{dx}\right),$$

and

$$B_2 = A^* = \frac{1}{\sqrt{2}}\left(x - \frac{d}{dx}\right).$$

Clearly,

$$H_0 = B_1B_2 - \frac{I_d}{2} = B_2B_1 + \frac{I_d}{2},$$

so that

$$[A, A^*] = [B_1, B_2] = B_1B_2 - B_2B_1 = I_d.$$

Similarly, as in the previous sections, by induction, we may obtain

$$[B_1, B_2^k] = kB_2^{k-1},\ \forall k \in \mathbb{N}.$$

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For

$$\phi_0 = \pi^{-1/4} e^{-\frac{x^2}{2}},$$

we define

$$\phi_k = \frac{1}{\sqrt{k}} B_2^k \phi_0, \ \forall k \in \mathbb{N}.$$

Also from the previous section, we may obtain

$$B_2 \phi_k = A^* \phi_k = \sqrt{k+1} \phi_{k+1},$$

$$B_1 \phi_k = A \phi_k = \sqrt{k} \phi_{k-1}, \ \forall k \in \mathbb{N}.$$

$$B_2 B_1 = A^* A \phi_k = k \phi_k,$$

and

$$B_1 B_2 \phi_k = A A^* \phi_k = (k+1) \phi_k, \forall k \in \mathbb{N} \cup \{0\}.$$

so that

$$H_0 \phi_k = (k + 1/2) \phi_k, \ \forall k \in \mathbb{N}.$$

Here we recall that

$$B_1 \phi_0 = A \phi_0 = 0,$$

and

$$\|\phi_0\|_{L^2} = 1.$$

In reference [21], page 54 it is proven that such a sequence $\{\phi_k\}$ is an ortho-normal basis for $L^2(\mathbb{R})$.

Finally, observe that for $\mathbb{R}^4$ we may define

$$(B_1)_j = A_j = \frac{1}{\sqrt{2}} \left(\frac{\partial}{\partial x_j} + x_j \right),$$

and

$$(B_2)_j = A_j^* = \frac{1}{\sqrt{2}} \left(-\frac{\partial}{\partial x_j} + x_j \right), \ \forall j \in \{0, 1, 2, 3\}.$$

Here generically,

$$\mathbf{x} = (x_0, x_1, x_2, x_3) \in \mathbb{R}^4.$$

Observe that clearly

$$\frac{\partial}{\partial x_j} = \frac{\sqrt{2}}{2} (A_j - A_j^*),$$

and

$$x_j I_d = \frac{\sqrt{2}}{2} (A_j + A_j^*), \ \forall j \in \{0, 1, 2, 3\}.$$

Denoting $x_0 = t$ where t stands for time, consider the relativistic Klein-Gordon equation,

$$-\frac{\partial^2 \phi}{\partial t^2} + \sum_{j=1}^{3} \frac{\partial^2 \phi}{\partial x_j^2} - m^2 \phi = 0.$$

From the previous results, we may represent such an equation by

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$$\left(-\frac{1}{2}(A_0 - A_0^*)^2 + \sum_{j=1}^{3} \frac{1}{2}(A_j - A_j^*)^2 - m^2 I_d\right)\phi = 0.$$

We highlight from the previous results we know the action of A_j and A_j^* on an appropriate basis of $L^2(\mathbb{R}^4)$ obtained though an appropriate tensorial product of the bases

$$\{\{\phi_k(x_j)\}, \text{ for } j \in \{0,1,2,3\}\}.$$

We shall call the operators A_j^* and A_j as the creation and annihilation operators concerning the original harmonic operator in quantum mechanics.

To justify such a nomenclature, we recall that $A_j^*\phi_0(x_j) = \phi_1(x_j)$ and $A_j\phi_0(x_j) = 0$, $\forall j \in \{0,1,2,3\}$.

27. A dual variational formulation for a related model

In this section we develop a concave dual variational formulation for a Ginzburg-Landau type equation.

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

Consider a functional $J : V \to \mathbb{R}$ defined by

$$\begin{aligned} J(u) &= \frac{\gamma}{2}\int_\Omega \nabla u \cdot \nabla u \, dx \\ &\quad + \frac{\alpha}{2}\int_\Omega (u^2 - \beta)^2 \, dx - \langle u, f\rangle_{L^2}, \end{aligned} \tag{168}$$

where $\gamma > 0$, $\alpha > 0$, $\beta > 0$, $f \in L^2(\Omega)$, and

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

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

Define now

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

for some appropriate $K_3 > 0$ and, $J_1 : V \times Y \to \mathbb{R}$ by

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

where

$$K_1 = \frac{1}{4\,\alpha K_3^2 + \varepsilon}$$

for some small parameter $0 < \varepsilon \ll 1$.

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Observe that

$$\begin{aligned} J(u,v_0^*) &= \frac{\gamma}{2}\int_\Omega \nabla u\cdot\nabla u\,dx + \langle u^2, v_0^*\rangle_{L^2} \\ &\quad + \frac{K_1}{2}\int_\Omega (-\gamma\nabla^2 u + 2v_0^* u - f)^2\,dx - \langle u, f\rangle_{L^2} \\ &\quad - \langle u^2, v_0^*\rangle_{L^2} + \frac{\alpha}{2}\int_\Omega (u^2-\beta)^2\,dx \\ &\geq \inf_{u\in V_1}\left\{\frac{\gamma}{2}\int_\Omega \nabla u\cdot\nabla u\,dx + \langle u^2, v_0^*\rangle_{L^2}\right. \\ &\quad \left. + \frac{K_1}{2}\int_\Omega (-\gamma\nabla^2 u + 2v_0^* u - f)^2\,dx - \langle u, f\rangle_{L^2}\right\} \\ &\quad + \inf_{v\in Y}\left\{-\langle v, v_0^*\rangle_{L^2} + \frac{\alpha}{2}\int_\Omega (v-\beta)^2\,dx\right\} \\ &= -F^*(v_0^*) - G^*(v_0^*) \\ &\equiv J^*(v_0^*), \forall u\in V_1,\ v_0^*\in Y^*, \end{aligned} \tag{169}$$

where we have denoted

$$F^*(v_0^*) = \sup_{u\in V_1}\{-\langle u^2, v_0^*\rangle_{L^2} - F(u,v_0^*)\},$$

$$F(u,v_0^*) = \frac{\gamma}{2}\int_\Omega \nabla u\cdot\nabla u\,dx + \frac{K_1}{2}\int_\Omega (-\gamma\nabla^2 u + 2v_0^* u - f)^2\,dx - \langle u, f\rangle_{L^2},$$

and

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

$$\begin{aligned} G^*(v_0^*) &= \sup_{v\in Y}\{\langle v, v_0^*\rangle_{L^2} - G(v)\} \\ &= \frac{1}{2\alpha}\int_\Omega (v_0^*)^2\,dx + \beta\int_\Omega v_0^*\,dx. \end{aligned} \tag{170}$$

Observe that

$$\frac{\partial F(u,v_0^*)}{\partial u^2} = -\gamma\nabla^2 + 2v_0^* + K_1(-\nabla^2 + 2v_0^*)^2,$$

so that we define

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

With such assumptions and definitions in mind, we may prove the following theorem:

Theorem 27.1. *For $J^*(v_0^*) = -F^*(v_0^*) - G^*(v_0^*)$, suppose $\hat{v}_0^*\in B^*$ is such that*

$$\delta J^*(\hat{v}_0^*) = \mathbf{0}.$$

Let $u_0\in Y$ be such that

$$\frac{\partial H(u_0,\hat{v}_0^*)}{\partial u} = \mathbf{0},$$

where

$$H(u,v_0^*) = F(u,v_0^*) + \langle u^2, v_0^*\rangle_{L^2}.$$

Suppose

$$u_0\in V_1.$$

Under such hypotheses,

$$F^*(\hat{v}_0^*) = H(u_0,\hat{v}_0^*),$$

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

and

$$\begin{aligned} J(u_0) &= J_1(u_0, \hat{v}_0^*) \\ &= \inf_{u \in V_1} J_1(u, \hat{v}_0^*) \\ &= \sup_{v_0^* \in Y^*} J^*(v_0^*) \\ &= J^*(\hat{v}_0^*). \end{aligned} \tag{171}$$

Proof. The proof that

$$F^*(\hat{v}_0^*) = H(u_0, \hat{v}_0^*),$$

is immediate from $\hat{v}_0 \in B^*$.

Moreover, the proof that

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

and

$$J(u_0) = J_1(u_0, \hat{v}_0^*) = J^*(\hat{v}_0^*)$$

may be done similarly as in the previous sections.

Observe that

$$J^*(v_0^*) = -F^*(v_0^*) - G^*(v_0^*) = \inf_{u \in V_1} \{H(u, v_0^*) - G^*(v_0^*)\},$$

so that J^* is concave in v_0^* as the infimum of a family of concave functionals in v_0^*.

From this and $\delta J^*(\hat{v}_0^*) = \mathbf{0}$ we get

$$J^*(\hat{v}_0^*) = \sup_{v_0^* \in Y^*} J^*(v_0^*).$$

Furthermore observe that

$$\begin{aligned} J(u_0) &= J_1(u_0, \hat{v}_0^*) \\ &\leq J_1(u, v_0^*) \\ &= F(u, \hat{v}_0^*) + \langle u^2, \hat{v}_0^* \rangle_{L^2} - G^*(\hat{v}_0^*) \\ &\leq F(u, \hat{v}_0^*) + \sup_{v_0^* \in Y^*} \left\{ \langle u^2, \hat{v}_0^* \rangle_{L^2} - G^*(\hat{v}_0^*) \right\} \\ &= F(u, \hat{v}_0^*) + G(u^2) \\ &= J_1(u, \hat{v}_0^*), \ \forall u \in V_1. \end{aligned} \tag{172}$$

Hence

$$J(u_0) = J_1(u_0, \hat{v}_0^*) = \inf_{u \in V_1} J_1(u, \hat{v}_0^*).$$

Joining the pieces, we have got

$$\begin{aligned} J(u_0) &= J_1(u_0, \hat{v}_0^*) \\ &= \inf_{u \in V_1} J_1(u, \hat{v}_0^*) \\ &= \sup_{v_0^* \in Y^*} J^*(v_0^*) \\ &= J^*(\hat{v}_0^*). \end{aligned} \tag{173}$$

The proof is complete. □

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28. The generalized method of lines applied to fourth order differential equations

In this sections we develop an application of the generalized method of lines to a fourth order equation.

We start by addressing the following ordinary differential equation (ode):

$$\varepsilon \frac{d^4 u(x)}{dx^4} - f = 0, \text{ in } [0,1],$$

with the boundary conditions

$$u(0) = u'(0) = 0$$

and

$$u(1) = u'(1) = 0.$$

In terms of linear elasticity, such a boundary conditions corresponds to a bi-clamped beam.

In a finite difference context, this last equation corresponds to

$$\varepsilon \left(\frac{u_{n+2} - 4u_{n+1} + 6u_n - 4u_{n-1} + u_{n-2}}{d^4} \right) - f_n = 0, \ \forall n \in \{1, \cdots N-2\},$$

where N is the number of nodes and $d = 1/N$.

Considering that, from the boundary conditions, $u_{-1} = u_0 = 0$, for $n = 1$ we get

$$6u_1 - 4u_2 + u_3 = \frac{f_1 d^4}{\varepsilon},$$

so that

$$u_1 = a_1 u_2 + b_1 u_3 + c_1,$$

where

$$a_1 = 2/3, \ \ b_1 - 1/6 \text{ and } c_1 = \frac{f_1 d^4}{6\varepsilon}.$$

Similarly, for $n = 2$, we obtain

$$-4u_1 + 6u_2 - 4u_3 + u_4 = \frac{f_2 d^4}{\varepsilon}.$$

Hence, replacing the value of u_1 previously obtained in this last equation, we have

$$-4(a_1 u_2 + b_1 u_3 + c_1) + 6u_2 - 4u_3 + u_4 = \frac{f_2 d^4}{\varepsilon},$$

so that

$$u_2 = a_2 u_3 + b_2 u_4 + c_2,$$

where defining $m_{12} = (6 - 4a_1)$, we have also

$$a_2 = \frac{4b_1 + 4}{m_{12}},$$

$$b_2 = -\frac{1}{m_{12}},$$

$$c_2 = \frac{1}{m_{12}} \left(\frac{f_2 d^4}{\varepsilon} + 4c_1 \right).$$

Now reasoning inductively, for n, having

$$u_{n-1} = a_{n-1} u_n + b_{n-1} u_{n+1} + c_{n-1},$$

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and

$$u_{n-2} = a_{n-2}u_{n-1} + b_{n-2}u_n + c_{n-2}$$

we obtain

$$u_{n-2} = a_{n-2}(a_{n-1}u_n + b_{n-1}u_{n+1} + c_{n-1}) + b_{n-2}u_n + c_{n-2},$$

so that from this and

$$u_{n+2} - 4u_{n+1} + 6u_n - 4u_{n-1} + u_{n-2} = \frac{f_n d^4}{\varepsilon},$$

we obtain

$$\begin{aligned} &a_{n-2}(a_{n-1}u_n + b_{n-1}u_{n+1} + c_{n-1}) + b_{n-2}u_n + c_{n-2} \\ &-4(a_{n-1}u_n + b_{n-1}u_{n+1} + c_{n-1}) + 6u_n - 4u_{n+1} + u_{n+2} = \frac{f_n d^4}{\varepsilon}, \end{aligned} \tag{174}$$

so that

$$u_n = a_n u_{n+1} + b_n u_{n+1} + c_n$$

where defining

$$m_{12} = (a_{n-2}(a_{n-1}) + b_{n-2} - 4a_{n-1} + 6)$$

we obtain

$$a_n = -\frac{1}{m_{12}}(a_{n-2}b_{n-1} - 4b_{n-1} - 4)$$

$$b_n = -\frac{1}{m_{12}},$$

and

$$c_n = \frac{1}{m_{12}}\left(a_{n-2}c_{n-1} + c_{n-2} - 4c_{n-1} - \frac{f_n d^4}{\varepsilon}\right).$$

Summarizing, we have got

$$u_n = a_n u_{n+1} + b_n u_{n+2} + c_n, \forall n \in \{1, \cdot N-2\}.$$

Observe now that from the boundary conditions,

$$u_{N-1} = u_N = 0.$$

From these last two equations, we may obtain

$$u_{N-2} = c_{N_2},$$

and

$$u_{N-3} = a_{N-3}u_{N-2} + b_{N-3}u_{N-1} + c_{N-3},$$

and so on up to obtaining

$$u_1 = a_1 u_2 + b_1 u_3 + c_1.$$

The problem is then solved.

28.1. *A numerical example*

We develop a numerical example considering

$$\varepsilon = 1,$$

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and

$$f \equiv 1, \text{ in } [0,1].$$

Thus, we have solved the equation

$$\varepsilon \frac{d^4 u(x)}{dx^4} - f = 0, \text{ in } [0,1],$$

with the boundary conditions

$$u(0) = u'(0) = 0$$

and

$$u(1) = u'(1) = 0.$$

In a finite differences context, we have used $N = 100$ nodes and $d = 1/N$. For a solution $u(x)$, please see Figure 19.

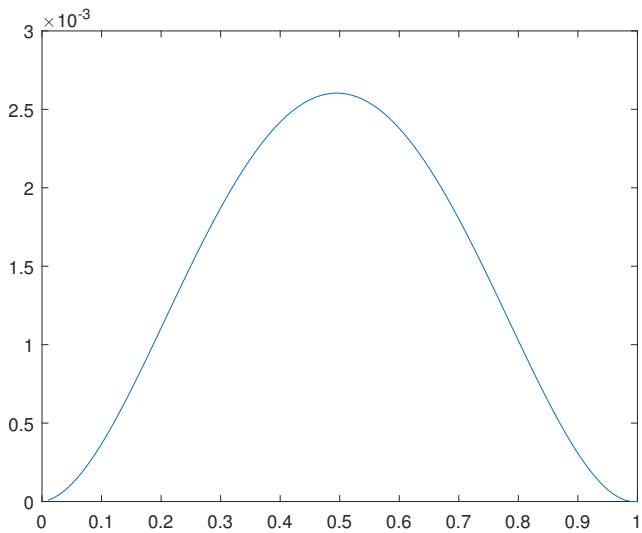

Figure 19. Solution $u(x)$ for the example B.

In the next lines, we present the concerning software in MAT-LAB
****

1. clear all

   m8=100;

   d=1/m8;

   e1=1.0;

   for i=1:m8

   f(i,1)=1.0;

   end;

   a(1)=2/3;

   b(1)=-1/6;

   c(1)=f(1,1)*d^4/(6e1);

   m12=(6-4*a(1));

   a(2)=(4*b(1)+4)/m12;

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```
b(2)=-1/m12;
c(2)=1/m12*(4*c(1)+f(2,1)*d^4/e1);
for i=3:m8-2
m12=(a(i-2)*a(i-1)+b(i-2)-4*a(i-1)+6);
a(i)=-1/m12*(a(i-2)*b(i-1)-4*b(i-1)-4);
b(i)=-1/m12;
c(i)=1/m12*(f(i,1)*d^4/e1-c(i-2)-a(i-2)*c(i-1)+4*c(i-1));
end;
u(m8,1)=0;
u(m8-1,1)=0;
for i=2:m8-1;
u(m8-i,1)=a(m8-i)*u(m8-i+1,1)+b(m8-i)*u(m8-i+2,1)+c(m8-i);
end;
for i=1:m8
x(i)=i*d;
end;
plot(x,u)
******************
```

29. Applications to the optimal shape design for a beam model

In this section, we present a numerical procedure for the shape optimization concerning the Bernoulli beam model.

Let $\Omega = [0,1] \subset \mathbb{R}$ corresponds to the horizontal axis of a straight beam with rectangular cross section $b \times h(x)$, that is, the beam has a variable thickness $h(x)$ distributed along such a horizontal axis x, where $x \in [0,1]$.

Define now

$$V = \{w \in W^{2,2}(\Omega) \ : \ w(0) = w(1) = 0\},$$

which corresponds to a simply supported beam.

Consider the problem of minimizing in $V \times B$ the functional

$$J(w,h) = \frac{1}{2}\int_{\Omega} H(x) w_{xx}(x)^2 \, dx$$

subject to

$$(H(x)w_{xx}(x))_{xx} - P(x) = 0, \text{ in } \Omega,$$

where

$$H(x) = \frac{h(x)^3 b}{12} E,$$

$h(x)$ is variable beam thickness, $A(x) = bh(x)$ corresponds to a rectangular cross section perpendicular to the x axis, and E is the young elasticity model.

Also, we define

$$B = \left\{ h : [0,1] \to \mathbb{R} \text{ measurable } : \ h_{min} \leq h(x) \leq h_{max} \text{ and } \int_0^1 h(x) \leq c_0 h_{max} \right\},$$

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where $0 < c_0 < 1$ and

$$C^* = \{w \in V \ : \ (H(x)w_{xx}(x))_{xx} - P(x) = 0, \text{ in } \Omega\}.$$

Observe that

$$\begin{aligned}
& \inf_{(w,h)\in C^*\times B} J(w,h) \\
= \ & \inf_{h\in B}\left\{\inf_{w\in C^*} J(w,h)\right\} \\
= \ & \inf_{h\in B}\left\{\sup_{\hat{w}\in V}\left\{\inf_{w\in V}\left\{\frac{1}{2}\int_\Omega H(x)w_{xx}(x)^2\,dx - \langle \hat{w}, (H(x)w_{xx}(x))_{xx} - P(x)\rangle_{L^2}\right\}\right\}\right\} \\
= \ & \inf_{h\in B}\left\{\sup_{\hat{w}\in V}\left\{-\frac{1}{2}\int_\Omega H(x)\hat{w}_{xx}^2\,dx + \langle \hat{w}, P\rangle_{L^2}\right\}\right\} \\
= \ & \inf_{h\in B}\left\{\inf_{M\in D^*}\left\{\frac{1}{2}\int_\Omega \frac{M^2}{H(x)}\,dx\right\}\right\}.
\end{aligned} \tag{175}$$

where

$$D^* = \{M \in Y^* \ : \ M_{xx} - P = 0, \text{ in } \Omega, \text{ and } M(0) = M(1) = 0\}.$$

Summarizing, we have got

$$\inf_{(w,h)\in C^*\times B} J(w,h) = \inf_{(M,h)\in D^*\times B}\left\{\frac{1}{2}\int_\Omega \frac{M^2}{H(x)}\,dx\right\}.$$

In order to obtain numerical results, we suggest the following primal dual procedure:

1. Set $n = 1$ and
$$h_n(x) = c_0 h_{max}.$$
2. Calculate $w_n \in V$ solution of equation
$$(H_n(x)(w_n)_{xx})_{xx} = P(x),$$
where
$$H_n(x) = \frac{Ebh_n(x)^3}{12}.$$
3. Calculate $h_{n+1}(x) \in B$ such that
$$J^*(M_n, h_{n+1}) = \inf_{h\in B} J^*(M_n, h),$$
where
$$M_n = H_n(w_n)_{xx},$$
$$J^*(M,h) = \frac{1}{2}\int_\Omega \frac{M^2}{H(x)}\,dx.$$
4. Set $n := n + 1$ and go to step 2 until an appropriate convergence criterion is satisfied.

We have developed numerical results for $c_0 = 0.65$, $E = 210\ 10^7$, $b = 0.1\ m$, $P(x) = 36\ 10^2\ N$, $h_{min} = 0.072\ m$ and $h_{max} = 0.18\ m$.

We have also defined

$$h(x) = t(x)h_{max},$$

where

$$0.4 \le t(x) \le 1, \text{ a.e. in } \Omega.$$

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For the optimal solution $w = w(x)$, please see Figure 20.
For a corresponding optimal solution $t = t(x)$, please see Figure 21.

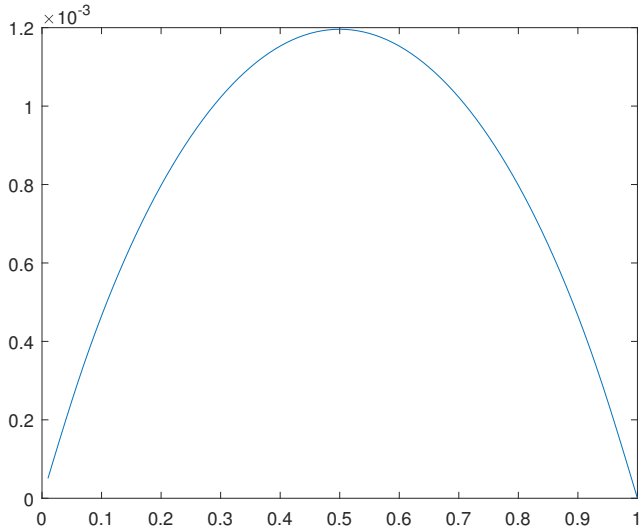

Figure 20. Optimal solution $w(x)$ for a simply supported beam.

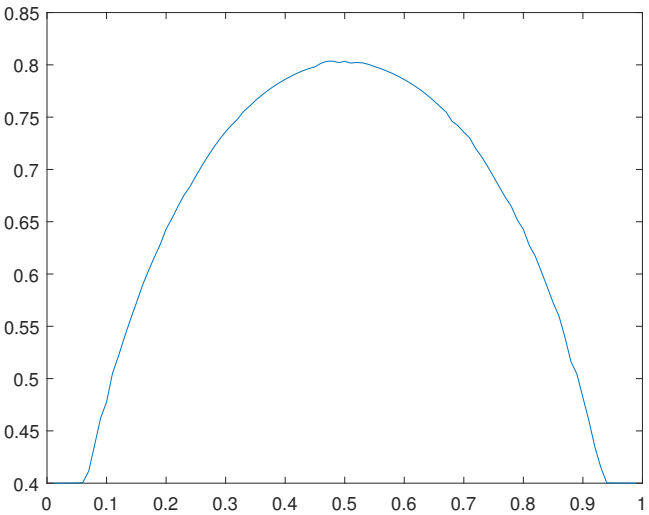

Figure 21. Optimal shape solution $t(x)$ for a simply supported beam.

Remark 29.1. *For such a simply-supported beam model, for the numerical solution of equation*

$$(H(x)w_{xx})_{xx} = P,$$

with the boundary conditions

$$w(0) = w(1) = w''(0) = w''(1) = 0$$

firstly we have solved the equation

$$v_{xx} - P = 0$$

with the boundary conditions

$$v(0) = v(1) = 0.$$

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Subsequently, we have solved the equation

$$H(x)w_{xx} = v$$

with the boundary conditions

$$w(0) = w(1) = 0.$$

Here we present the software developed in MAT-LAB.

****

1. clear all
   global m8 d d2wo H e1 ho h1 xo b5
   m8=100;
   d=1.0/m8;
   b5=0.1;
   e1=210*10^7;
   ho=0.18;
   A=zeros(m8-1,m8-1);
   for i=1:m8-1
   A(1,i)=1.0;
   xo(i,1)=0.55;
   x3(i,1)=0.55;
   end;
   lb=0.4*ones(m8-1,1);
   ub=ones(m8-1,1);
   b=zeros(m8-1,1);
   b(1,1)=0.65*(m8-1);
   for i=1:m8
   f(i,1)=1.0;
   L(i,1)=1/2;
   P(i,1)=36.0*10^2;
   end;
   i=1;
   m12=2;
   m50(i)=1/m12;
   z(i)=1/m50(i)*(-P(i,1)*d^2);
   for i=2:m8-1
   m12=2-m50(i-1);
   m50(i)=1/m12;
   z(i)=m50(i)*(-P(i,1)*d^2+z(i-1));
   end;
   v(m8,1)=0;

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```
for i=1:m8-1
v(m8-i,1)=m50(m8-i)*v(m8-i+1,1)+z(m8-i);
end;
k=1;
b12=1.0;
while (b12 > 10^-4) and (k < 10)
k
k=k+1;
for i=1:m8-1
H(i,1)=b5*L(i,1)^3 * ho^3/12*e1;
f1(i,1)=v(i,1)/H(i,1);
end;
i=1;
m12=2;
m70(i)=1/m12;
z1(i)=m70(i)*(-f1(i,1)*d^2);
for i=2:m8-1
m12=2-m70(i-1);
m70(i)=1/m12;
z1(i)=m70(i)*(-f1(i,1)*d^2+z1(i-1));
end;
w(m8,1)=0;
for i=1:m8-1
w(m8-i,1)=m70(m8-i)*w(m8-i+1,1)+z1(m8-i);
end;
d2wo(1,1)=(-2*w(1,1)+w(2,1))/d^2;
for i=2:m8-1
d2wo(i,1)=(w(i+1,1)-2*w(i,1)+w(i-1,1))/d^2;
end;
k9=1;
b14=1.0;
while (b14 > 10^-4) and (k9 < 120)
k9
k9=k9+1;
X=fmincon('beamNov2023',xo,A,b,[ ],[ ],lb,ub);
b14=max(abs(xo-X))
xo=X;
end;
b12=max(abs(xo-x3))
```

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```
x3=xo;
for i=1:m8-1
L(i,1)=xo(i,1);
end;
end;
**************
```

With the auxiliary function "beamNov2023":

```
********************
```

```
function S=beamNov2023(x)
global m8 d d2wo H e1 ho h1 xo b5
S=0;
for i=1:m8-1
S=S+1/(x(i,1)^3)/ho^3/b5/e1*(H(i,1)*d2wo(i,1))^2*12;
end;
****************************
```

We develop numerical results also for

$$V = W_0^{2,2}(\Omega) = \{w \in W^{2,2}(\Omega) \text{ such that } w(0) = w(1) = w'(0) = w'(1) = 0\}.$$

Such boundary conditions corresponds to bi-clamped beam. The remaining data is equal to the previous example

For the optimal solution $w = w(x)$, please see Figure 22.

For a corresponding optimal solution $t = t(x)$, please see Figure 23.

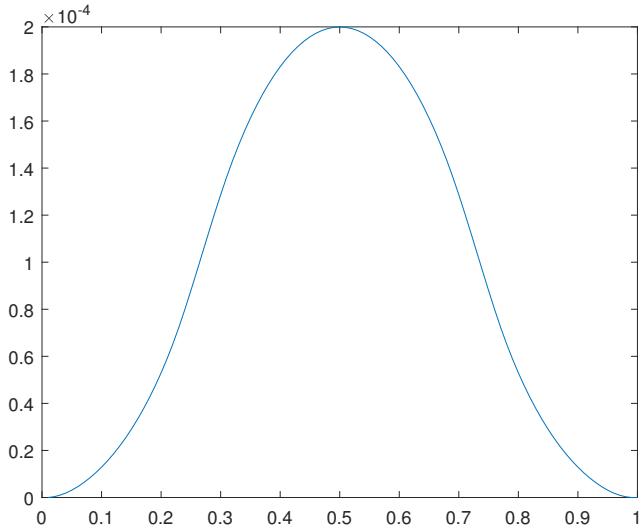

Figure 22. Optimal solution $w(x)$ for a bi-clamped beam.

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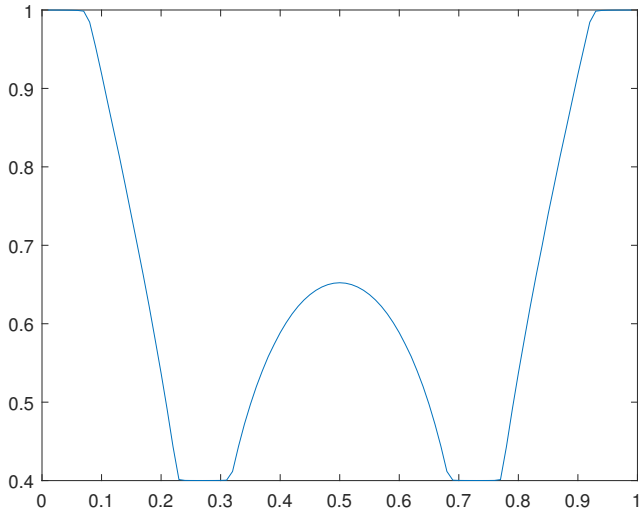

Figure 23. Optimal shape solution $t(x)$ for a bi-clamped beam.

Remark 29.2. *For such a bi-clamped beam model, for the numerical solution of equation*

$$(H(x)w_{xx})_{xx} = P,$$

with the boundary conditions

$$w(0) = w(1) = w'(0) = w'(1) = 0,$$

firstly we have solved the equation

$$v_{xx} - P = 0$$

with the boundary conditions

$$v(0) = v(1) = 0.$$

Subsequently, we solved the equation

$$H(x)w_{xx} = v + ax + b$$

with the boundary conditions

$$w(0) = w(1) = 0,$$

obtaining $a, b \in \mathbb{R}$ such that the boundary conditions

$$w'(0) = w'(1) = 0$$

are also satisfied.

Here we present the software developed in MAT-LAB.

****

1. clear all
   global m8 d d2wo H e1 ho h1 xo b5
   m8=100;
   d=1.0/m8;
   b5=0.1;
   e1=210*10^7;

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```
ho=0.18;
A=zeros(m8-1,m8-1);
for i=1:m8-1
A(1,i)=1.0;
xo(i,1)=0.55;
x3(i,1)=0.55;
end;
lb=0.4*ones(m8-1,1);
ub=ones(m8-1,1);
b=zeros(m8-1,1);
b(1,1)=0.65*(m8-1);
for i=1:m8
f(i,1)=1.0;
L(i,1)=1/2;
P(i,1)=36.0*10^2;
end;
i=1;
m12=2;
m50(i)=1/m12;
z(i)=1/m50(i)*(-P(i,1)*d^2);
for i=2:m8-1
m12=2-m50(i-1);
m50(i)=1/m12;
z(i)=m50(i)*(-P(i,1)*d^2+z(i-1));
end;
v(m8,1)=0;
for i=1:m8-1
v(m8-i,1)=m50(m8-i)*v(m8-i+1,1)+z(m8-i);
end;
k=1;
b12=1.0;
while (b12 > 10^-4) and (k < 10)
k
k=k+1;
for i=1:m8-1
H(i,1)=b5*L(i,1)^3 * ho^3/12*e1;
f1(i,1)=v(i,1)/H(i,1);
f2(i,1)=i*d/H(i,1);
f3(i,1)=1/H(i,1);
```

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```
end;
i=1;
m12=2;
m70(i)=1/m12;
z1(i)=m70(i)*(-f1(i,1)*d^2);
z2(i)=m70(i)*(-f2(i,1)*d^2);
z3(i)=m70(i)*(-f3(i,1)*d^2);
for i=2:m8-1
m12=2-m70(i-1);
m70(i)=1/m12;
z1(i)=m70(i)*(-f1(i,1)*d^2+z1(i-1));
z2(i)=m70(i)*(-f2(i,1)*d^2+z2(i-1));
z3(i)=m70(i)*(-f3(i,1)*d^2+z3(i-1));
end;
w1(m8,1)=0;
w2(m8,1)=0;
w3(m8,1)=0;
for i=1:m8-1
w1(m8-i,1)=m70(m8-i)*w1(m8-i+1,1)+z1(m8-i);
w2(m8-i,1)=m70(m8-i)*w2(m8-i+1,1)+z2(m8-i);
w3(m8-i,1)=m70(m8-i)*w3(m8-i+1,1)+z3(m8-i);
end;
m3(1,1)=w2(1,1);
m3(1,2)=w3(1,1);
m3(2,1)=w2(m8-1,1);
m3(2,2)=w3(m8-1,1);
h3(1,1)=-w1(1,1);
h3(2,1)=-w1(m8-1,1);
h5(:,1)=inv(m3)*h3;
for i=1:m8
wo(i,1)=w1(i,1)+h5(1,1)*w2(i,1)+h5(2,1)*w3(i,1);
end;
d2wo(1,1)=(-2*wo(1,1)+wo(2,1))/d^2;
for i=2:m8-1
d2wo(i,1)=(wo(i+1,1)-2*wo(i,1)+wo(i-1,1))/d^2;
end;
k9=1;
b14=1.0;
while (b14 > 10^-4) and (k9 < 120)
```

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```
k9
k9=k9+1;
X=fmincon('beamNov2023',xo,A,b,[ ], [ ],lb,ub);
b14=max(abs(xo-X))
xo=X;
end;
b12=max(abs(xo-x3))
x3=xo;
for i=1:m8-1
L(i,1)=xo(i,1);
end;
end;
****************************
```

Remark 29.3. *About the numerical results obtained for these two beam models, a final word of caution is necessary.*

Indeed, the full convergence in such cases is hard to obtain so that we have obtained just approximations of critical points with the functionals close to their optimal values. It is also worth emphasizing we have fixed the number of iterations so that the solutions and shapes obtained are just approximate ones.

30. Applications to the optimal shape design for a plate model

In this section, we present a numerical procedure for the shape optimization concerning a thin plate model.

Let $\Omega = [0,1] \times [0,1] \subset \mathbb{R}^2$ corresponds to the middle surface of a thin plate with a variable thickness $h(x,y)$.

Define now

$$V = \{w \in W^{2,2}(\Omega) \ : \ w = 0 \text{ on } \partial\Omega\},$$

which corresponds to a simply supported plate.

Consider the problem of minimizing in $V \times B$ the functional

$$J(w,h) = \frac{1}{2}\int_\Omega H(x,y)(\nabla^2 w(x,y))^2 \, dx$$

subject to

$$\nabla^2[(H(x,y)\nabla^2 w(x,y))] - P(x,y) = 0, \text{ in } \Omega,$$

where

$$H(x,y) = \frac{h(x,y)^3}{12} E/(1 - w_5^2),$$

$h = h(x,y)$ is variable plate thickness, E is the young elasticity model and $w_5 = 0.3$.

Also, we define

$$B = \left\{ h : \Omega \to \mathbb{R} \text{ measurable } \ : \ h_{min} \le h(x,y) \le h_{max} \text{ and } \int_\Omega h(x,y) \le c_0 h_{max} \right\},$$

where $0 < c_0 < 1$ and

$$C^* = \{w \in V \ : \ \nabla^2[H(x,y)\nabla^2 w(x,y))] - P(x,y) = 0, \text{ in } \Omega\}.$$

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Observe that

$$\begin{aligned}
&\inf_{(w,h)\in C^*\times B} J(w,h)\\
=\ &\inf_{h\in B}\left\{\inf_{w\in C^*} J(w,h)\right\}\\
=\ &\inf_{h\in B}\left\{\sup_{\hat{w}\in V}\left\{\inf_{w\in V}\left\{\frac{1}{2}\int_\Omega H(x,y)[\nabla^2\, w(x,y)]^2\, dx - \langle \hat{w}, \nabla^2[H(x,y)\nabla^2 w(x,y)] - P(x,y)\rangle_{L^2}\right\}\right\}\right\}\\
=\ &\inf_{h\in B}\left\{\sup_{\hat{w}\in V}\left\{-\frac{1}{2}\int_\Omega H(x,y)[\nabla^2\hat{w}(x,y)]^2\, dx + \langle \hat{w}, P\rangle_{L^2}\right\}\right\}\\
=\ &\inf_{h\in B}\left\{\inf_{\tilde{M}\in D^*}\left\{\frac{1}{2}\int_\Omega \frac{\tilde{M}^2}{H(x,y)}\, dx\right\}\right\}. \qquad (176)
\end{aligned}$$

where

$$D^* = \{\tilde{M}\in Y^* \quad \nabla^2\tilde{M} - P = 0, \text{ in } \Omega, \text{ and } \tilde{M} = 0, \text{ on } \Omega\}.$$

Summarizing, we have got

$$\inf_{(w,h)\in C^*\times B} J(w,h) = \inf_{(\tilde{M},h)\in D^*\times B}\left\{\frac{1}{2}\int_\Omega \frac{\tilde{M}^2}{H(x,y)}\, dx\right\}.$$

In order to obtain numerical results, we suggest the following primal dual procedure:

1. Set $n = 1$ and
$$h_n(x) = c_0 h_{max}.$$
2. Calculate $w_n \in V$ solution of equation
$$\nabla^2(H_n(x,y)\nabla^2 w_n(x,y)) = P(x,y),$$
where
$$H_n(x,y) = \frac{E h_n(x)^3}{12(1-w_5^2)}.$$
3. Calculate $h_{n+1}\in B$ such that
$$J^*(\tilde{M}_n, h_{n+1}) = \inf_{h\in B} J^*(\tilde{M}_n, h),$$
where
$$\tilde{M}_n = H_n(x,y)\nabla^2\, w_n,$$
$$J^*(\tilde{M},h) = \frac{1}{2}\int_\Omega \frac{\tilde{M}^2}{H(x,y)}\, dx.$$
4. Set $n := n+1$ and go to step 2 until an appropriate convergence criterion is satisfied.

We have developed numerical results for $c_0 = 0.75$, $E = 200\ 10^5$, $P(x,y) = 2\ 10^2\ N$, $h_{min} = 0.45 * (0.12)\ m$ and $h_{max} = 0.12\ m$.

We have also defined

$$h(x,y) = t(x,y)h_{max},$$

where

$$0.45 \le t(x,y) \le 1, \text{ a.e. in } \Omega.$$

For the optimal solution $w = w(x,y)$, please see Figure 24.

For a corresponding optimal solution $t = t(x,y)$, please see Figure 25.

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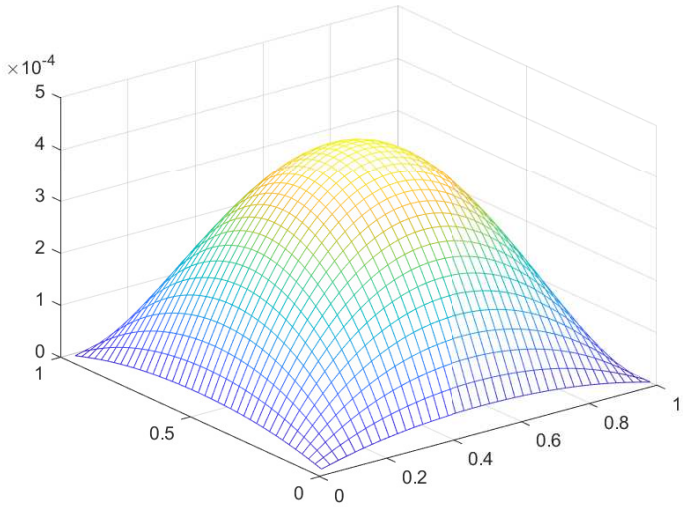

Figure 24. Optimal solution $w(x, y)$ for a simply supported plate.

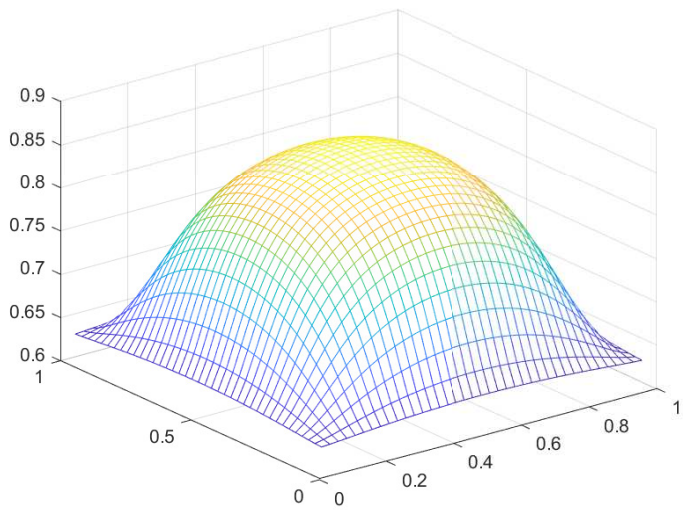

Figure 25. Optimal shape solution $t(x, y)$ for a simply supported plate.

Remark 30.1. *For such a simply-supported plate model, for the numerical solution of equation*

$$\nabla^2[H(x, y)\nabla^2 w(x, y)] = P,$$

with the boundary conditions

$$w = 0 \text{ on } \partial\Omega,$$

firstly we have solved the equation

$$\nabla^2 v - P = 0$$

with the boundary conditions

$$v = 0 \text{ on } \partial\Omega.$$

Subsequently, we have solved the equation

$$H(x, y)\nabla^2 w(x, y) = v(x, y)$$

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with the boundary conditions

$$w = 0 \text{ on } \partial\Omega.$$

Here we present the software developed in MAT-LAB.

****

1. clear all
   global m8 d d2xwo d2ywo H e1 ho xo b5
   m8=40;
   d=1.0/m8;
   w5=0.3;
   e1=200*$10^5/(1-w5^2)$;
   ho=0.12;
   A=zeros($(m8-1)^2$, $(m8-1)^2$);
   for i=1:$(m8-1)^2$
   A(1,i)=1.0;
   xo(i,1)=0.55;
   x3(i,1)=0.55;
   end;
   lb=0.45*ones($(m8-1)^2$,1);
   ub=ones($(m8-1)^2$,1);
   b=zeros($(m8-1)^2$,1);
   b(1,1)=0.75*$(m8-1)^2$;
   for i=1:(m8-1)
   for j=1:m8-1
   f(i,j,1)=1.0;
   L(i,j,1)=1/2;
   P(i,j,1)=2*10^2; end;
   end;
   for i=1:m8
   wo(:,i)=0.001*ones(m8-1,1);
   end;
   m2=zeros(m8-1,m8-1);
   for i=2:m8-2
   m2(i,i)=-2.0;
   m2(i,i-1)=1.0;
   m2(i,i+1)=1.0;
   end;
   m2(1,1)=-2.0;
   m2(1,2)=1.0;
   m2(m8-1,m8-1)=-2.0;

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```
m2(m8-1,m8-2)=1.0;
Id=eye(m8-1);
i=1;
m12=2*Id-m2*d^2/d^2; m50(:,:,i)=inv(m12);
z(:,i)=m50(:,:,i)*(-P(:,i,1)*d^2);
for i=2:m8-1
m12=2*Id-m2*d^2/d^2-m50(:,:,i-1);
m50(:,:,i)=inv(m12);
z(:,i)=m50(:,:,i)*(-P(:,i,1)*d^2+z(:,i-1));
end; v(:,m8)=zeros(m8-1,1);
for i=1:m8-1
v(:,m8-i)=m50(:,:,m8-i)*v(:,m8-i+1)+z(:,m8-i);
end;
k=1;
b12=1.0;
while (b12 > 10^-4) and (k < 12)
k
k=k+1;
for i=1:m8-1
for j=1:m8-1
H(j,i,1)=L(j,i,1)^3 * ho^3/12*e1;
f1(j,i,1)=v(j,i)/H(j,i,1);
end;
end;
i=1;
m12=2*Id-m2*d^2/d^2;
m70(:,:,i)=inv(m12);
z1(:,i)=m70(:,:,i)*(-f1(:,i,1)*d^2);
for i=2:m8-1
m12=2*Id-m2*d^2/d^2-m70(:,:,i-1);
m70(:,:,i)=inv(m12);
z1(:,i)=m70(:,:,i)*(-f1(:,i,1)*d^2+z1(:,i-1));
end;
w(:,m8)=zeros(m8-1,1);
for i=1:m8-1
w(:,m8-i)=m70(:,:,m8-i)*w(:,m8-i+1)+z1(:,m8-i);
end;
d2xwo(:,1)=(-2*w(:,1)+w(:,2))/d^2;
for i=2:m8-1
```

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```
d2xwo(:,i)=(w(:,i+1)-2*w(:,i)+w(:,i-1))/d^2;
end;
for i=1:m8-1
d2ywo(:,i)=m2*w(:,i)/d^2;
end;
k9=1; b14=1.0;
while (b14 > 10^-4) and (k9 < 30)
k9
k9=k9+1;
X=fmincon('beamNov2023A3',xo,A,b,[ ], [ ],lb,ub);
b14=max(abs(xo-X))
xo=X;
end;
b12=max(max(abs(w-wo)))
wo=w;
x3=xo;
for i=1:m8-1
for j=1:m8-1
L(j,i,1)=xo((i-1)*(m8-1)+j,1);
end;
end;
end;
for i=1:m8-1
x8(i,1)=i*d;
end;
mesh(x8,x8,L);
********************
```

With the auxiliary function "beamNov2023A3', where

****

1. function S=beamNov2023A3(x)

```
global m8 d d2xwo d2ywo H e1 ho xo b5
S=0;
for i=1:m8-1
for j=1:m8-1
x1(j,i)=x((m8-1)*(i-1)+j,1);
end;
end;
for i=1:m8-1
```

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```
for j=1:m8-1
S=S+1/((x1(j,i))^3)/ho^3/e1*(H(j,i,1))^2*(d2xwo(j,i)+d2ywo(j,i))^2*12;
end;
end;
*****************************
```

Remark 30.2. *About the numerical results obtained for this plate model, a final word of caution is necessary.*

Indeed, the full convergence in such a case is hard to obtain so that we have obtained just approximations of critical points with the functional close to its optimal value. It is also worth emphasizing we have fixed the number of iterations so that the solution and shape obtained are just approximate ones.

31. A note on the first Maxwell equation of electromagnetism

Let $\Omega_1 \subset \mathbb{R}^3$ be an open, bounded and connected set with a regular (Lipschitzian) boundary denoted by $\partial\Omega_1$.

Suppose $\mathbf{E} : \Omega_1 \to \mathbb{R}^3$ is an electric field of C^1 class in Ω.

Let $\Omega \subset \Omega_1$ be also an open, bounded and connected set with a regular (Lipschitzian) boundary denoted by $S = \partial\Omega$.

Observe that there exists a scalar field $V : \Omega \to \mathbb{R}$ such that

$$\nabla^2 V = \text{ div } \mathbf{E}, \text{ in } \Omega,$$

and

$$\nabla V \cdot \mathbf{n} = 0, \text{ on } S = \partial\Omega.$$

Here $\mathbf{n}$ denotes the normal outward field to S.

Observe also that

$$\nabla^2 V = \text{ div } \nabla V = \text{ div } \mathbf{E},$$

so that defining

$$\mathbf{h} = \nabla V - \mathbf{E},$$

we have that

$$\text{div } \mathbf{h} = 0, \text{ in } \Omega.$$

Hence, from such results and the divergence Theorem, we get

$$\begin{aligned} \int_S \mathbf{E} \cdot \mathbf{n} \, dS &= \int_S (\nabla V) \cdot \mathbf{n} \, dS - \int_S \mathbf{h} \cdot \mathbf{n} \, dS \\ &= -\int_\Omega \text{ div } \mathbf{h} \, dV = 0. \end{aligned} \tag{177}$$

Summarizing, we have got

$$\int_S \mathbf{E} \cdot \mathbf{n} \, dS = 0.$$

Consider now a charge q_0 localized at the center of a sphere Ω_2 of radius $R > 0$ and boundary $S_2 = \partial\Omega_2$.

The electric field on the sphere surface generated by q_0 is given by

$$\mathbf{E}_2 = \frac{1}{4\pi\varepsilon_0} \frac{q_0}{R^2} \mathbf{n}_2,$$

where $\mathbf{n}_2$ is the normal outward field to S_2.

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Clearly

$$\int_{S_2} \mathbf{E}_2 \cdot \mathbf{n}_2 \, dS_2 = \frac{1}{4\pi\varepsilon_0} \frac{q_0}{R^2} (4\pi R^2) = \frac{q_0}{\varepsilon_0}.$$

Consider again the set Ω but now with a charge q_0 localized at a point $\mathbf{x}$ inside the interior of Ω, which is denoted by Ω^0.

At first the electric field $\mathbf{E}$ generated by q_0 is not of C^1 class on Ω.

However, there exists $R > 0$ such that

$$B_R(\mathbf{x}) \subset \Omega = \Omega^0.$$

Define $\Omega_3 = \Omega \setminus B_R(\mathbf{x})$.

Therefore, $\mathbf{E}$ is of C^1 class on Ω_3.

Denoting the boundary of Ω_3 by S_3, from the previous results, we may infer that

$$\int_{S_3} \mathbf{E} \cdot \mathbf{n} \, dS_3 = 0,$$

so that

$$\begin{aligned} \int_{S_3} \mathbf{E} \cdot \mathbf{n} \, dS_3 &= \int_S \mathbf{E} \cdot \mathbf{n} \, dS - \int_{\partial B_R(\mathbf{x})} \mathbf{E} \cdot \mathbf{n} \, dS_2 \\ &= \int_S \mathbf{E} \cdot \mathbf{n} \, dS - \frac{q_0}{\varepsilon_0} \\ &= 0. \end{aligned} \tag{178}$$

Therefore, we have got

$$\int_S \mathbf{E} \cdot \mathbf{n} \, dS = \frac{q_0}{\varepsilon_0}.$$

Assume now on Ω we have a density of charges $\rho(\mathbf{x})$.

For a small volume ΔV consider a punctual charge q_0 localized in $\mathbf{x} \in \Omega$ such that

$$q_0 \approx \rho(x) \Delta V.$$

Denoting by $\Delta\mathbf{E}$ the electric field generated by q_0, from the previous results we may infer that

$$\int_S \Delta\mathbf{E} \cdot \mathbf{n} \, dS = \frac{q_0}{\varepsilon_0} \approx \frac{\rho(\mathbf{x}) \Delta V}{\varepsilon_0}.$$

Such an equation in its differential form, stands for:

$$\int_S d\mathbf{E} \cdot \mathbf{n} \, dS = \frac{\rho(\mathbf{x}) \, dV}{\varepsilon_0}.$$

Integrating in Ω we may obtain

$$\begin{aligned} \int_S \mathbf{E} \cdot \mathbf{n} \, dS &= \int_S \int_\Omega d\mathbf{E} \cdot \mathbf{n} \, dV \, dS \\ &= \int_\Omega \frac{\rho(\mathbf{x})}{\varepsilon_0} \, dV, \end{aligned} \tag{179}$$

so that

$$\int_S \mathbf{E} \cdot \mathbf{n} \, dS = \int_\Omega \frac{\rho(\mathbf{x})}{\varepsilon_0} \, dV.$$

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From this and the Divergence Theorem, we have

$$\int_S \mathbf{E}\cdot\mathbf{n}\, dS = \int_\Omega \operatorname{div}\mathbf{E}\, dV = \int_\Omega \frac{\rho(\mathbf{x})}{\varepsilon_0}\, dV.$$

Summarizing, we have got

$$\int_\Omega \operatorname{div}\mathbf{E}\, dV = \int_\Omega \frac{\rho(\mathbf{x})}{\varepsilon_0}\, dV.$$

This is the integral form of the first Maxwell equation of electromagnetism.

For this last equation, the set $\Omega \subset \Omega_1$ is rather arbitrary so that for Ω as a ball of small radius $r > 0$ with center at a point $\mathbf{x} \in \Omega_1$, from the Mean Value Theorem fot integrals and letting $r \to 0^+$, we obtain

$$\operatorname{div}\mathbf{E} = \frac{\rho}{\varepsilon_0}, \text{ in } \Omega_1.$$

This last equation stands for the differential form of the first Maxwell equation of electromagnetism.

Remark 31.1. *Summarizing, in this section we have formally obtained a mathematical deduction of the first Maxwell equation of electromagnetism.*

32. A note on relaxation for a general model in the vectorial calculus of variations

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

Consider a function $g : \mathbb{R}^{N\times n} \to \mathbb{R}$ twice differentiable and such that

$$g(y) \to +\infty, \text{ as } |y| \to +\infty.$$

Define a functional $G : V \to \mathbb{R}$ by

$$G(\nabla u) = \frac{1}{2}\int_\Omega g(\nabla u)\, dx,$$

where

$$V = \{W^{1,2}(\Omega;\mathbb{R}^N) \ : \ u = u_0 \text{ on } \partial\Omega\}.$$

Moreover, for $f \in L^2(\Omega;\mathbb{R}^N)$, define also

$$J(u) = G(\nabla u) - \langle u, f\rangle_{L^2}.$$

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

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

Observe that from the convex analysis basic theory, we have that

$$\begin{aligned} \alpha &= \inf_{u\in V} J(u) \\ &= \inf_{u\in V} J^{**}(u) \\ &= \inf_{u\in V}\{(G\circ\nabla)^{**}(u) - \langle u, f\rangle_{L^2}\}. \end{aligned} \tag{180}$$

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On the other hand

$$\begin{aligned}(G\circ\nabla)^{**}(u) &\leq H(u)\\ &\equiv \inf_{(\lambda,(v,w))\in[0,1]\times B(u,\lambda)}\{\lambda G(\nabla w)+(1-\lambda)G(\nabla v)\}\\ &\leq G(\nabla u),\end{aligned} \tag{181}$$

where

$$B(u,\lambda)=\{(v,w)\in V\ :\ \lambda w+(1-\lambda)v=u\}.$$

From such results, we may infer that

$$\inf_{u\in V} J^{**}(u)=\inf_{u\in V}\{H(u)-\langle u,f\rangle_{L^2}\}=\inf_{u\in V} J(u).$$

Furthermore, observe that

$$\lambda\nabla w+(1-\lambda)\nabla v=\nabla u,$$

so that

$$\begin{aligned}\nabla v &= \nabla u+\lambda(\nabla v-\nabla w)\\ &= \nabla u+\lambda\nabla\phi,\end{aligned} \tag{182}$$

where $\phi=v-w\in W_0^{1,2}(\Omega;\mathbb{R}^N)$ so that

$$\nabla\phi=\nabla v-\nabla w,$$

and

$$\nabla w=\nabla v-\nabla\phi.$$

Therefore,

$$\nabla w=\nabla v-\nabla\phi=\nabla u+\lambda\nabla\phi-\nabla\phi=\nabla u-(1-\lambda)\nabla\phi.$$

Replacing such results into the expression of H, we have

$$H(u)=\inf_{(\lambda,\phi)\in[0,1]\times V_0}\{\lambda G(\nabla u-(1-\lambda)\nabla\phi)+(1-\lambda)G(\nabla u+\lambda\nabla\phi)\},$$

where

$$V_0=W_0^{1,2}(\Omega;\mathbb{R}^N).$$

Joining the pieces, we have got

$$\begin{aligned}\inf_{u\in V} J(u) &= \inf_{u\in V} J^{**}(u)\\ &= \inf_{u\in V}\{H(u)-\langle u,f\rangle_{L^2}\}\\ &= \inf_{(\lambda,\phi,u)\in[0,1]\times V_0\times V}\{\lambda G(\nabla u-(1-\lambda)\nabla\phi)+(1-\lambda)G(\nabla u+\lambda\nabla\phi)-\langle u,f\rangle_{L^2}\}.\end{aligned}$$

This last functional corresponds to a relaxation for the original non-convex functional.
The note is complete.

32.1. *Some related numerical results*

In this subsection we present numerical results for an one-dimensional model and related relaxed formulation.

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For $\Omega = [0,1] \subset \mathbb{R}$, consider the functional $J : V \to \mathbb{R}$ where

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

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

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

Based on the results of the previous section, denoting $V_0 = W_0^{1,2}(\Omega)$, we define the following relaxed functional $J_1 : [0,1] \times V \times V_0 \to \mathbb{R}$, where

$$J_1(\lambda, u, \phi) = \frac{\lambda}{2}\int_\Omega ((u' - (1-\lambda)\phi')^2 - 1)^2\, dx + \frac{1-\lambda}{2}\int_\Omega ((u' + \lambda\phi')^2 - 1)^2\, dx + \frac{1}{2}\int_\Omega (u - f)^2\, dx.$$

Indeed, we have developed an algorithm for minimizing the following regularized functional $J_2 : [0,1] \times V \times V_0 \to \mathbb{R}$, where

$$J_2(\lambda, u, \phi) = J_1(\lambda, u, \phi) + \frac{\varepsilon_3}{2}\int_\Omega (u'')^2\, dx,$$

for a small parameter $\varepsilon_3 > 0$.

For the case in which $f(x) = \sin(\pi x)/2$, for the optimal solution u, please see Figure 26.

For the case in which $f(x) = \cos(\pi x)/2$, for the optimal solution u, please see Figure 27.

For the case in which $f(x) = 0$, for the optimal solution u, please see Figure 28.

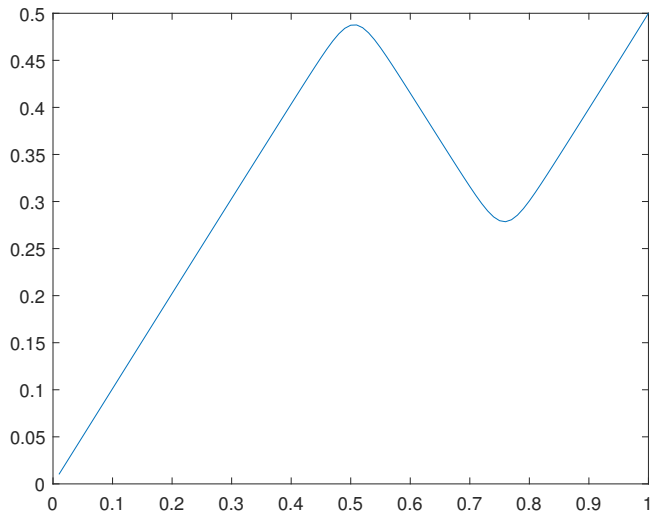

Figure 26. Optimal solution $u(x)$ for the case $f(x) = \sin(\pi x)/2$.

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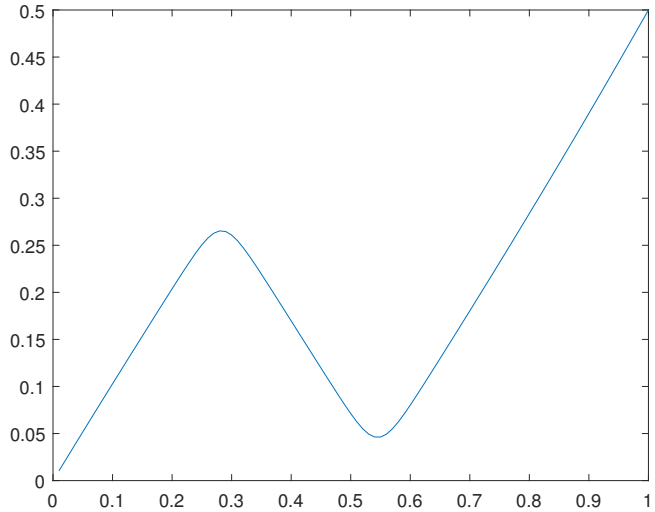

Figure 27. Optimal solution $u(x)$ for the case $f(x) = \cos(\pi x)/2$.

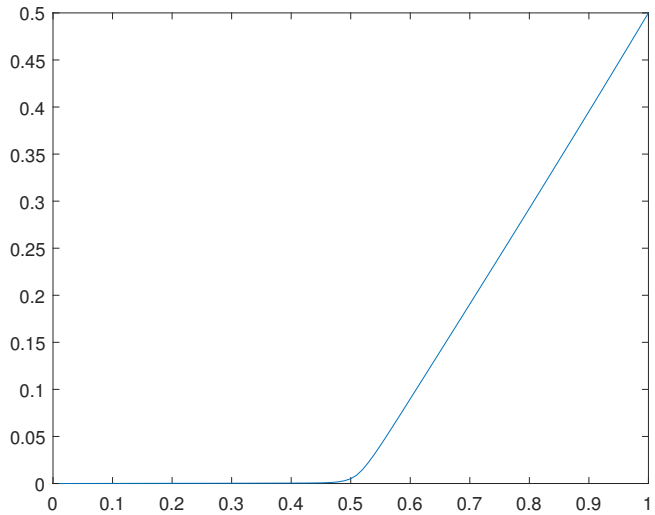

Figure 28. Optimal solution $u(x)$ for the case $f(x) = 0$.

We highlight to obtain the solution for this last case which $f = 0$ is harder. A good solution was possible only using

$$x_0 = 0$$

as the initial solution concerning the iterative process.

Here we present the software in MAT-LAB developed.

****

1. clear all

   global m8 d u e3

   m8=100;

   d=1/m8;

   e3=0.0005;

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```
for i=1:2*m8+1
xo(i,1)=0.36;
end;
b12=1.0;
k=1;
while (b12 > 10^-7) and (k < 60)
k
k=k+1;
X=fminunc('funDecember2023',xo);
b12=max(abs(xo-X))
xo=X;
u(m8/2)
end;
for i=1:m8
x(i,1)=i*d;
end;
plot(x,u);
**********************
```

With the main function "funDecember2023"
****

```
1. function S=funDecember2023(x)
   global m8 d u e3
   for i=1:m8
   u(i,1)=x(i,1);
   v(i,1)=x(i+m8,1);
   yo(i,1)=sin(pi*i*d)/2;
   end;
   L=(1+sin(x(2*m8+1,1)))/2;
   u(m8,1)=1/2;
   v(m8,1)=0.0;
   du(1,1)=u(1,1)/d;
   dv(1,1)=v(1,1)/d;
   for i=2:m8
   du(i,1)=(u(i,1)-u(i-1,1))/d;
   dv(i,1)=(v(i,1)-v(i-1,1))/d;
   end;
   d2u(1,1)=(-2*u(1,1)+u(2,1))/d^2;
   for i=2:m8-1
   d2u(i,1)=(u(i-1,1)-2*u(i,1)+u(i+1,1))/d^2;
```

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```
end;
S=0;
for i=1:m8
S=S+1/2*L*((du(i,1)-(1-L)*dv(i,1))^2-1)^2;
S=S+1/2*(1-L)*((du(i,1)+L*dv(i,1))^2-1)^2;
S=S+(u(i,1)-yo(i,1))^2;
end;
for i=1:m8-1
S=S+e3*d2u(i,1)^2;
end;
******************
```

33. A general concave primal dual formulation for an originally non-convex primal one

In this section we develop a general concave dual formulation related to a primal one which is originally non-convex.

Let $\Omega \subset \mathbb{R}^3$ be an open, bounded and connected set with a regular (Lipschitzian) boundary denoted by $\partial\Omega$. Consider a Fréchet differentiable functional $J : V \to \mathbb{R}$ where

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

Assume there exists $K_1, K_3, K > 0$ such that

$$-K_1 I_d \leq \delta^2 J(u) \leq K_1 I_d, \ \forall \ \|u\|_\infty \leq K_3,$$

where

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

Observe that

$$\begin{aligned} J(u) &= -\langle u, e^{Kv_1^*}\rangle_{L^2} + \frac{1}{2}\int_\Omega (\sqrt[4]{K}u + 2K)^2 \, dx \\ &\quad + \langle u, e^{Kv_1^*}\rangle_{L^2} - \frac{1}{2}\int_\Omega (\sqrt[4]{K}u + 2K)^2 \, dx + J(u) \\ &\geq \inf_{u \in L^2} \left\{ -\langle u, e^{Kv_1^*}\rangle_{L^2} + \frac{1}{2}\int_\Omega (\sqrt[4]{K}u + 2K)^2 \, dx \right\} \\ &\quad + \langle u, e^{Kv_1^*}\rangle_{L^2} - \frac{1}{2}\int_\Omega (\sqrt[4]{K}u + 2K)^2 \, dx + J(u) \\ &= -\frac{1}{2}\int_\Omega \frac{e^{2Kv_1^*}}{\sqrt{K}} \, dx + 2\,K \int_\Omega \frac{e^{Kv_1^*}}{\sqrt[4]{K}} \, dx \\ &\quad + \langle u, e^{Kv_1^*}\rangle_{L^2} - \frac{1}{2}\int_\Omega (\sqrt[4]{K}u + 2K)^2 \, dx + J(u) \\ &\equiv J_1^*(u, v_1^*), \end{aligned} \tag{183}$$

where we have denoted

$$\begin{aligned} J_1^*(u, v_1^*) &= -\frac{1}{2}\int_\Omega \frac{e^{2Kv_1^*}}{\sqrt{K}} \, dx + 2\,K \int_\Omega \frac{e^{Kv_1^*}}{\sqrt[4]{K}} \, dx \\ &\quad + \langle u, e^{Kv_1^*}\rangle_{L^2} - \frac{1}{2}\int_\Omega (\sqrt[4]{K}u + 2K)^2 \, dx + J(u). \end{aligned} \tag{184}$$

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We observe that the calculation of the concerning polar functional is made through the extremal equation

$$\frac{\partial}{\partial u}\left\{-\langle u, e^{Kv_1^*}\rangle_{L^2} + \frac{1}{2}\int_\Omega (\sqrt[4]{K}u + 2K)^2\, dx\right\} = \mathbf{0},$$

which stands for

$$-e^{Kv_1^*} + (\sqrt[4]{K}u + 2K)\ \sqrt[4]{K} = 0,$$

so that

$$e^{Kv_1^*} \approx 2K\ \sqrt[4]{K},$$

and thus

$$Kv_1^* \approx \ln(2K\ \sqrt[4]{K}),$$

that is

$$v_1^* \approx \frac{\ln(2K\ \sqrt[4]{K})}{K}.$$

With such results in mind, we define the non-active restriction

$$v_1^* \geq \frac{3}{4}\frac{\ln(2K\ \sqrt[4]{K})}{K},\ \text{in } \Omega.$$

Defining now

$$A^* = \left\{(u, v_1^*) \in V \times Y^*\ :\ v_1^* \geq \frac{3}{4}\frac{\ln(2K\ \sqrt[4]{K})}{K},\ \text{in } \Omega\right\}$$

where $Y = Y^* = L^2(\Omega)$, by just directly computing

$$\delta^2 J_1^*(u, v_1^*)$$

we may easily obtain that such a Hessian is positive definite in A^* so that J_1^* is concave on the convex set A^*.

Defining

$$B^* = \{(u, v_1^*) \in V \times Y^*\ :\ \|u\|_\infty \leq K_3\},$$

suppose now $(u_0, \hat{v}_1^*) \in A^* \cap B^*$ is such that

$$\delta J_1^*(u_0, \hat{v}_1^*) = \mathbf{0}.$$

From the variation of J^* in v_1^*, we have

$$-K\frac{e^{2K\hat{v}_1^*}}{\sqrt{K}} + 2K^2\frac{e^{K\hat{v}_1^*}}{\sqrt[4]{K}} + Ke^{K\hat{v}_1^*}u_0 = \mathbf{0},$$

so that

$$-e^{K\hat{v}_1^*} + (\sqrt[4]{K}u_0 + 2K)\ \sqrt[4]{K} = 0,$$

From the variation of J_1^* in u, we obtain

$$e^{K\hat{v}_1^*} - (\sqrt[4]{K}u_0 + 2K)\ \sqrt[4]{K} + \delta J(u_0) = \mathbf{0}$$

so that

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

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Remark 33.1. *Summarizing, the functional J_1^* is concave on $A^* \cap B^*$ (which corresponds to a non-active restriction) and a critical point of J_1^* corresponds to a critical point of the original primal functional J. Therefore, J_1^* corresponds to a concave primal dual formulation for a originally non-convex primal functional J.*

34. Conclusion

In the first part of this article we have developed a relaxation proposal and duality principles suitable for a large class of models in physics and engineering.

In a second part we develop duality principles for the quasi-convex envelop of some vectorial models in the calculus of variations.

We highlight such dual variational formulations established are in general convex (in fact concave).

Finally, in the last sections, we develop mathematical models for some types of chemical reactions, including the hydrogen nuclear fusion and the water hydrolysis. Among such results, we highlight our proposal of modeling the Ginzburg-Landau theory in super-conductivity as a two-phase eigenvalue approach.

Data Availability Statement: Details on the software for numerical results avaialable upon request e-mail: fabio.botelho@ufsc.br.

Conflicts of Interest: The author declares no conflict of interest concerning this article.

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