Article

Not peer-reviewed version

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

Fabio Botelho *

Posted Date: 21 August 2023

doi: 10.20944/preprints202302.0051.v29

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

Article

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

Fabio Silva Botelho

Department of Mathematics, Federal University of Santa Catarina, Florianópolis - SC, Brazil; fabio.botelho@ufsc.br

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. Finally, in the last section we present a concerning numerical example and the respective software.

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

MSC: 49N15

---

1. Introduction

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

The main duality principle is applied to 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 [2,3,15,16] and on a D.C. optimization approach developed in Toland [17].

About the other references, details on the Sobolev spaces involved are found in [1]. Related results on convex analysis and duality theory are addressed in [5,7,8,10,14].

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 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

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

and where

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

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

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

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

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

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

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

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

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

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

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

Observe that

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

Preprints (www.preprints.org) | NOT PEER-REVIEWED | Posted: 21 August 2023 doi:10.20944/preprints202302.0051.v29

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

From the general results in [17], we may infer that

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

On the other hand

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

From these last two results we may obtain

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

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

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

where

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

$$F_1^*(v_1^* + z_1^*, \nabla \phi) = \sup_{v_1 \in Y_1} \{\langle v_1, z_1^* + v_1^* \rangle_{L^2} - F_1(v_1, \nabla \phi)\},$$

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

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

we have got

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

Finally, observe that

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

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 $J : V \rightarrow \mathbb{R}$ where

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

and where

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

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

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

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

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

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

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

and

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

Observe 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

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

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

and

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

by

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

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

and

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

 doi:10.20944/preprints202302.0051.v29

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 $n = 1$.
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;
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;
```

 doi:10.20944/preprints202302.0051.v29


```
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
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.

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.*

Preprints (www.preprints.org) | NOT PEER-REVIEWED | Posted: 21 August 2023 doi:10.20944/preprints202302.0051.v29

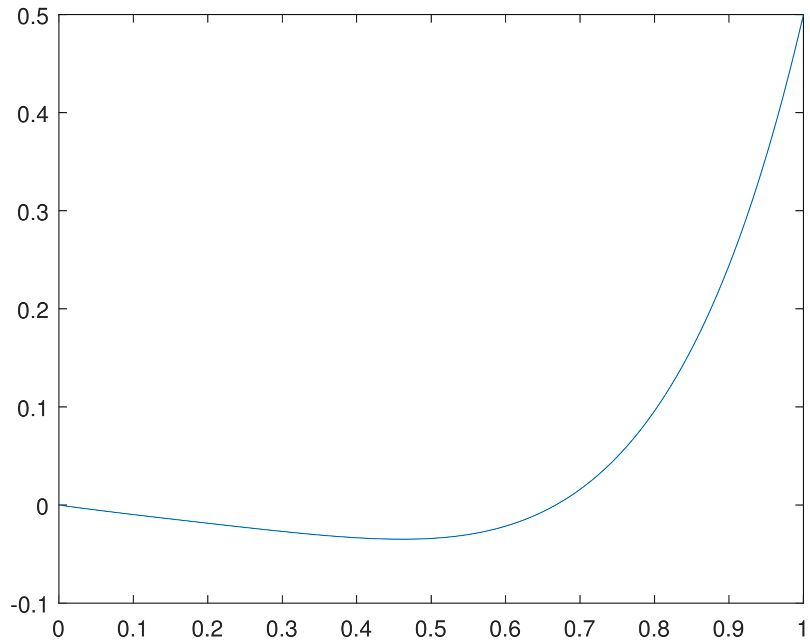

Figure 1. solution $u_0(x)$ for the case $f(x) = 0$.

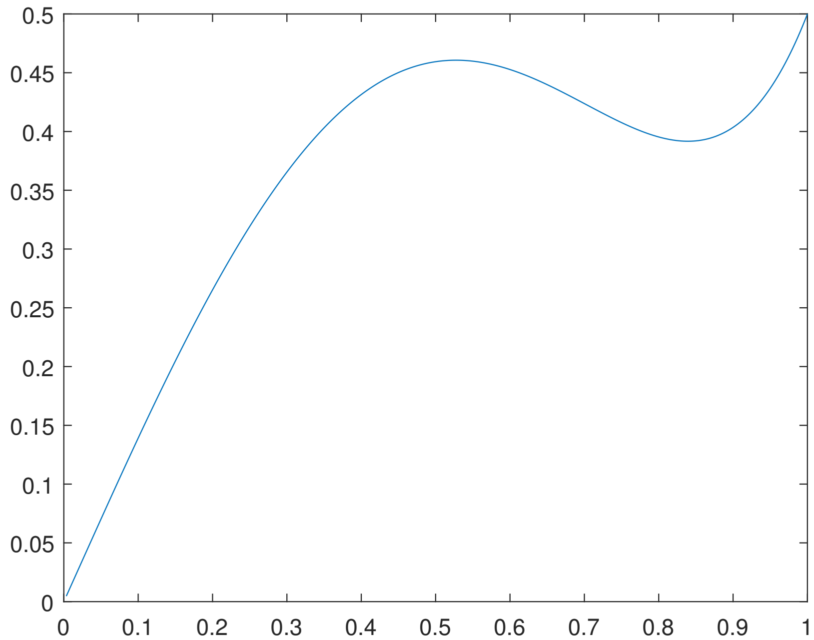

Figure 2. solution $u_0(x)$ for the case $f(x) = \sin(\pi x)/2$.

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

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

and define also

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

At this point we define

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

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

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

Preprints (www.preprints.org) | NOT PEER-REVIEWED | Posted: 21 August 2023 doi:10.20944/preprints202302.0051.v29

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

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

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

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

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

Preprints (www.preprints.org) | NOT PEER-REVIEWED | Posted: 21 August 2023 doi:10.20944/preprints202302.0051.v29

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

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

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

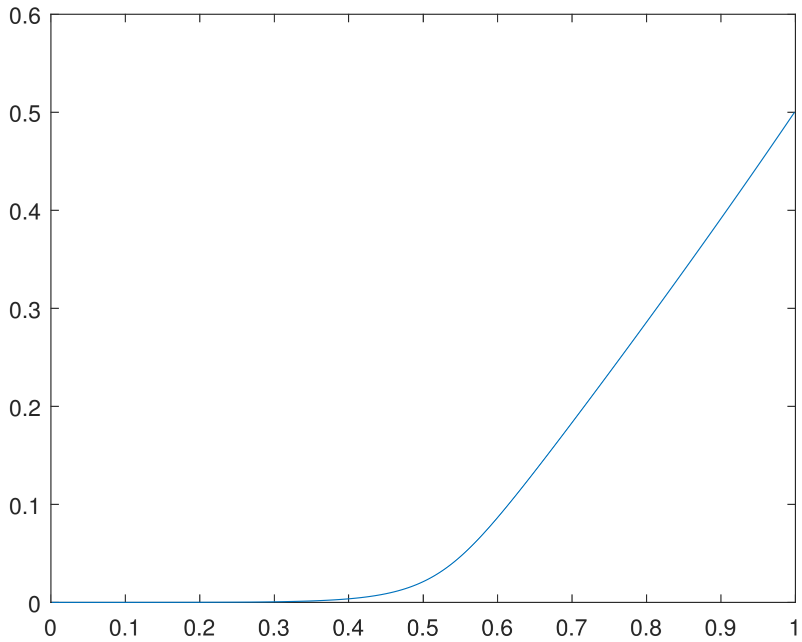

Figure 3. solution $u_0(x)$ for the case $f(x) = 0$.

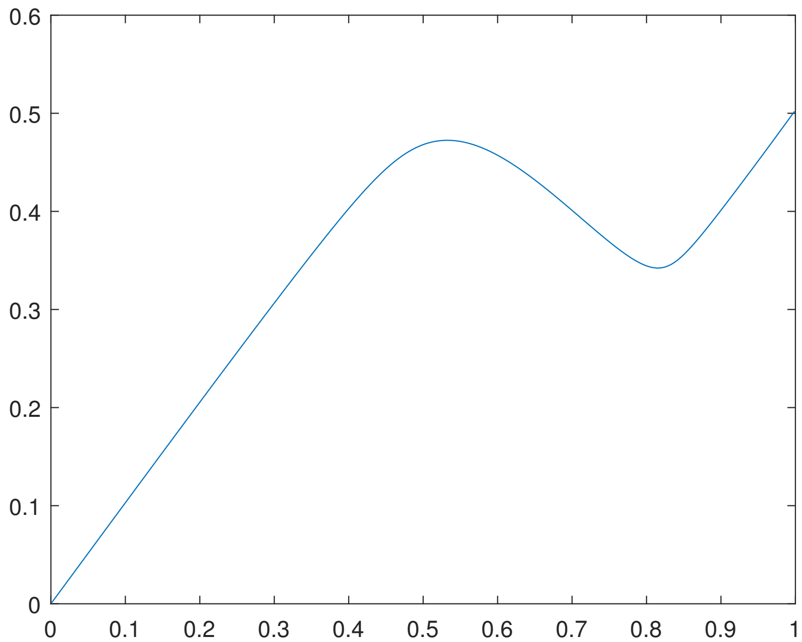

Figure 4. solution $u_0(x)$ for the case $f(x) = \sin(\pi x)/2$.

Preprints (www.preprints.org) | NOT PEER-REVIEWED | Posted: 21 August 2023 doi:10.20944/preprints202302.0051.v29

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

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

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. $for\ i = 1 : m_8 - 1$

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

    $end;$

Preprints (www.preprints.org) | NOT PEER-REVIEWED | Posted: 21 August 2023 doi:10.20944/preprints202302.0051.v29

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. $for\ i = 1 : m_8 - 1$

    $x(i) = i * d;$

    $end;$

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

****

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, [11].

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

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

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

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

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

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

Preprints (www.preprints.org) | NOT PEER-REVIEWED | Posted: 21 August 2023 doi:10.20944/preprints202302.0051.v29

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

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

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 $\mathcal{O}(700 - 1000)$.

Preprints (www.preprints.org) | NOT PEER-REVIEWED | Posted: 21 August 2023 doi:10.20944/preprints202302.0051.v29

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.

6. 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

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

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

$$\begin{aligned} J^*(v^*) &= -F_1^*(v^*) + F_2^*(v^*) \\ &= -F_1^*(v^*) + \frac{1}{2\varepsilon}\int_\Omega (v_1^* + f_1)^2\,dx + \frac{1}{2\varepsilon}\int_\Omega (v_2^*)^2\,dx. \end{aligned} \quad (24)$$

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

$$\begin{aligned} J_1^*(v^*) &= -F_1^*(v^*) + \frac{1}{2\varepsilon}\int_\Omega (v_1^* + f_1)^2\,dx + \frac{1}{2\varepsilon}\int_\Omega (v_2^*)^2\,dx \\ &\quad + \langle \varphi, (v_1^* + f)_y - (v_2^*)_x \rangle_{L^2}. \end{aligned} \quad (25)$$

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

$$-\frac{\partial F_1^*(v^*)}{\partial v_1^*} + \frac{v_1^* + f}{\varepsilon} - \frac{\partial \varphi}{\partial y} = 0. \quad (26)$$

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

$$-\frac{\partial F_1^*(v^*)}{\partial v_2^*} + \frac{v_2^*}{\varepsilon} + \frac{\partial \varphi}{\partial x} = 0. \quad (27)$$

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

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

 doi:10.20944/preprints202302.0051.v29

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 (26) and (27) we have

$$\begin{aligned} & -\varepsilon \left(\frac{\partial F_1^*(v^*)}{\partial v_1^*}\right)_x - \varepsilon \left(\frac{\partial F_1^*(v^*)}{\partial v_2^*}\right)_y \\ & +(v_1^* + f_1)_x + (v_2^*)_y \\ = & -\varepsilon u_{xx} - \varepsilon u_{yy} + (v_1^*)_x + (v_2^*)_y + f = 0. \end{aligned} \tag{28}$$

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

$$\left(\frac{\partial F(u_x - \varphi_y, u_y + \varphi_x)}{\partial v_1}\right)_x + \left(\frac{\partial F(u_x - \varphi_y, u_y + \varphi_x)}{\partial v_2}\right)_y + f = 0, \text{ in } \Omega. \tag{29}$$

Observe that if

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

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 (29) 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 $r > 0$

7. 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 $\partial\Omega$.

Preprints (www.preprints.org) | NOT PEER-REVIEWED | Posted: 21 August 2023 doi:10.20944/preprints202302.0051.v29

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

$$\begin{aligned} J(u) &= \frac{\gamma}{2}\int_\Omega \nabla u \cdot \nabla u \, dx + \frac{\alpha}{2}\int_\Omega (u^2-\beta)^2 \, dx \\ &\quad -\langle u, f\rangle_{L^2}, \end{aligned} \tag{30}$$

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

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

$$\begin{aligned} J_1^*(u, v_0^*) &= -\frac{\gamma}{2}\int_\Omega \nabla u \cdot \nabla u \, dx - \langle u^2, v_0^*\rangle_{L^2} \\ &\quad +\frac{K_1}{2}\int_\Omega (-\gamma\nabla^2 u + 2v_0^* u - f)^2 \, dx + \langle u, f\rangle_{L^2} \\ &\quad +\frac{1}{2\alpha}\int_\Omega (v_0^*)^2 \, dx + \beta\int_\Omega v_0^* \, dx, \end{aligned} \tag{31}$$

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

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

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

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

$$\begin{aligned} &\det\{\delta^2 J_1^*(u, v_0^*)\} \\ &= \frac{\partial^2 J_1^*(u, v_0^*)}{\partial (v_0^*)^2}\frac{\partial^2 J_1^*(u, v_0^*)}{\partial u^2} - \left(\frac{\partial^2 J_1^*(u, v_0^*)}{\partial u \partial v_0^*}\right)^2 \\ &= \frac{K_1(-\gamma\nabla^2 + 2v_0^*)^2}{\alpha} - \frac{\gamma\nabla^2 + 2v_0^* + 4\alpha u^2}{\alpha} \\ &\quad -4K_1^2\varphi^2 - 8K_1\varphi(-\gamma\nabla^2 + 2v_0^*)u + 8K_1\varphi u \\ &\quad +4K_1(-\gamma\nabla^2 u + 2v_0^* u)u. \end{aligned} \tag{32}$$

Observe now that a critical point $\varphi = 0$ and $(-\gamma\nabla^2 u + 2v_0^* u)u = fu \geq 0$ in Ω.

Preprints (www.preprints.org) | NOT PEER-REVIEWED | Posted: 21 August 2023 doi:10.20944/preprints202302.0051.v29

Therefore, for an appropriate large $K_1 > 0$, also at a critical point, we have

$$\begin{aligned} & \det\{\delta^2 J_1^*(u, v_0^*)\} \\ = \; & 4K_1 f u - \frac{\delta^2 J(u)}{\alpha} + K_1 \frac{(-\gamma \nabla^2 + 2v_0^*)^2}{\alpha} > \mathbf{0}. \end{aligned} \tag{33}$$

Remark 7.1. *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 7.2. *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

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

8. 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 $J : V \rightarrow \mathbb{R}$ where

$$\begin{aligned} J(u) \;=\; & \frac{\gamma}{2} \int_\Omega \nabla u \cdot \nabla u \, dx + \frac{\alpha}{2} \int_\Omega (u^2 - \beta)^2 \, dx \\ & - \langle u, f \rangle_{L^2}, \end{aligned} \tag{34}$$

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

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

$$\begin{aligned} J_1^*(u, v_0^*, v_1^*) \;=\; & \frac{\gamma}{2} \int_\Omega \nabla u \cdot \nabla u \, dx + \frac{1}{2} \int_\Omega K \, u^2 \, dx \\ & - \langle u, v_1^* \rangle_{L^2} + \frac{1}{2} \int_\Omega \frac{(v_1^*)^2}{(-2v_0^* + K)} \, dx \\ & + \frac{1}{2(\alpha + \varepsilon)} \int_\Omega (v_0^* - \alpha(u^2 - \beta))^2 \, dx + \langle u, f \rangle_{L^2} \\ & - \frac{1}{2\alpha} \int_\Omega (v_0^*)^2 \, dx - \beta \int_\Omega v_0^* \, dx, \end{aligned} \tag{35}$$

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 8.1. *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

$$sign\ (u_1) = \ sign\ (u_2)\ in\ \Omega,$$

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

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

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

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

 doi:10.20944/preprints202302.0051.v29

so that

$$\begin{aligned}
& \det\left\{\frac{\partial^2 J_1^*(u,v_0^*,v_1^*)}{\partial u \partial v_1^*}\right\} \\
= & \frac{\partial^2 J_1^*(u,v_1^*,v_0^*)}{\partial (v_1^*)^2}\frac{\partial^2 J_1^*(u,v_1^*,v_0^*)}{\partial u^2}-\left(\frac{\partial^2 J_1^*(u,v_1^*,v_0^*)}{\partial u \partial v_1^*}\right)^2 \\
= & \frac{-\gamma\nabla^2+2v_0^*+4\frac{\alpha^2}{\alpha+\varepsilon}u^2-2\frac{\alpha}{\alpha+\varepsilon}\varphi}{-2v_0^*+K} \\
\equiv & H(u,v_0^*). \qquad (36)
\end{aligned}$$

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 8.2. *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

$$\begin{aligned}
J(u_0) &= \inf_{u \in (C_1)^*_{\hat{v}_0^*}} J(u) \\
&= J_1^*(u_0,\hat{v}_1^*,\hat{v}_0^*) \\
&= \inf_{(u,v_1^*)\in (C_1)^*_{\hat{v}_0^*}\times D^*}\left\{\sup_{v_0^*\in B^*} J_1^*(u,v_1^*,v_0^*)\right\} \\
&= \sup_{v_0^*\in B^*}\left\{\inf_{(u,v_1^*)\in (C_1)^*_{\hat{v}_0^*}\times D^*} J_1^*(u,v_1^*,v_0^*)\right\}. \qquad (37)
\end{aligned}$$

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

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

Preprints (www.preprints.org) | NOT PEER-REVIEWED | Posted: 21 August 2023 doi:10.20944/preprints202302.0051.v29

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

$$\begin{aligned} J(u_0) &= J_1^*(u_0, \hat{v}_1^*, \hat{v}_0^*) \\ &= \inf_{(u,v_1^*) \in (C_1)^*_{\hat{v}_0^*} \times D^*} \left\{ \sup_{v_0^* \in B^*} J_1^*(u, v_1^*, v_0^*) \right\} \\ &= \sup_{v_0^* \in B^*} \left\{ \inf_{(u,v_1^*) \in (C_1)^*_{\hat{v}_0^*} \times D^*} J_1^*(u, v_1^*, v_0^*) \right\}. \end{aligned} \tag{38}$$

Moreover, observe that

$$\begin{aligned} J_1^*(u_0, \hat{v}_1^*, \hat{v}_0^*) &= \inf_{(u,v_1^*) \in (C_1)^*_{\hat{v}_0^*} \times D^*} J_1^*(u, v_1^*, \hat{v}_0^*) \\ &\leq \frac{\gamma}{2} \int_\Omega \nabla u \cdot \nabla u \, dx + \frac{K}{2} \int_\Omega u^2 \, dx \\ &\quad + \langle u^2, \hat{v}_0^* \rangle_{L^2} - \frac{K}{2} \int_\Omega u^2 \, dx \\ &\quad - \frac{1}{2\alpha} \int_\Omega (\hat{v}_0^*)^2 \, dx - \beta \int_\Omega \hat{v}_0^* \, dx \\ &\quad + \frac{1}{2(\alpha + \varepsilon)} \int_\Omega (\hat{v}_0^* - \alpha(u^2 - \beta))^2 \, dx - \langle u, f \rangle_{L^2} \\ &\leq \sup_{v_0^* \in Y^*} \left\{ \frac{\gamma}{2} \int_\Omega \nabla u \cdot \nabla u \, dx + \langle u^2, v_0^* \rangle \right. \\ &\quad - \frac{1}{2\alpha} \int_\Omega (v_0^*)^2 \, dx - \beta \int_\Omega v_0^* \, dx \\ &\quad \left. + \frac{1}{2(\alpha + \varepsilon)} \int_\Omega (v_0^* - \alpha(u^2 - \beta))^2 \, dx - \langle u, f \rangle_{L^2} \right\} \\ &= \frac{\gamma}{2} \int_\Omega \nabla u \cdot \nabla u \, dx + \frac{\alpha}{2} \int_\Omega (u^2 - \beta)^2 \, dx \\ &\quad - \langle u, f \rangle_{L^2}, \; \forall u \in (C_1)^*_{\hat{v}_0^*}. \end{aligned} \tag{39}$$

Summarizing, we have got

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

 doi:10.20944/preprints202302.0051.v29

From such results, we may infer that

$$
\begin{aligned}
J(u_0) &= \inf_{u \in (C_1)^*_{\hat{v}_0^*}} J(u) \\
&= J_1^*(u_0, \hat{v}_1^*, \hat{v}_0^*) \\
&= \inf_{(u, v_1^*) \in (C_1)^*_{\hat{v}_0^*} \times D^*} \left\{ \sup_{v_0^* \in B^*} J_1^*(u, v_1^*, v_0^*) \right\} \\
&= \sup_{v_0^* \in B^*} \left\{ \inf_{(u, v_1^*) \in (C_1)^*_{\hat{v}_0^*} \times D^*} J_1^*(u, v_1^*, v_0^*) \right\}. \qquad (40)
\end{aligned}
$$

The proof is complete. □

9. 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 [5], Chapter 21.

9.1. 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

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

subject to

$$
\begin{cases}
(H_{ijkl}(t)e_{kl}(u))_{,j} + f_i = 0 \text{ in } \Omega, \\
H_{ijkl}(t)e_{kl}(u)n_j - \hat{f}_i = 0, \text{ on } \Gamma_t, \ \forall i \in \{1,2,3\}.
\end{cases} \qquad (41)
$$

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

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

Preprints (www.preprints.org) | NOT PEER-REVIEWED | Posted: 21 August 2023 doi:10.20944/preprints202302.0051.v29

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 [2,3]. Similar theoretical results have been developed in [10], 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 [1]. In addition, the primal variational development of the topology optimization problem has been described in [10].

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.

9.2. Mathematical formulation of the topology optimization problem

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

Theorem 9.1. *Consider the statements and assumptions indicated in the last section, in particular those refereing to Ω and the functional $\hat{J} : U \times B \to \mathbb{R}$.*

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

$$dx = dx_1dx_2dx_3.$$

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

$$\begin{aligned} J^*(u) &= \inf_{t\in B}\{J_1(u,t)\} \\ &= \inf_{t\in B}\{-G(e(u),t) + \langle u_i, f_i\rangle_{L^2(\Omega)} + \langle u_i, \hat{f}_i\rangle_{L^2(\Gamma_t)}\}. \end{aligned} \tag{42}$$

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

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

Preprints (www.preprints.org) | NOT PEER-REVIEWED | Posted: 21 August 2023 doi:10.20944/preprints202302.0051.v29

where

$$Ind(u,t) = \begin{cases} 0, & \text{if } (u,t) \in A^*, \\ +\infty, & \text{otherwise}, \end{cases} \tag{43}$$

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*

$$\begin{aligned} J(u_0,t_0) &= \inf_{(u,t)\in U\times B} J(u,t) \\ &= \sup_{\hat{u}\in U} J^*(\hat{u}) \\ &= J^*(u_0) \\ &= \hat{J}(u_0,t_0) \\ &= \inf_{(t,\sigma)\in B\times C^*} G^*(\sigma,t) \\ &= G^*(\sigma(u_0),t_0), \end{aligned} \tag{44}$$

where

$$\begin{aligned} G^*(\sigma,t) &= \sup_{v\in Y}\{\langle v_{ij},\sigma_{ij}\rangle_{L^2(\Omega)} - G(v,t)\} \\ &= \frac{1}{2}\int_\Omega \overline{H}_{ijkl}(t)\sigma_{ij}\sigma_{kl}\,dx, \end{aligned} \tag{45}$$

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

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

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

and

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

Proof. Observe that

$$\begin{aligned}
\inf_{(u,t)\in U\times B} J(u,t) &= \inf_{t\in B}\left\{\inf_{u\in U} J(u,t)\right\} \\
&= \inf_{t\in B}\left\{\sup_{\hat{u}\in U}\left\{\inf_{u\in U}\left\{\frac{1}{2}\int_\Omega H_{ijkl}(t)e_{ij}(u)e_{kl}(u)\,dx\right.\right.\right. \\
&\quad +\langle \hat{u}_i, (H_{ijkl}(t)e_{kl}(u))_{,j}+f_i\rangle_{L^2(\Omega)} \\
&\quad \left.\left.\left.-\langle \hat{u}_i, H_{ijkl}(t)e_{kl}(u)n_j-\hat{f}_i\rangle_{L^2(\Gamma_t)}\right\}\right\}\right\} \\
&= \inf_{t\in B}\left\{\sup_{\hat{u}\in U}\left\{\inf_{u\in U}\left\{\frac{1}{2}\int_\Omega H_{ijkl}(t)e_{ij}(u)e_{kl}(u)\,dx\right.\right.\right. \\
&\quad -\int_\Omega H_{ijkl}(t)e_{ij}(\hat{u})e_{kl}(u)\,dx \\
&\quad \left.\left.\left.+\langle \hat{u}_i, f_i\rangle_{L^2(\Omega)}+\langle \hat{u}_i, \hat{f}_i\rangle_{L^2(\Gamma_t)}\right\}\right\}\right\} \\
&= \inf_{t\in B}\left\{\sup_{\hat{u}\in U}\left\{-\int_\Omega H_{ijkl}(t)e_{ij}(\hat{u})e_{kl}(\hat{u})\,dx\right.\right. \\
&\quad \left.\left.\langle \hat{u}_i, f_i\rangle_{L^2(\Omega)}+\langle \hat{u}_i, \hat{f}_i\rangle_{L^2(\Gamma_t)}\right\}\right\} \\
&= \inf_{t\in B}\left\{\inf_{\sigma\in C^*} G^*(\sigma,t)\right\}. \qquad (46)
\end{aligned}$$

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

$$\begin{aligned}
\inf_{(u,t)\in U\times B} J(u,t) &= \inf_{t\in B}\left\{\sup_{\hat{u}\in U} J_1(u,t)\right\} \\
&= \sup_{u\in U}\left\{\inf_{t\in B} J_1(u,t)\right\} \\
&= J_1(u_0,t_0) \\
&= \inf_{t\in B} J_1(u_0,t) \\
&= J^*(u_0). \qquad (47)
\end{aligned}$$

Finally, from the extremal necessary condition

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

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 $\sigma(u_0)\in C^*$.

Preprints (www.preprints.org) | NOT PEER-REVIEWED | Posted: 21 August 2023 doi:10.20944/preprints202302.0051.v29

Moreover

$$\begin{aligned} J^*(u_0) &= -G(e(u_0)) + \langle (u_0)_i, f_i \rangle_{L^2(\Omega)} + \langle (u_0)_i, \hat{f}_i \rangle_{L^2(\Gamma_t)} \\ &= G(e(u_0)) \\ &= G(e(u_0)) + Ind(u_0, t_0) \\ &= J(u_0, t_0) \\ &= G^*(\sigma(u_0), t_0). \end{aligned} \tag{48}$$

This completes the proof. □

9.3. 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);
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;
```

Preprints (www.preprints.org) | NOT PEER-REVIEWED | Posted: 21 August 2023 doi:10.20944/preprints202302.0051.v29

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;

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);
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
```

Preprints (www.preprints.org) | NOT PEER-REVIEWED | Posted: 21 August 2023 doi:10.20944/preprints202302.0051.v29


```
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.

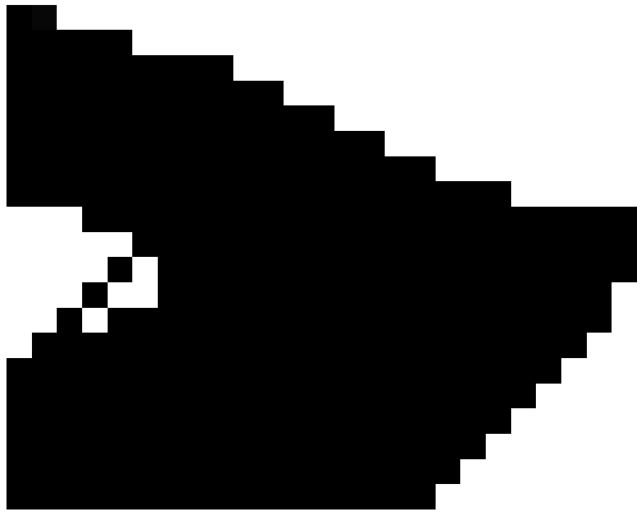

Figure 5. Density $t(x,y)$ for the Case A.

Preprints (www.preprints.org) | NOT PEER-REVIEWED | Posted: 21 August 2023 doi:10.20944/preprints202302.0051.v29

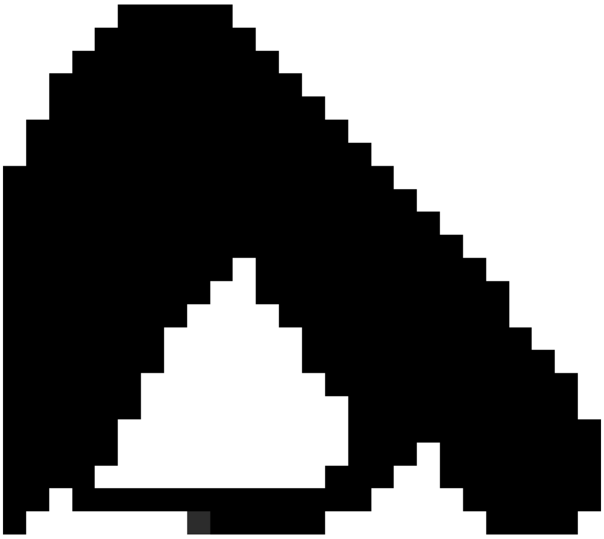

Figure 6. Density $t(x, y)$ for the Case B.

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

10. 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

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

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

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

 doi:10.20944/preprints202302.0051.v29

It is well known that

$$\begin{aligned}\alpha &= \inf_{u\in V} J(u) \\ &= \inf_{u\in V} J^{**}(u) \\ &= \inf_{u\in V}\{(G\circ\nabla)^{**}(u) - \langle u,f\rangle_{L^2}\}. \end{aligned} \tag{49}$$

Under some mild hypotheses, from convexity, we have that

$$\begin{aligned} &\inf_{u\in V}\{(G\circ\nabla)^{**}(u) - \langle u,f\rangle_{L^2}\} \\ = &\sup_{v^*\in A^*}\{-(G\circ\nabla)^*(-div\ v^*)\} = -(G\circ\nabla)^*(f), \end{aligned} \tag{50}$$

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

$$\begin{aligned}(G\circ\nabla)^*(-div\ v^*) &= \sup_{u\in V}\{\langle u, -div\ v^*\rangle_{L^2} - G(\nabla u)\} \\ &= \sup_{u\in V}\{\langle \nabla u, v^*\rangle_{L^2} - G(\nabla u)\} \\ &\leq \inf_{\phi\in Y^*}\left\{\sup_{v\in Y}\{\langle v,v^*\rangle_{L^2} - G(v) + \langle\phi,\text{curl } v\rangle_{L^2}\right\} \\ &= \inf_{\phi\in Y^*} G^*(v^* + \text{curl } \phi). \end{aligned} \tag{51}$$

where we have denoted

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

and

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

Joining the pieces, we have got

$$\begin{aligned}\inf_{u\in V} J(u) &= \inf_{u\in V}\{G(\nabla u) - \langle u,f\rangle_{L^2}\} \\ &\geq \sup_{(v^*,\phi)\in A^*\times Y^*}\{-G^*(v^* + \text{curl } \phi)\}, \end{aligned} \tag{52}$$

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).

11. 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 $\partial\Omega$.

Preprints (www.preprints.org) | NOT PEER-REVIEWED | Posted: 21 August 2023 doi:10.20944/preprints202302.0051.v29

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

$$J(u) = \frac{\gamma}{2}\int_\Omega \nabla u \cdot \nabla u \, dx + \frac{\alpha}{4}\int_\Omega u^4 \, dx \\ -\frac{\beta}{2}\int_\Omega u^2 \, dx - \langle u, f\rangle_{L^2} \quad (53)$$

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

$$\frac{\partial^2 J_1(u)}{\partial u^2} = (-\gamma\nabla u + \alpha u^3 - \beta u - f)6\alpha u \\ +(-\gamma\nabla^2 + 3\alpha u^2 - \beta)^2. \quad (54)$$

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

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

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

$$\begin{aligned} J_3(u) &= K_1 J_1(u) + J(u) \\ &= \frac{K_1}{2}\int_\Omega (-\gamma \nabla^2 u + \alpha u^3 - \beta u - f)^2 \, dx \\ &\quad + \frac{\gamma}{2}\int_\Omega \nabla u \cdot \nabla u \, dx + \frac{\alpha}{4}\int_\Omega u^4 \, dx \\ &\quad - \frac{\beta}{2}\int_\Omega u^2 \, dx - \langle u, f \rangle_{L^2}, \end{aligned} \tag{55}$$

subject to

$$u \in B_3.$$

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

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

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

12. 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

$$\begin{aligned} J(u) &= \frac{\gamma}{2}\int_\Omega \nabla u \cdot \nabla u \, dx + \frac{\alpha}{4}\int_\Omega u^4 \, dx \\ &\quad - \frac{\beta}{2}\int_\Omega u^2 \, dx - \langle u, f \rangle_{L^2} \end{aligned} \tag{56}$$

 doi:10.20944/preprints202302.0051.v29

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

$$\begin{aligned} F_1^*(v_1^*) &= \sup_{u\in V}\{\langle u, v_1^*\rangle_{L^2} - F_1(u)\} \\ &= \frac{1}{2}\int_\Omega \frac{(v_1^*)^2}{-\gamma\nabla^2}\, dx, \end{aligned} \tag{57}$$

$$\begin{aligned} F_2^*(v_2^*) &= \sup_{u\in V}\{\langle u, v_2^*\rangle_{L^2} - F_2(u)\} \\ &= \frac{3}{4}\int_\Omega \frac{(v_2^*)^{4/3}}{\alpha^{1/3}}\, dx, \end{aligned} \tag{58}$$

$$\begin{aligned} F_3^*(v_3^*) &= \sup_{u\in V}\{\langle u, v_3^*\rangle_{L^2} - F_3(u)\} \\ &= \frac{1}{2\beta}\int_\Omega (v_3^*)^2\, dx. \end{aligned} \tag{59}$$

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

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

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

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

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

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

Preprints (www.preprints.org) | NOT PEER-REVIEWED | Posted: 21 August 2023 doi:10.20944/preprints202302.0051.v29

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

$$F_4^*(v^*) = \begin{cases} 0, & \text{if } v_1^* + v_2^* - v_3^* - f = 0, \text{ in } \Omega, \\ +\infty, & \text{otherwise.} \end{cases} \tag{60}$$

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

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

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

$$\begin{aligned} J^*(v^*) &= \frac{1}{2}\int_\Omega \left(-v_2^* + v_3^* + f + \frac{\gamma \nabla^2 v_3^*}{\beta}\right)^2 dx \\ &+ \frac{1}{2}\int_\Omega \left(v_2^* - \alpha \left(\frac{v_3^*}{\beta}\right)^3\right)^2 dx. \end{aligned} \tag{61}$$

At this point, defining

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

we obtain

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

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

Preprints (www.preprints.org) | NOT PEER-REVIEWED | Posted: 21 August 2023 doi:10.20944/preprints202302.0051.v29

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

From such results we may infer that

$$\begin{aligned} \det\left(\frac{\partial^2 J^*(v^*)}{\partial v_2^* \partial v_3^*}\right) &= \frac{\partial^2 J^*(v^*)}{\partial (v_2^*)^2}\frac{\partial^2 J^*(v^*)}{\partial (v_3^*)^2} - \left(\frac{\partial^2 J^*(v^*)}{\partial v_2^* \partial v_3^*}\right)^2 \\ &= \left(-1 - \frac{\gamma\nabla^2}{\beta} + 3\alpha\frac{(v_3^*)^2}{\beta^3}\right)^2 + \mathcal{O}(\varphi) \end{aligned} \quad (62)$$

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,

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

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

12.1. 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.

Preprints (www.preprints.org) | NOT PEER-REVIEWED | Posted: 21 August 2023 doi:10.20944/preprints202302.0051.v29

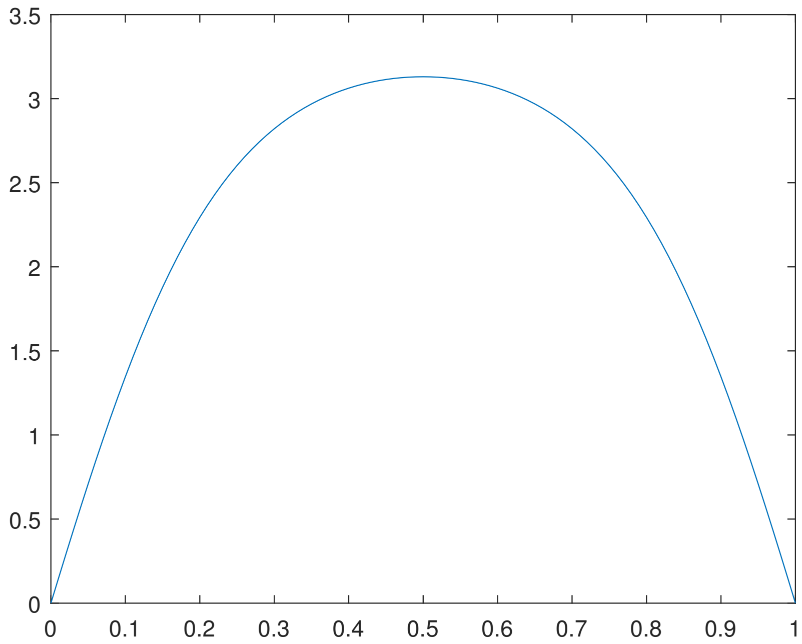

Figure 7. Solution $u(x) = v_3^*(x)/\beta$ for the example 1.

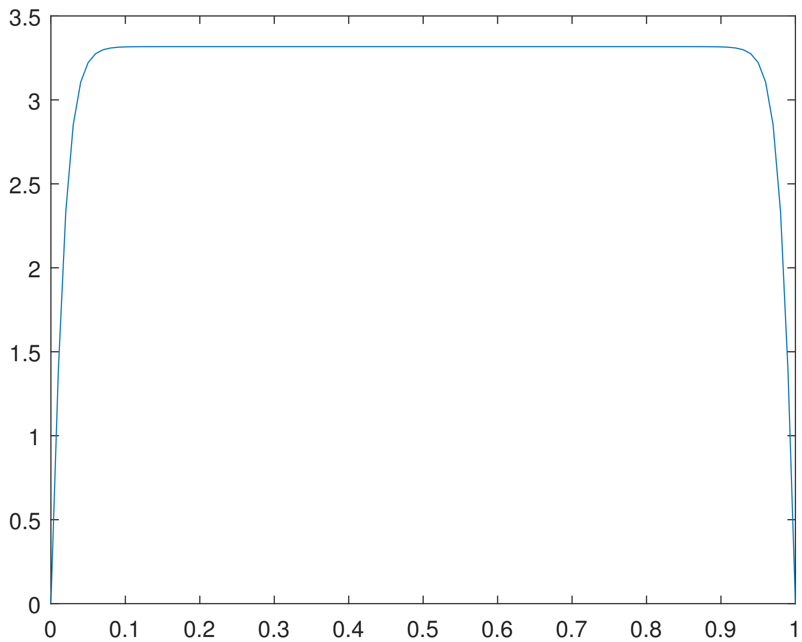

Figure 8. Solution $u(x) = v_3^*(x)/\beta$ for the example 2.

13. 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

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

 doi:10.20944/preprints202302.0051.v29

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

$$\begin{aligned} G_1^*(v^*, u) &= \sup_{v \in Y} \{ \langle v, v^* \rangle_{L^2} - G_1(u, v) \} \\ &= -G_{K_\varepsilon}^*(v^* + Ku) + \frac{K}{2} \int_\Omega u^2 \, dx, \end{aligned} \tag{63}$$

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

and

$$\begin{aligned} F^*(-v^*) &= \sup_{u \in V} \{ -\langle u, v^* \rangle_{L^2} - F(u) \} \\ &= \frac{1}{2\varepsilon} \int_\Omega (v^* - f)^2 \, dx. \end{aligned} \tag{64}$$

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

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

and

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

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

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

14. 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

$$\begin{aligned} J(u) &= \frac{1}{2}\int_\Omega \min\{(u'+1)^2, (u'-1)^2\}\, dx \\ &+\frac{1}{2}\int_\Omega u^2\, dx - \langle u, f\rangle_{L^2} \\ &= \frac{1}{2}\int_\Omega (u')^2\, dx - \int_\Omega |u'|\, dx + 1/2 \\ &+\frac{1}{2}\int_\Omega u^2\, dx - \langle u, f\rangle_{L^2}. \end{aligned} \tag{65}$$

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

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

Preprints (www.preprints.org) | NOT PEER-REVIEWED | Posted: 21 August 2023 doi:10.20944/preprints202302.0051.v29

Observe now that

$$
\begin{aligned}
J_2(u,v,\phi) &= J_1(u,v)+\frac{1}{2}\langle \phi^2,(v')^2-K_2\rangle_{L^2} \\
&= G(u',v')+\frac{1}{2}\langle \phi^2,(v')^2-K_2\rangle_{L^2} \\
&\quad +F(u,v) \\
&= -\langle u',v_1^*\rangle_{L^2}-\langle v',v_2^*\rangle_{L^2}+G(u',v') \\
&\quad +\frac{1}{2}\langle \phi^2,(v')^2-K_2\rangle_{L^2} \\
&\quad \langle u',v_1^*\rangle_{L^2}+\langle v',v_2^*\rangle_{L^2}+F(u,v) \\
&\geq \inf_{(v_1,v_2)\in Y\times Y}\Big\{-\langle v_1,v_1^*\rangle_{L^2}-\langle v_2,v_2^*\rangle_{L^2}+G_1(v_1,v_2,\phi) \\
&\quad +\frac{1}{2}\langle \phi^2,(v_2)^2-K_2\rangle_{L^2}\Big\} \\
&\quad +\inf_{(u,v)\in V\times V_1}\{\langle u',v_1^*\rangle_{L^2}+\langle v',v_2^*\rangle_{L^2}+F(u,v)\} \\
&= -G_1^*(v_1^*,v_2^*,\phi)-\tilde{F}^*(v_1^*,v_2^*),\ \forall (u,v)\in V\times V_1,(v_1^*,v_2^*,\phi)\in [Y^*]^3, \qquad (66)
\end{aligned}
$$

where

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

Also,

$$
\begin{aligned}
G_1^*(v_1^*,v_2^*,\phi) &= \sup_{(v_1,v_2)\in Y\times Y}\{\langle v_1,v_1^*\rangle_{L^2}+\langle v_1,v_1^*\rangle_{L^2}-G_1(v_1,v_2,\phi)\} \\
&= \frac{1}{2}\int_\Omega (v_1^*)^2\,dx \\
&\quad +\int_\Omega |v_1^*|\,dx+\frac{1}{2}\int_\Omega \frac{(v_1^*-v_2^*)^2}{\phi^2} \\
&\quad +\frac{K_2}{2}\int_\Omega \phi^2\,dx, \qquad (67)
\end{aligned}
$$

where

$$\tilde{F}^*(v^*)=\begin{cases} \frac{1}{2}\int_\Omega((v_1^*)'+f)^2\,dx-v_1^*(1)u(1), & \text{if } (v_2^*)'=0, \text{ in } \Omega, \\ +\infty, & \text{otherwise.}\end{cases} \qquad (68)$$

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

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

Preprints (www.preprints.org) | NOT PEER-REVIEWED | Posted: 21 August 2023 doi:10.20944/preprints202302.0051.v29

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.

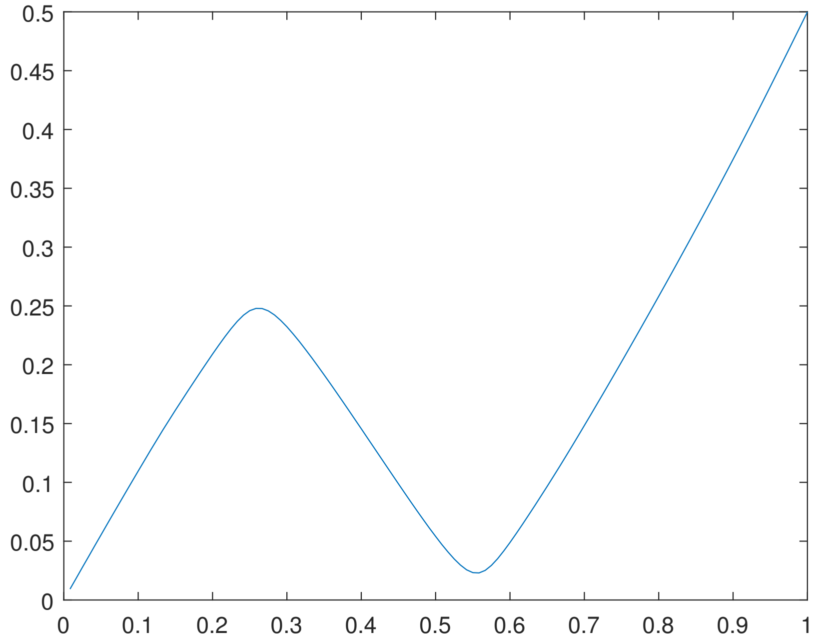

Figure 9. Solution $u_0(x)$ for the example A.

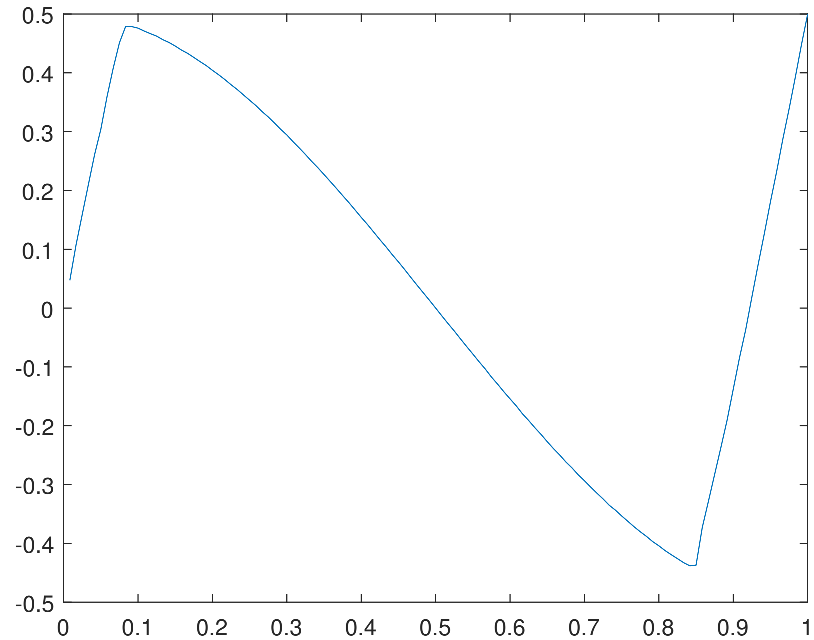

Figure 10. Solution $u_0(x)$ for the example B.

15. 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

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

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

$$\begin{aligned}
& \frac{1}{2}\int_\Omega ((u' + v')^2 - 1)^2\, dx + \frac{1}{2}\int_\Omega u^2\, dx - \langle u, f\rangle_{L^2} + \langle \Lambda^2, (v')^2 - K\rangle_{L^2} \\
= & -\langle v_0^*, (u' + v')^2 - 1\rangle_{L^2} + \frac{1}{2}\int_\Omega ((u' + v')^2 - 1)^2\, dx \\
& +\langle v_0^*, (u' + v')^2 - 1\rangle_{L^2} + \langle \Lambda^2, (v')^2 - K\rangle_{L^2} - \langle u', v_1^*\rangle_{L^2} - \langle v', v_2^*\rangle_{L^2} \\
& +\langle u', v_1^*\rangle_{L^2} + \langle v', v_2^*\rangle_{L^2} + \frac{1}{2}\int_\Omega u^2\, dx - \langle u, f\rangle_{L^2} \\
\geq & \inf_{w \in Y}\left\{-\langle v_0^*, w\rangle_{L^2} + \frac{1}{2}\int_\Omega (w)^2\, dx\right\} \\
& \inf_{(v_1, v_2) \in Y \times Y}\left\{\langle v_0^*, (v_1 + v_2)^2 - 1\rangle_{L^2} + \langle \Lambda^2, (v_2)^2 - K\rangle_{L^2} - \langle v_1, v_1^*\rangle_{L^2} - \langle v_2, v_2^*\rangle_{L^2}\right\} \\
& + \inf_{(u,v) \in V \times V_0}\left\{\langle u', v_1^*\rangle_{L^2} + \langle v', v_2^*\rangle_{L^2} + \frac{1}{2}\int_\Omega u^2\, dx - \langle u, f\rangle_{L^2}\right\} \\
= & -\frac{1}{2}\int_\Omega (v_0^*)^2\, dx - \int_\Omega v_0^*\, dx \\
& -\frac{1}{4}\int_\Omega \frac{(v_1^*)^2}{v_0^*}\, dx - \frac{1}{2}\int_\Omega \frac{(v_1^* - v_2^*)^2}{2\Lambda^2}\, dx \\
& -\frac{1}{2}\int_\Omega ((v_1^*)' + f)^2\, dx - \frac{1}{2}\int_\Omega K\Lambda^2\, dx + v_1^*(1)u(1).
\end{aligned} \tag{69}$$

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

$$\begin{aligned}
J_1^*(v^*, \Lambda) = & -\frac{1}{2}\int_\Omega (v_0^*)^2\, dx - \int_\Omega v_0^*\, dx \\
& -\frac{1}{4}\int_\Omega \frac{(v_1^*)^2}{v_0^*}\, dx - \frac{1}{2}\int_\Omega \frac{(v_1^* - v_2^*)^2}{2\Lambda^2}\, dx \\
& -\frac{1}{2}\int_\Omega ((v_1^*)' + f)^2\, dx - \frac{1}{2}\int_\Omega K\Lambda^2\, dx + v_1^*(1)u(1)
\end{aligned} \tag{70}$$

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 $A^* \times [Y^*] \times \mathbb{R} \times Y^*$.

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

Remark 15.1. *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 $K > 0$.*

16. 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 $\partial\Omega = \Gamma$.

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

Preprints (www.preprints.org) | NOT PEER-REVIEWED | Posted: 21 August 2023 doi:10.20944/preprints202302.0051.v29

$$
\begin{aligned}
J_1(u,\phi) &= G_1(\nabla u+\nabla_y\phi)+F(u)-\langle u,f\rangle_{L^2} \\
&= -\frac{1}{|\Omega|}\int_\Omega\int_\Omega v^*(x,y)\cdot(\nabla u+\nabla_y\phi(x,y))\,dy\,dx+G_1(\nabla u+\nabla_y\phi) \\
&\quad +\frac{1}{|\Omega|}\int_\Omega\int_\Omega v^*(x,y)\cdot(\nabla u+\nabla_y\phi(x,y))\,dy\,dx+F(u)-\langle u,f\rangle_{L^2} \\
&\geq \inf_{v\in Y_2}\left\{-\frac{1}{|\Omega|}\int_\Omega\int_\Omega v^*(x,y)\cdot v(x,y)\,dy\,dx+G_1(v)\right\} \\
&\quad +\inf_{(v,\phi)\in V\times V_0}\left\{\frac{1}{|\Omega|}\int_\Omega\int_\Omega v^*(x,y)\cdot(\nabla u+\nabla_y\phi(x,y))\,dy\,dx+F(u)-\langle u,f\rangle_{L^2}\right\} \\
&= -G_1^*(v^*)-F^*\left(\operatorname{div}_x\left(\frac{1}{|\Omega|}\int_\Omega v^*(x,y)\,dy\right)+f\right) \\
&\quad +\frac{1}{|\Omega|}\int_{\partial\Omega}\left(\int_\Omega v^*(x,y)\,dy\right)\otimes\mathbf{n}u_0\,d\Gamma, \qquad (71)
\end{aligned}
$$

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

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

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

$$
\begin{aligned}
&F^*\left(\operatorname{div}_x\left(\frac{1}{|\Omega|}\int_\Omega v^*(x,y)\,dy\right)+f\right)-\frac{1}{|\Omega|}\int_{\partial\Omega}\left(\int_\Omega v^*(x,y)\,dy\right)\otimes\mathbf{n}u_0\,d\Gamma \\
=&\sup_{(v,\phi)\in V\times V_0}\left\{-\frac{1}{|\Omega|}\int_\Omega\int_\Omega v^*(x,y)\cdot(\nabla u+\nabla_y\phi(x,y))\,dy\,dx-F(u)+\langle u,f\rangle_{L^2}\right\}, \qquad (72)
\end{aligned}
$$

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

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

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).

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.

Preprints (www.preprints.org) | NOT PEER-REVIEWED | Posted: 21 August 2023 doi:10.20944/preprints202302.0051.v29

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

$$\begin{aligned} J(u,v,E) &= \frac{\gamma_1}{2}\int_\Omega \nabla u\cdot\nabla u\,dx + \frac{\alpha_1}{2}\int_\Omega |u|^4\,dx \\ &-\frac{\omega^2}{2}\int_\Omega |u|^2\,dx \\ &+\frac{\gamma_2}{2}\int_\Omega \nabla v\cdot\nabla v\,dx + \frac{\alpha_2}{2}\int_\Omega |v|^4\,dx \\ &-\frac{\omega_1^2}{2K_3^2}\int_\Omega |v|^2\,dx \\ &-\frac{E}{2}\left(\int_\Omega (|u|^2+|v|^2)\,dx - m_T\right). \end{aligned} \quad (73)$$

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

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

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.

Preprints (www.preprints.org) | NOT PEER-REVIEWED | Posted: 21 August 2023 doi:10.20944/preprints202302.0051.v29

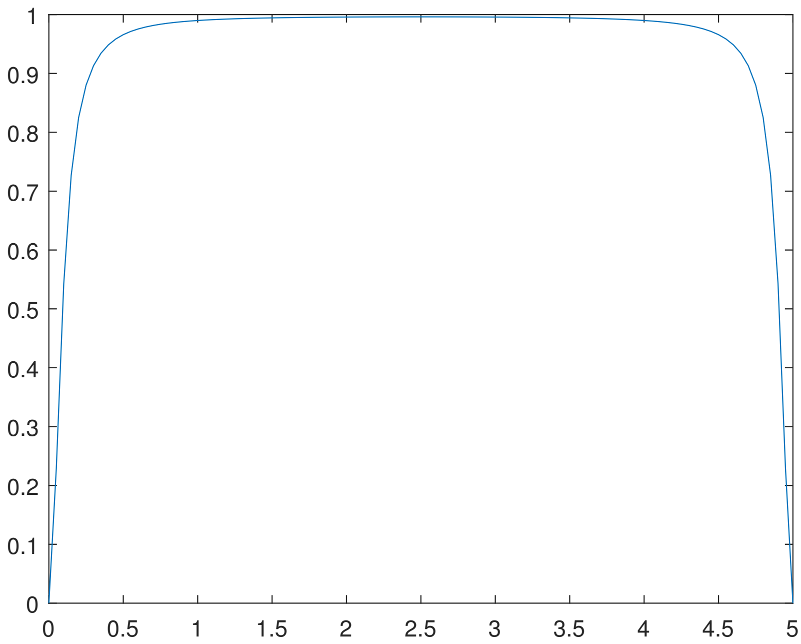

Figure 11. Solution $\phi_N(x)$ for the $\omega = 1.8$.

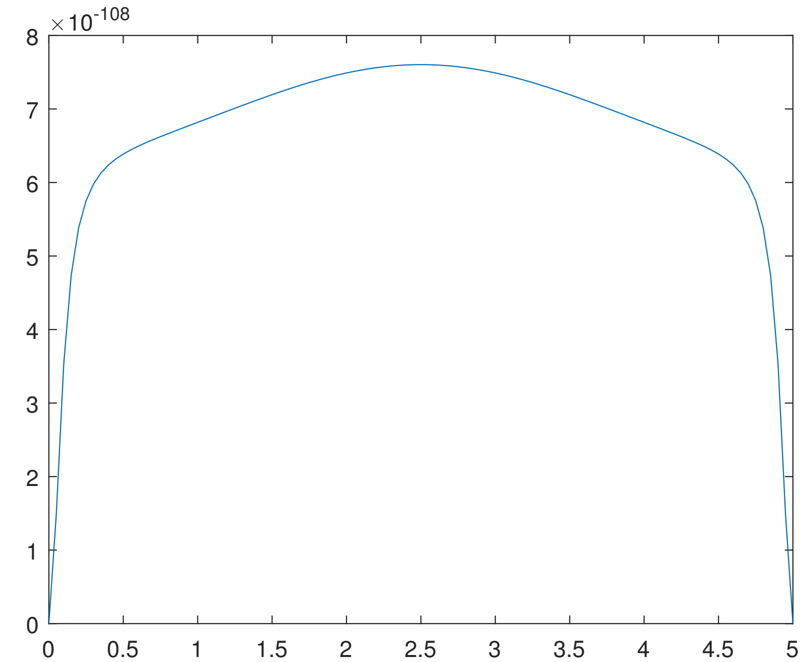

Figure 12. Solution $\phi_S(x)$ for the $\omega = 1.8$.

Preprints (www.preprints.org) | NOT PEER-REVIEWED | Posted: 21 August 2023 doi:10.20944/preprints202302.0051.v29

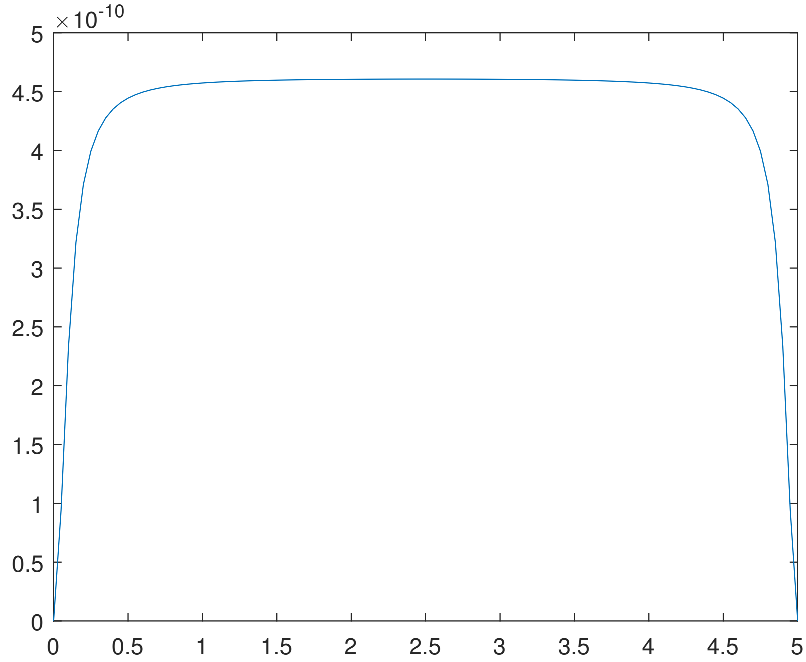

Figure 13. Solution $\phi_N(x)$ for the $\omega = 1.0$.

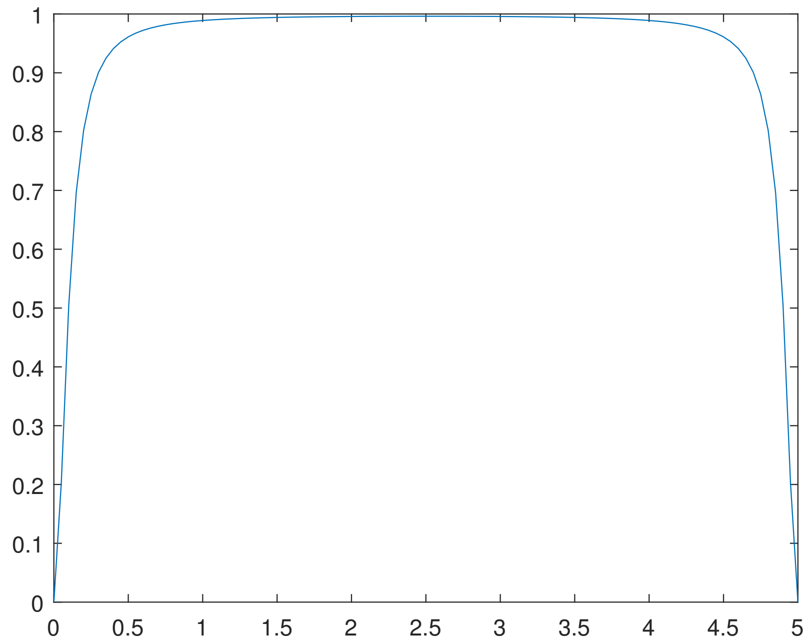

Figure 14. Solution $\phi_S(x)$ for the $\omega = 1.0$.

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.

 doi:10.20944/preprints202302.0051.v29

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 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.

Preprints (www.preprints.org) | NOT PEER-REVIEWED | Posted: 21 August 2023 doi:10.20944/preprints202302.0051.v29

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

$$\begin{aligned} G(\nabla\phi) \quad = \quad & \frac{\gamma_p^D}{2}\int_\Omega (\nabla\phi_p^D)\cdot(\nabla\phi_p^D)\ dy \\ & +\frac{\gamma_N^D}{2}\int_\Omega (\nabla\phi_N^D)\cdot(\nabla\phi_N^D)\ dx\ dy \\ & \frac{\gamma_p^T}{2}\int_\Omega (\nabla\phi_p^T)\cdot(\nabla\phi_p^T)\ dy \\ & +\frac{\gamma_{N_1}^T}{2}\int_\Omega (\nabla\phi_{N_1}^T)\cdot(\nabla\phi_{N_1}^T)\ dx\ dy \\ & +\frac{\gamma_{N_2}^T}{2}\int_\Omega (\nabla\phi_{N_2}^T)\cdot(\nabla\phi_{N_2}^T)\ dx\ dy \\ & +\frac{\gamma_{2p}^{H_e}}{2}\int_\Omega (\nabla\phi_{2p}^{H_e})\cdot(\nabla\phi_{2p}^{H_e})\ dy \\ & +\frac{\gamma_{N_1}^{H_e}}{2}\int_\Omega (\nabla\phi_{N_1}^{H_e})\cdot(\nabla\phi_{N_1}^{H_e})\ dx\ dy \\ & +\frac{\gamma_{N_2}^{H_e}}{2}\int_\Omega (\nabla\phi_{N_2}^{H_e})\cdot(\nabla\phi_{N_2}^{H_e})\ dx\ dy \\ & +\frac{\gamma_N}{2}\int_\Omega (\nabla\phi_N)\cdot(\nabla\phi_N)\ dx, \end{aligned} \tag{74}$$

and,

$$\begin{aligned} F(\phi) \quad = \quad & \frac{\alpha_D}{2}\int_\Omega \frac{|\phi_D(x-\xi_1,y-\xi_2)|^2|\phi_D(\xi_1,\xi_2)|^2}{|(x,y)-(\xi_1,\xi_2)|}\ dx\ dy\ d\xi_1\ d\xi_2 \\ & +\frac{\alpha_T}{2}\int_\Omega \frac{|\phi_T(x-\xi_1,y-\xi_2)|^2|\phi_T(\xi_1,\xi_2)|^2}{|(x,y)-(\xi_1,\xi_2)|}\ dx\ dy\ d\xi_1\ d\xi_2 \\ & +\frac{\alpha_{DT}}{2}\int_\Omega \frac{|\phi_D(x-\xi_1,y-\xi_2)|^2|\phi_T(\xi_1,\xi_2)|^2}{|(x,y)-(\xi_1,\xi_2)|}\ dx\ dy\ d\xi_1\ d\xi_2 \\ & +\frac{\alpha_{H_e}}{2}\int_\Omega \frac{|\phi_{H_e}(x-\xi_1,y-\xi_2)|^2|\phi_{H_e}(\xi_1,\xi_2)|^2}{|(x,y)-(\xi_1,\xi_2)|}\ dx\ dy\ d\xi_1\ d\xi_2 \\ & +\frac{\alpha_N}{2}\int_0^{t_f}\int_\Omega \frac{|\phi_N(x-\xi)|^2|\phi_N(\xi)|^2}{|x-\xi|}\ dx\ d\xi \\ & +\sum_{j=1}^{2}\frac{\alpha_{H_e\,N}}{2}\int_\Omega \frac{|\phi_{H_e}(x_1-\xi_1,y-\xi_2)|^2|\phi_N(\xi_j)|^2}{|(x,y)-(\xi_1,\xi_2)|}\ dx\ dy\ d\xi_1\ d\xi_2 \end{aligned} \tag{75}$$

and the kinetics energy is expressed by

$$\begin{aligned} E_c(\phi,\mathbf{r}) \quad = \quad & \frac{1}{2}\int_\Omega |\phi_D|^2\,\frac{\partial\mathbf{r}_D}{\partial t}\cdot\frac{\partial\mathbf{r}_D}{\partial t}\ dx\ dy \\ & +\frac{1}{2}\int_\Omega |\phi_T|^2\,\frac{\partial\mathbf{r}_T}{\partial t}\cdot\frac{\partial\mathbf{r}_T}{\partial t}\ dx\ dy \\ & +\frac{1}{2}\int_\Omega |\phi_{H_e}|^2\,\frac{\partial\mathbf{r}_{H_e}}{\partial t}\cdot\frac{\partial\mathbf{r}_{H_e}}{\partial t}\ dx\ dy \\ & +\frac{1}{2}\int_\Omega |\phi_N|^2\,\frac{\partial\mathbf{r}_N}{\partial t}\cdot\frac{\partial\mathbf{r}_N}{\partial t}\ dx\ dy, \end{aligned} \tag{76}$$

 doi:10.20944/preprints202302.0051.v29

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.
$$\int_\Omega |\phi_N|^2 \, dx \, dy = \lambda_2 (m_N)_T,$$

Preprints (www.preprints.org) | NOT PEER-REVIEWED | Posted: 21 August 2023 doi:10.20944/preprints202302.0051.v29

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

$$\begin{aligned} J_1(\phi, \omega, E, \lambda) &= \frac{\gamma_p^D}{2} \int_\Omega (\nabla \phi_p^D) \cdot (\nabla \phi_p^D) \, dy \\ &+ \frac{\gamma_N^D}{2} \int_\Omega (\nabla \phi_N^D) \cdot (\nabla \phi_N^D) \, dx \, dy \\ &\frac{\gamma_p^T}{2} \int_\Omega (\nabla \phi_p^T) \cdot (\nabla \phi_p^T) \, dy \\ &+ \frac{\gamma_{N_1}^T}{2} \int_\Omega (\nabla \phi_{N_1}^T) \cdot (\nabla \phi_{N_1}^T) \, dx \, dy \\ &+ \frac{\gamma_{N_2}^T}{2} \int_\Omega (\nabla \phi_{N_2}^T) \cdot (\nabla \phi_{N_2}^T) \, dx \, dy \\ &+ \frac{\gamma_{2p}^{H_e}}{2} \int_\Omega (\nabla \phi_{2p}^{H_e}) \cdot (\nabla \phi_{2p}^{H_e}) \, dy \\ &+ \frac{\gamma_{N_1}^{H_e}}{2} \int_\Omega (\nabla \phi_{N_1}^{H_e}) \cdot (\nabla \phi_{N_1}^{H_e}) \, dx \, dy \\ &+ \frac{\gamma_{N_2}^{H_e}}{2} \int_\Omega (\nabla \phi_{N_2}^{H_e}) \cdot (\nabla \phi_{N_2}^{H_e}) \, dx \, dy \\ &+ \frac{\gamma_N}{2} \int_\Omega (\nabla \phi_N) \cdot (\nabla \phi_N) \, dx \\ &+ \frac{\alpha_D}{2} \int_\Omega |\phi_D|^4 \, dx + \frac{\alpha_T}{2} \int_\Omega |\phi_T|^4 \, dx \\ &+ \frac{\alpha_{H_e}}{2} \int_\Omega |\phi_{H_e}|^4 \, dx + \frac{\alpha_N}{2} \int_\Omega |\phi_N|^4 \, dx \\ &- \omega^2 \int_\Omega (|\phi_D|^2 + |\phi_T|^2) \, dx \\ &- \omega_1^2 \int_\Omega |\phi_N|^2 \, dx + J_{Aux}, \end{aligned} \tag{77}$$

Preprints (www.preprints.org) | NOT PEER-REVIEWED | Posted: 21 August 2023 doi:10.20944/preprints202302.0051.v29

where the functional J_{Aux} stands for

$$\begin{aligned}
J_{Aux} &= -\int_\Omega (E_N^D)_5(y)\left(\int_\Omega |\phi_N^D(x,y)|^2\,dx - m_N\right)\,dy \\
&\quad -\int_\Omega (E_{N_1}^T)_6(y)\left(\int_\Omega |\phi_{N_1}^T(x,y)|^2\,dx - m_N\right)\,dy \\
&\quad -\int_\Omega (E_{N_2}^T)_7(y)\left(\int_\Omega |\phi_{N_2}^T(x,y)|^2\,dx - m_N\right)\,dy \\
&\quad -\int_\Omega (E_{N_1}^{H_e})_8(y)\left(\int_\Omega |\phi_{N_1}^{H_e}(x,y)|^2\,dx - m_N\right)\,dy \\
&\quad -\int_\Omega (E_{N_2}^{H_e})_9(y)\left(\int_\Omega |\phi_{N_2}^{H_e}(x,y)|^2\,dx - m_N\right)\,dy \\
&\quad -(E_D)_2\left(\int_\Omega |\phi_p^D(y)|^2\,dy - \lambda_1 c m_p\right) \\
&\quad -(E_T)_3\left(\int_\Omega |\phi_p^T(y)|^2\,dy - \lambda_1 c m_p\right) \\
&\quad -(E_{H_e})_3\left(\int_\Omega |\phi_{2P}^{H_e}(x,y)|^2\,dy - \lambda_2\, 2 c m_p\right) \\
&\quad -E_5\left(\int_\Omega |\phi_D|^2\,dx\,dy - \lambda_1 (m_D)_T\right) \\
&\quad -E_6\left(\int_\Omega |\phi_T|^2\,dx\,dy - \lambda_1 (m_T)_T\right) \\
&\quad -E_7\left(\int_\Omega |\phi_{H_e}|^2\,dx\,dy - \lambda_2 (m_{H_e})_T\right) \\
&\quad -E_8\left(\int_\Omega |\phi_N|^2\,dx\,dy - \lambda_2 (m_N)_T\right) \\
&\quad -E_9(\lambda_1+\lambda_2-1). \qquad (78)
\end{aligned}$$

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.

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 Hellion and a field of single energetic Neutrons.

Symbolically such a reaction stands for

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

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.

Preprints (www.preprints.org) | NOT PEER-REVIEWED | Posted: 21 August 2023 doi:10.20944/preprints202302.0051.v29

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

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

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

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

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

Preprints (www.preprints.org) | NOT PEER-REVIEWED | Posted: 21 August 2023 doi:10.20944/preprints202302.0051.v29

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.
$$m_e(t) = \int_\Omega \rho_e(x,t)\, dx.$$
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

 doi:10.20944/preprints202302.0051.v29

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

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

$$\begin{aligned}
G(\nabla\phi) \quad = \quad & \frac{\gamma_p^D}{2}\int_0^{t_f}\int_\Omega (\nabla\phi_p^D)\cdot(\nabla\phi_p^D)\ dy\ dt \\
& + \frac{\gamma_N^D}{2}\int_0^{t_f}\int_\Omega (\nabla\phi_N^D)\cdot(\nabla\phi_N^D)\ dx\ dy\ dt \\
& \frac{\gamma_p^T}{2}\int_0^{t_f}\int_\Omega (\nabla\phi_p^T)\cdot(\nabla\phi_p^T)\ dy\ dt \\
& + \frac{\gamma_{N_1}^T}{2}\int_0^{t_f}\int_\Omega (\nabla\phi_{N_1}^T)\cdot(\nabla\phi_{N_1}^T)\ dx\ dy\ dt \\
& + \frac{\gamma_{N_2}^T}{2}\int_0^{t_f}\int_\Omega (\nabla\phi_{N_2}^T)\cdot(\nabla\phi_{N_2}^T)\ dx\ dy\ dt \\
& + \frac{\gamma_{2p}^{H_e}}{2}\int_0^{t_f}\int_\Omega (\nabla\phi_{2p}^{H_e})\cdot(\nabla\phi_{2p}^{H_e})\ dy\ dt \\
& + \frac{\gamma_{N_1}^{H_e}}{2}\int_0^{t_f}\int_\Omega (\nabla\phi_{N_1}^{H_e})\cdot(\nabla\phi_{N_1}^{H_e})\ dx\ dy\ dt \\
& + \frac{\gamma_{N_2}^{H_e}}{2}\int_0^{t_f}\int_\Omega (\nabla\phi_{N_2}^{H_e})\cdot(\nabla\phi_{N_2}^{H_e})\ dx\ dy\ dt \\
& + \frac{\gamma_N}{2}\int_0^{t_f}\int_\Omega (\nabla\phi_N)\cdot(\nabla\phi_N)\ dx\ dt \\
& + \frac{\gamma_e}{2}\int_0^{t_f}\int_\Omega (\nabla\phi_e)\cdot(\nabla\phi_e)\ dx\ dy\ dt, \qquad (79)
\end{aligned}$$

and

$$\begin{aligned}
F(\phi) \quad = \quad & \frac{\alpha_D}{2}\int_0^{t_f}\int_\Omega \frac{|\phi_D(x-\xi_1, y-\xi_2, t)|^2|\phi_D(\xi_1,\xi_2,t)|^2}{|(x,y)-(\xi_1,\xi_2)|}\ dx\ dy\ d\xi_1\ d\xi_2\ dt \\
& + \frac{\alpha_T}{2}\int_0^{t_f}\int_\Omega \frac{|\phi_T(x-\xi_1, y-\xi_2, t)|^2|\phi_T(\xi_1,\xi_2,t)|^2}{|(x,y)-(\xi_1,\xi_2)|}\ dx\ dy\ d\xi_1\ d\xi_2\ dt \\
& + \frac{\alpha_{DT}}{2}\int_0^{t_f}\int_\Omega \frac{|\phi_D(x-\xi_1, y-\xi_2, t)|^2|\phi_T(\xi_1,\xi_2,t)|^2}{|(x,y)-(\xi_1,\xi_2)|}\ dx\ dy\ d\xi_1\ d\xi_2\ dt \\
& + \frac{\alpha_{H_e}}{2}\int_0^{t_f}\int_\Omega \frac{|\phi_{H_e}(x-\xi_1, y-\xi_2, t)|^2|\phi_{H_e}(\xi_1,\xi_2,t)|^2}{|(x,y)-(\xi_1,\xi_2)|}\ dx\ dy\ d\xi_1\ d\xi_2\ dt \\
& + \frac{\alpha_N}{2}\int_0^{t_f}\int_\Omega \frac{|\phi_N(x-\xi, t)|^2|\phi_N(\xi)|^2}{|x-\xi, t|}\ dx\ d\xi\ dt \\
& + \sum_{j=1}^{2}\frac{\alpha_{H_e\,N}}{2}\int_0^{t_f}\int_\Omega \frac{|\phi_{H_e}(x_1-\xi_1, y-\xi_2, t)|^2|\phi_N(\xi_j,t)|^2}{|(x,y)-(\xi_1,\xi_2)|}\ dx\ dy\ d\xi_1\ d\xi_2\ dt \\
& + \frac{\alpha_{H_e,\,e}}{2}\int_0^{t_f}\int_\Omega \frac{|\phi_{H_e}(x-\xi_1, y-\xi_2, t)|^2|\phi_e(\xi_1,\xi_2,t)|^2}{|(x,y)-(\xi_1,\xi_2)|}\ dx\ dy\ d\xi_1\ d\xi_2\ dt \\
& + \frac{\alpha_{e,e}}{2}\int_0^{t_f}\int_\Omega \frac{|\phi_e(x-\xi_1, y-\xi_2, t)|^2|\phi_e(\xi_1,\xi_2,t)|^2}{|(x,y)-(\xi_1,\xi_2)|}\ dx\ dy\ d\xi_1\ d\xi_2\ dt \qquad (80)
\end{aligned}$$

and the internal kinetics energy is expressed by

$$\begin{aligned} E_c(\phi,\mathbf{r}) &= \frac{1}{2}\int_0^{t_f}\int_\Omega |\phi_D|^2 \frac{\partial \mathbf{r}_D}{\partial t}\cdot\frac{\partial \mathbf{r}_D}{\partial t}\,dx\,dy\,dt \\ &+\frac{1}{2}\int_0^{t_f}\int_\Omega |\phi_T|^2 \frac{\partial \mathbf{r}_T}{\partial t}\cdot\frac{\partial \mathbf{r}_T}{\partial t}\,dx\,dy\,dt \\ &+\frac{1}{2}\int_0^{t_f}\int_\Omega |\phi_{H_e}|^2 \frac{\partial \mathbf{r}_{H_e}}{\partial t}\cdot\frac{\partial \mathbf{r}_{H_e}}{\partial t}\,dx\,dy\,dt \\ &+\frac{1}{2}\int_0^{t_f}\int_\Omega |\phi_N|^2 \frac{\partial \mathbf{r}_N}{\partial t}\cdot\frac{\partial \mathbf{r}_N}{\partial t}\,dx\,dy\,dt \\ &+\frac{1}{2}\int_0^{t_f}\int_\Omega |\phi_e|^2 \frac{\partial \mathbf{r}_e}{\partial t}\cdot\frac{\partial \mathbf{r}_e}{\partial t}\,dx\,dy\,dt, \end{aligned} \quad (81)$$

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,

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

$$\begin{aligned} F_2 &= \int_0^{t_f}\int_\Omega \mathbf{E}_{ind}\cdot K_p|\phi_p^D|^2\left(\mathbf{u}+\frac{\partial \mathbf{r}_D}{\partial t}\right)dx\,dy\,dt \\ &+\int_0^{t_f}\int_\Omega \mathbf{E}_{ind}\cdot K_p|\phi_p^T|^2\left(\mathbf{u}+\frac{\partial \mathbf{r}_T}{\partial t}\right)dx\,dy\,dt \\ &+\int_0^{t_f}\int_\Omega \mathbf{E}_{ind}\cdot K_p|\phi_{2p}^{H_e}|^2\left(\mathbf{u}+\frac{\partial \mathbf{r}_{H_e}}{\partial t}\right)dx\,dy\,dt \\ &+\int_0^{t_f}\int_\Omega \mathbf{E}_{ind}\cdot K_e|\phi_e|^2\left(\mathbf{u}+\frac{\partial \mathbf{r}_e}{\partial t}\right)dx\,dy\,dt, \end{aligned} \quad (82)$$

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 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,

$$\begin{aligned} F_3 &= \frac{C_D}{2}\int_0^{t_f}\int_\Omega \nabla_{(x,y)}\mathbf{r}_D\cdot\nabla_{(x,y)}\mathbf{r}_D\,dx\,dy\,dt + \frac{C_T}{2}\int_0^{t_f}\int_\Omega \nabla_{(x,y)}\mathbf{r}_T\cdot\nabla_{(x,y)}\mathbf{r}_T\,dx\,dy\,dt \\ &\frac{C_{H_e}}{2}\int_0^{t_f}\int_\Omega \nabla_{(x,y)}\mathbf{r}_{H_e}\cdot\nabla_{(x,y)}\mathbf{r}_{H_e}\,dx\,dy\,dt + \frac{C_N}{2}\int_0^{t_f}\int_\Omega \nabla_{(x,y)}\mathbf{r}_N\cdot\nabla_{(x,y)}\mathbf{r}_N\,dx\,dy\,dt \\ &\frac{C_e}{2}\int_0^{t_f}\int_\Omega \nabla_{(x,y)}\mathbf{r}_e\cdot\nabla_{(x,y)}\mathbf{r}_e\,dx\,dy\,dt, \end{aligned} \quad (83)$$

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

$$\rho\left(\frac{\partial u_k}{\partial t} + u_j\frac{\partial u_k}{\partial x_j}\right) = \rho f_k - \frac{\partial P}{\partial x_k} + \tau_{kj,j} + (F_E)_k + (F_M)_k,$$

Preprints (www.preprints.org) | NOT PEER-REVIEWED | Posted: 21 August 2023 doi:10.20944/preprints202302.0051.v29

$\forall k \in \{1,2,3\}$.

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

$$\begin{aligned} \mathbf{F}_M &= \{(F_M)_k\} \\ &= \left(K_p \left(|\phi_p^D|^2 \left(\mathbf{u} + \frac{\partial \mathbf{r}_D}{\partial t} \right) \right. \right. \\ & |\phi_p^T|^2 \left(\mathbf{u} + \frac{\partial \mathbf{r}_T}{\partial t} \right) \\ & \left. + |\phi_{2p}^{H_e}|^2 \left(\mathbf{u} + \frac{\partial \mathbf{r}_{H_e}}{\partial t} \right) \right) \\ & \left. + K_e |\phi_e|^2 \left(\mathbf{u} + \frac{\partial \mathbf{r}_e}{\partial t} \right) \right) \times \mathbf{B}. \end{aligned} \tag{84}$$

2. Mass conservation equation:

$$\frac{\partial \rho}{\partial t} + \text{div}\,(\rho \mathbf{u}) = 0.$$

3. Energy equation

$$\rho \frac{De}{Dt} + P(\,\text{div}\,\mathbf{u}) = \frac{\partial Q}{\partial t} - \text{div}\,\mathbf{q},$$

where we assume the Fourier law

$$\mathbf{q} = -K \nabla T,$$

where $T = T(x,t)$ is the scalar field of temperature.

Also,

$$\begin{aligned} e &= \frac{\rho}{2} \mathbf{u} \cdot \mathbf{u} + \frac{\rho_D}{2} \frac{\partial \mathbf{r}_D}{\partial t} \cdot \frac{\partial \mathbf{r}_D}{\partial t} \\ & + \frac{\rho_T}{2} \frac{\partial \mathbf{r}_T}{\partial t} \cdot \frac{\partial \mathbf{r}_T}{\partial t} \\ & + \frac{\rho_{H_e}}{2} \frac{\partial \mathbf{r}_{H_e}}{\partial t} \cdot \frac{\partial \mathbf{r}_{H_e}}{\partial t} \\ & + \frac{\rho_N}{2} \frac{\partial \mathbf{r}_N}{\partial t} \cdot \frac{\partial \mathbf{r}_N}{\partial t} \\ & + \frac{\rho_e}{2} \frac{\partial \mathbf{r}_e}{\partial t} \cdot \frac{\partial \mathbf{r}_e}{\partial t} \end{aligned} \tag{85}$$

and

$$\frac{De}{Dt} = \frac{\partial e}{\partial t} + u_j \frac{\partial e}{\partial x_j}.$$

4.

$$P = F_7(\rho, T),$$

Preprints (www.preprints.org) | NOT PEER-REVIEWED | Posted: 21 August 2023 doi:10.20944/preprints202302.0051.v29

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,

(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

$$\begin{aligned}
&\text{curl } \mathbf{E}_{ind} + \frac{1}{c}\text{ curl } \left(\hat{K}_p|\phi_p^D|^2\left(\mathbf{u} + \frac{\partial \mathbf{r}_D}{\partial t}\right)\right.\\
&+\hat{K}_p|\phi_p^T|^2\left(\mathbf{u} + \frac{\partial \mathbf{r}_T}{\partial t}\right)\\
&+\hat{K}_p|\phi_{2p}^{H_e}|^2\left(\mathbf{u} + \frac{\partial \mathbf{r}_{H_e}}{\partial t}\right)\\
&\left.+\ \hat{K}_e\int_\Omega |\phi_e(x,y,t)|^2\left(\mathbf{u}(y,t) + \frac{\partial \mathbf{r}_e(x,y,t)}{\partial t}\,dx\right)\right)\\
&\times(\text{ curl } \mathbf{A} - \mathbf{B}_0) - \frac{1}{c}\frac{\partial}{\partial t}(\text{ curl } \mathbf{A} - \mathbf{B}_0) = \mathbf{0},
\end{aligned} \tag{86}$$

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

$$\mathbf{B} = \mathbf{B}_0 - \text{ curl } \mathbf{A}.$$

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

$$\langle h_1,h_2\rangle_{L^2} = \int_0^{t_f}\int_\Omega h_1\,h_2\,dx\,dy\,dt.$$

Preprints (www.preprints.org) | NOT PEER-REVIEWED | Posted: 21 August 2023 doi:10.20944/preprints202302.0051.v29

Thus, already including the Lagrange multipliers concerning the restrictions indicated, the extended functional J_3 stands for=

$$\begin{aligned}
& J_3 = J_3(\phi, \mathbf{u}, \mathbf{r}, P, \mathbf{A}, \mathbf{B}, \mathbf{E}, \Lambda, E) \\
= \; & G(\nabla\phi) + F(\phi) + E_c(\phi, \mathbf{r}) + F_1 + F_2 + F_3 \\
& + \left\langle \Lambda_k, \rho \left(\frac{\partial u_k}{\partial t} + u_j \frac{\partial u_k}{\partial x_j} \right) - \rho f_k + \frac{\partial P}{\partial x_k} - \tau_{kj,j} - (F_E)_k - (F_M)_k \right\rangle_{L^2} \\
& + \left\langle \Lambda_4, \frac{\partial \rho}{\partial t} + \text{ div } (\rho \mathbf{u}) \right\rangle_{L^2} + J_{Aux_1} + J_{Aux_2} + J_{Aux_3} + J_{Aux_4},
\end{aligned} \tag{87}$$

where,

$$\begin{aligned}
J_{Aux_1} &= \left\langle \Lambda_5, \; \rho \frac{De}{Dt} + P(\text{ div } \mathbf{u}) - \frac{\partial Q}{\partial t} + \text{ div } \mathbf{q} \right\rangle_{L^2} \\
& + \langle \Lambda_6, \; P - F_7(\rho, T) \rangle_{L^2},
\end{aligned} \tag{88}$$

$$\begin{aligned}
J_{Aux_2} &= \left\langle \Lambda_7, m_D(t) - \int_\Omega \rho_D(x,t)\, dx \right\rangle_{L^2} \\
& + \left\langle \Lambda_8, m_T(t) - \int_\Omega \rho_T(x,t)\, dx \right\rangle_{L^2} \\
& \left\langle \Lambda_9, m_{H_e}(t) - \int_\Omega \rho_{H_e}(x,t)\, dx \right\rangle_{L^2} \\
& \left\langle \Lambda_{10}, m_N(t) - \int_\Omega \rho_N(x,t)\, dx \right\rangle_{L^2} \\
& \left\langle \Lambda_{11}, m_e(t) - \int_\Omega \rho_e(x,t)\, dx \right\rangle_{L^2} \\
& \int_0^{t_f} E_12(t)(\alpha_N m_{H_e})_T(t) - \alpha_{H_e}(m_N)_T(t))\, dt,
\end{aligned} \tag{89}$$

$$\begin{aligned}
J_{Aux_3} &= -\int_0^{t_f} \int_\Omega (E_N^D)_5(y,t) \left(\int_\Omega |\phi_N^D(x,y,t)|^2\, dx - m_N \right) dy\, dt \\
& - \int_0^{t_f} \int_\Omega (E_{N_1}^T)_6(y,t) \left(\int_\Omega |\phi_{N_1}^T(x,y,t)|^2\, dx - m_N \right) dy\, dt \\
& - \int_0^{t_f} \int_\Omega (E_{N_2}^T)_7(y,t) \left(\int_\Omega |\phi_{N_2}^T(x,y,t)|^2\, dx - m_N \right) dy\, dt \\
& - \int_0^{t_f} \int_\Omega (E_{N_1}^{H_e})_8(y,t) \left(\int_\Omega |\phi_{N_1}^{H_e}(x,y,t)|^2\, dx - m_N \right) dy\, dt \\
& - \int_0^{t_f} \int_\Omega (E_{N_2}^{H_e})_9(y,t) \left(\int_\Omega |\phi_{N_2}^{H_e}(x,y,t)|^2\, dx - m_N \right) dy\, dt,
\end{aligned} \tag{90}$$

Preprints (www.preprints.org) | NOT PEER-REVIEWED | Posted: 21 August 2023 doi:10.20944/preprints202302.0051.v29

$$\begin{aligned} J_{Aux_4} &= \langle \Lambda_{12}, \text{ curl } \mathbf{E}_{ind} \\ &+\frac{1}{c} \text{ curl } \left(\hat{K}_p |\phi_p^D|^2 \left(\mathbf{u} + \frac{\partial \mathbf{r}_D}{\partial t} \right) \right. \\ &+\hat{K}_p |\phi_p^T|^2 \left(\mathbf{u} + \frac{\partial \mathbf{r}_T}{\partial t} \right) \\ &+\hat{K}_p |\phi_{2p}^{H_e}|^2 \left(\mathbf{u} + \frac{\partial \mathbf{r}_{H_e}}{\partial t} \right) \\ &\left. + \hat{K}_e \int_\Omega |\phi_e(x,y,t)|^2 \left(\mathbf{u}(y,t) + \frac{\partial \mathbf{r}_e(x,y,t)}{\partial t} \, dx \right) \right) \\ &\times (\text{ curl } \mathbf{A} - \mathbf{B}_0) - \frac{1}{c} \frac{\partial}{\partial t} (\text{ curl } \mathbf{A} - \mathbf{B}_0) \Big\rangle_{L^2} \\ &+ \langle \Lambda_{13}, \text{ div } \mathbf{B} \rangle_{L^2} \\ &+ \left\langle \Lambda_{14}, \text{ div } \mathbf{E} - 4\pi \left(K_p(|\phi_p^D|^2 + |\phi_p^T|^2 + |\phi_{2p}^{H_e}|^2) + K_e \int_\Omega |\phi_e(x,y,t)|^2 \, dx \right) \right\rangle_{L^2}. \quad (91) \end{aligned}$$

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.

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

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,

$$\rho = \rho_D + \rho_T + \rho_{H_e} + \rho_N + \rho_e,$$

Preprints (www.preprints.org) | NOT PEER-REVIEWED | Posted: 21 August 2023 doi:10.20944/preprints202302.0051.v29

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

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.

Preprints (www.preprints.org) | NOT PEER-REVIEWED | Posted: 21 August 2023 doi:10.20944/preprints202302.0051.v29

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

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

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

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

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.
$$(m_T)(t) = (m_T)_0 - \int_0^t \int_{\partial\Omega_1 \cup \partial\Omega_2} (\rho_T(x,\tau))\mathbf{u} \cdot \mathbf{n} \, dS \, d\tau - \alpha_T (m_{H_e,N})_T(t),$$

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.
$$(m_e)_T(t) = m_e(t) + \int_0^t \int_{\partial\Omega_2} (\rho_e(x,\tau))\mathbf{u} \cdot \mathbf{n} \, dS \, d\tau,$$

Preprints (www.preprints.org) | NOT PEER-REVIEWED | Posted: 21 August 2023 doi:10.20944/preprints202302.0051.v29

11.
$$m_e(t) = \int_\Omega \rho_e(x,t)\,dx.$$

12.
$$\begin{aligned} m_e(t) &= \int_0^{N_D(t)} \int_\Omega |\phi_p^D(y,t,s)|^2\,dy\,ds\frac{m_e}{m_p} + \int_0^{N_T(t)} \int_\Omega |\phi_p^T(y,t,s)|^2\,dy\,ds\frac{m_e}{m_p} \\ &+ \int_0^{N_p(t)} \int_\Omega |\phi_{2p}^{H_e}(y,t,s)|^2\,dy\,ds\frac{m_e}{m_p}. \end{aligned} \tag{92}$$

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

$$J = G(\nabla u) + F(\phi) + E_c(\phi,\mathbf{r}) + F_1 + F_2 + F_3 + F_4,$$

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

$$\begin{aligned} G(\nabla\phi) &= \frac{\gamma_p^D}{2}\int_0^{t_f}\int_0^{N_D(t)}\int_\Omega (\nabla\phi_p^D)\cdot(\nabla\phi_p^D)\,dy\,ds\,dt \\ &+\frac{\gamma_N^D}{2}\int_0^{t_f}\int_0^{N_D(t)}\int_\Omega (\nabla\phi_N^D)\cdot(\nabla\phi_N^D)\,dx\,dy\,ds\,dt \\ &\frac{\gamma_p^T}{2}\int_0^{t_f}\int_0^{N_T(t)}\int_\Omega (\nabla\phi_p^T)\cdot(\nabla\phi_p^T)\,dy\,ds\,dt \\ &+\frac{\gamma_{N_1}^T}{2}\int_0^{t_f}\int_0^{N_T(t)}\int_\Omega (\nabla\phi_{N_1}^T)\cdot(\nabla\phi_{N_1}^T)\,dx\,dy\,ds\,dt \\ &+\frac{\gamma_{N_2}^T}{2}\int_0^{t_f}\int_0^{N_T(t)}\int_\Omega (\nabla\phi_{N_2}^T)\cdot(\nabla\phi_{N_2}^T)\,dx\,dy\,ds\,dt \\ &+\frac{\gamma_{2p}^{H_e}}{2}\int_0^{t_f}\int_0^{N_{H_e}(t)}\int_\Omega (\nabla\phi_{2p}^{H_e})\cdot(\nabla\phi_{2p}^{H_e})\,dy\,ds\,dt \\ &+\frac{\gamma_{N_1}^{H_e}}{2}\int_0^{t_f}\int_0^{N_{H_e}(t)}\int_\Omega (\nabla\phi_{N_1}^{H_e})\cdot(\nabla\phi_{N_1}^{H_e})\,dx\,dy\,ds\,dt \\ &+\frac{\gamma_{N_2}^{H_e}}{2}\int_0^{t_f}\int_0^{N_{H_e}(t)}\int_\Omega (\nabla\phi_{N_2}^{H_e})\cdot(\nabla\phi_{N_2}^{H_e})\,dx\,dy\,ds\,dt \\ &+\frac{\gamma_N}{2}\int_0^{t_f}\int_0^{N_N(t)}\int_\Omega (\nabla\phi_N)\cdot(\nabla\phi_N)\,dx\,ds\,dt \\ &+\frac{\gamma_e}{2}\int_0^{t_f}\int_0^{N_e(t)}\int_\Omega (\nabla\phi_e)\cdot(\nabla\phi_e)\,dx\,dy\,ds\,dt, \end{aligned} \tag{93}$$

and

Preprints (www.preprints.org) | NOT PEER-REVIEWED | Posted: 21 August 2023 doi:10.20944/preprints202302.0051.v29

$$F(\phi) =$$
$$\frac{\alpha_D}{2}\int_0^{t_f}\int_0^{N_D(t)}\int_0^{N_D(t)}\int_\Omega \frac{|\phi_D(x-\xi_1,y-\xi_2,t,s-s_1)|^2|\phi_D(\xi_1,\xi_2,t,s_1)|^2}{|(x,y)-(\xi_1,\xi_2)|}\,dx\,dy\,d\xi_1\,d\xi_2\,ds\,ds_1\,dt$$
$$+\frac{\alpha_T}{2}\int_0^{t_f}\int_0^{N_T(t)}\int_0^{N_T(t)}\int_\Omega \frac{|\phi_T(x-\xi_1,y-\xi_2,t,s-s_1)|^2|\phi_T(\xi_1,\xi_2,t,s_1)|^2}{|(x,y)-(\xi_1,\xi_2)|}\,dx\,dy\,d\xi_1\,d\xi_2\,ds\,ds_1\,dt$$
$$+\frac{\alpha_{DT}}{2}\int_0^{t_f}\int_0^{N_D(t)}\int_0^{N_T(t)}\int_\Omega \frac{|\phi_D(x-\xi_1,y-\xi_2,t,s-s_1)|^2|\phi_T(\xi_1,\xi_2,t,s_1)|^2}{|(x,y)-(\xi_1,\xi_2)|}\,dx\,dy\,d\xi_1\,d\xi_2\,dt$$
$$+\frac{\alpha_{H_e}}{2}\int_0^{t_f}\int_0^{N_{H_e}(t)}\int_0^{N_{H_e}(t)}\int_\Omega \frac{|\phi_{H_e}(x-\xi_1,y-\xi_2,t,s-s_1)|^2|\phi_{H_e}(\xi_1,\xi_2,t)|^2}{|(x,y)-(\xi_1,\xi_2,s_1)|}\,dx\,dy\,d\xi_1\,d\xi_2\,ds\,ds_1\,dt$$
$$+\frac{\alpha_N}{2}\int_0^{t_f}\int_0^{N_N(t)}\int_0^{N_N(t)}\int_\Omega \frac{|\phi_N(x-\xi,t,s-s_1)|^2|\phi_N(\xi,t,s_1)|^2}{|x-\xi|}\,dx\,d\xi\,ds\,ds_1\,dt$$
$$+\sum_{j=1}^{2}\frac{\alpha_{H_e\,N}}{2}\int_0^{t_f}\int_0^{N_{H_e}(t)}\int_0^{N_D(t)}\int_\Omega \frac{|\phi_{H_e}(x_1-\xi_1,y-\xi_2,t)|^2|\phi_N(\xi_j,t)|^2}{|(x,y)-(\xi_1,\xi_2)|}\,dx\,dy\,d\xi_1\,d\xi_2\,ds\,ds_1\,dt$$
$$+\frac{\alpha_{H_e,\,e}}{2}\int_0^{t_f}\int_0^{N_{H_e}(t)}\int_0^{N_e(t)}\int_\Omega \frac{|\phi_{H_e}(x-\xi_1,y-\xi_2,t,s-s_1)|^2|\phi_e(\xi_1,\xi_2,t,s_1)|^2}{|(x,y)-(\xi_1,\xi_2)|}\,dx\,dy\,d\xi_1\,d\xi_2\,ds\,ds_1\,dt$$
$$+\frac{\alpha_{e,e}}{2}\int_0^{t_f}\int_0^{N_e(t)}\int_0^{N_e(t)}\int_\Omega \frac{|\phi_e(x-\xi_1,y-\xi_2,t,s-s_1)|^2|\phi_e(\xi_1,\xi_2,t,s_1)|^2}{|(x,y)-(\xi_1,\xi_2)|}\,dx\,dy\,d\xi_1\,d\xi_2\,ds\,ds_1\,dt \quad (94)$$

and the internal kinetics energy is expressed by

$$\begin{aligned}E_c(\phi,\mathbf{r}) &= \frac{1}{2}\int_0^{t_f}\int_0^{N_D(t)}\int_\Omega |\phi_D|^2\,\frac{\partial \mathbf{r}_D}{\partial t}\cdot\frac{\partial \mathbf{r}_D}{\partial t}\,dx\,dy\,ds\,dt \\ &+\frac{1}{2}\int_0^{t_f}\int_0^{N_T(t)}\int_\Omega |\phi_T|^2\,\frac{\partial \mathbf{r}_T}{\partial t}\cdot\frac{\partial \mathbf{r}_T}{\partial t}\,dx\,dy\,ds\,dt \\ &+\frac{1}{2}\int_0^{t_f}\int_0^{N_{H_e}(t)}\int_\Omega |\phi_{H_e}|^2\,\frac{\partial \mathbf{r}_{H_e}}{\partial t}\cdot\frac{\partial \mathbf{r}_{H_e}}{\partial t}\,dx\,dy\,ds\,dt \\ &+\frac{1}{2}\int_0^{t_f}\int_0^{N_N(t)}\int_\Omega |\phi_N|^2\,\frac{\partial \mathbf{r}_N}{\partial t}\cdot\frac{\partial \mathbf{r}_N}{\partial t}\,dx\,dy\,ds\,dt \\ &+\frac{1}{2}\int_0^{t_f}\int_0^{N_e(t)}\int_\Omega |\phi_e|^2\,\frac{\partial \mathbf{r}_e}{\partial t}\cdot\frac{\partial \mathbf{r}_e}{\partial t}\,dx\,dy\,ds\,dt, \end{aligned} \quad (95)$$

Moreover,

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

$$\begin{aligned}F_2 &= \int_0^{t_f}\int_0^{N_D(t)}\int_\Omega \mathbf{E}_{ind}\cdot K_p|\phi_p^D|^2\left(\mathbf{u}+\frac{\partial \mathbf{r}_D}{\partial t}\right)\,dx\,dy\,ds\,dt \\ &+\int_0^{t_f}\int_0^{N_T(t)}\int_\Omega \mathbf{E}_{ind}\cdot K_p|\phi_p^T|^2\left(\mathbf{u}+\frac{\partial \mathbf{r}_T}{\partial t}\right)\,dx\,dy\,ds\,dt \\ &+\int_0^{t_f}\int_0^{N_{H_e}(t)}\int_\Omega \mathbf{E}_{ind}\cdot K_p|\phi_{2p}^{H_e}|^2\left(\mathbf{u}+\frac{\partial \mathbf{r}_{H_e}}{\partial t}\right)\,dx\,dy\,ds\,dt \\ &+\int_0^{t_f}\int_0^{N_e(t)}\int_\Omega \mathbf{E}_{ind}\cdot K_e|\phi_e|^2\left(\mathbf{u}+\frac{\partial \mathbf{r}_e}{\partial t}\right)\,dx\,dy\,ds\,dt, \end{aligned} \quad (96)$$

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

Preprints (www.preprints.org) | NOT PEER-REVIEWED | Posted: 21 August 2023 doi:10.20944/preprints202302.0051.v29

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,

$$\begin{aligned} F_3 &= \frac{C_D}{2}\int_0^{t_f}\int_0^{N_D(t)}\int_\Omega \nabla_{(x,y)}\mathbf{r}_D\cdot\nabla_{(x,y)}\mathbf{r}_D\;dx\,dy\,ds\,dt \\ &+\frac{C_T}{2}\int_0^{t_f}\int_0^{N_T(t)}\int_\Omega \nabla_{(x,y)}\mathbf{r}_T\cdot\nabla_{(x,y)}\mathbf{r}_T\;dx\,dy\,ds\,dt \\ &+\frac{C_{H_e}}{2}\int_0^{t_f}\int_0^{N_{H_e}(t)}\int_\Omega \nabla_{(x,y)}\mathbf{r}_{H_e}\cdot\nabla_{(x,y)}\mathbf{r}_{H_e}\;dx\,dy\,ds\,dt \\ &+\frac{C_N}{2}\int_0^{t_f}\int_0^{N_N(t)}\int_\Omega \nabla_{(x,y)}\mathbf{r}_N\cdot\nabla_{(x,y)}\mathbf{r}_N\;dx\,dy\,ds\,dt \\ &\frac{C_e}{2}\int_0^{t_f}\int_0^{N_e(t)}\int_\Omega \nabla_{(x,y)}\mathbf{r}_e\cdot\nabla_{(x,y)}\mathbf{r}_e\;dx\,dy\,ds\,dt, \end{aligned} \tag{97}$$

for appropriate real positive constants $C_D\ C_T,\ C_{H_e},\ C_N,\ C_e$.

Finally,

$$\begin{aligned} F_4 &= \frac{\varepsilon_D}{2}\int_0^{t_f}\left(\frac{\partial N_D(t)}{\partial t}\right)^2 dt+\frac{\varepsilon_T}{2}\int_0^{t_f}\left(\frac{\partial N_D(t)}{\partial t}\right)^2 dt \\ &+\frac{\varepsilon_N}{2}\int_0^{t_f}\left(\frac{\partial N_N(t)}{\partial t}\right)^2 dt+\frac{\varepsilon_{H_e}}{2}\int_0^{t_f}\left(\frac{\partial N_{H_e}(t)}{\partial t}\right)^2 dt \\ &+\frac{\varepsilon_e}{2}\int_0^{t_f}\left(\frac{\partial N_e(t)}{\partial t}\right)^2 dt, \end{aligned} \tag{98}$$

where $\varepsilon_D,\ \varepsilon_T,\ \varepsilon_N,\ \varepsilon_{H_e},\ \varepsilon_e$ 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,

$$\tau_{ij}=\mu\left(\frac{\partial u_i}{\partial x_j}+\frac{\partial u_j}{\partial x_i}-\frac{2}{3}\delta_{ij}\sum_{k=1}^3\frac{\partial u_k}{\partial x_k}\right),$$

$\forall i,j\in\{1,2,3\}$,

$$\mathbf{F}_E=\{(F_E)_k\}=$$
$$\left(K_p\left(\int_0^{N_D(t)}|\phi_p^D|^2\,ds+\int_0^{N_T(t)}|\phi_p^T|^2\,ds+\int_0^{N_{H_e}(t)}|\phi_{2p}^{H_e}|^2\,ds\right)+K_e\int_0^{N_e(t)}|\phi_e|^2\,ds\right)\mathbf{E},$$

Preprints (www.preprints.org) | NOT PEER-REVIEWED | Posted: 21 August 2023 doi:10.20944/preprints202302.0051.v29

and

$$\begin{aligned}
\mathbf{F}_M &= \{(F_M)_k\} \\
&= \left(K_p \left(\int_0^{N_D(t)} |\phi_p^D|^2 \left(\mathbf{u} + \frac{\partial \mathbf{r}_D}{\partial t} \right) ds \right.\right. \\
&\quad \int_0^{N_T(t)} |\phi_p^T|^2 \left(\mathbf{u} + \frac{\partial \mathbf{r}_T}{\partial t} \right) ds \\
&\quad \left. + \int_0^{N_{H_e}(t)} |\phi_{2p}^{H_e}|^2 \left(\mathbf{u} + \frac{\partial \mathbf{r}_{H_e}}{\partial t} \right) ds \right) \\
&\quad \left. + K_e \int_0^{N_e(t)} |\phi_e|^2 \left(\mathbf{u} + \frac{\partial \mathbf{r}_e}{\partial t} \right) ds \right) \times \mathbf{B}. \qquad (99)
\end{aligned}$$

2. Mass conservation equation:

$$\frac{\partial \rho}{\partial t} + \text{div } (\rho \mathbf{u}) = 0.$$

3. Energy equation

$$\rho \frac{De}{Dt} + P(\text{ div } \mathbf{u}) = \frac{\partial Q}{\partial t} - \text{ div } \mathbf{q},$$

where we assume the Fourier law

$$\mathbf{q} = -K \nabla T,$$

where $T = T(x,t)$ is the scalar field of temperature.

Also,

$$\begin{aligned}
e &= \frac{\rho}{2} \mathbf{u} \cdot \mathbf{u} + \frac{\rho_D}{2} \frac{\partial \mathbf{r}_D}{\partial t} \cdot \frac{\partial \mathbf{r}_D}{\partial t} \\
&\quad + \frac{\rho_T}{2} \frac{\partial \mathbf{r}_T}{\partial t} \cdot \frac{\partial \mathbf{r}_T}{\partial t} \\
&\quad + \frac{\rho_{H_e}}{2} \frac{\partial \mathbf{r}_{H_e}}{\partial t} \cdot \frac{\partial \mathbf{r}_{H_e}}{\partial t} \\
&\quad + \frac{\rho_N}{2} \frac{\partial \mathbf{r}_N}{\partial t} \cdot \frac{\partial \mathbf{r}_N}{\partial t} \\
&\quad + \frac{\rho_e}{2} \frac{\partial \mathbf{r}_e}{\partial t} \cdot \frac{\partial \mathbf{r}_e}{\partial t} \qquad (100)
\end{aligned}$$

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)

$$m_T(t) = \int_\Omega \rho_T(x,t)\, dx,$$

 doi:10.20944/preprints202302.0051.v29

(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)
$$(m_{H_e})_T(t) = \int_\Omega \rho_{H_e}(x,t)\, dx + \int_0^t \int_{\partial\Omega_2} \rho_{H_e}(x,\tau)\mathbf{u}\cdot\mathbf{n}\, d\Gamma d\tau,$$
(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)
$$\begin{aligned} m_e(t) &= \int_0^{N_D(t)} \int_\Omega |\phi_p^D(y,t,s)|^2\, dy\, dy\, ds\frac{m_e}{m_p} + \int_0^{N_T(t)} \int_\Omega |\phi_p^T(y,t,s)|^2\, dy\, ds\frac{m_e}{m_p} \\ &+ \int_0^{N_p(t)} \int_\Omega |\phi_{2p}^{H_e}(y,t,s)|^2\, dy\, ds\frac{m_e}{m_p}. \end{aligned} \tag{101}$$

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)
$$\int_\Omega |\phi_{N_2}^T(x,y,t,s)|^2\, dx = m_N,$$

 doi:10.20944/preprints202302.0051.v29

(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

$$\begin{aligned}
&\text{curl } \mathbf{E}_{ind} + \frac{1}{c}\text{ curl }\left(\hat{K}_p \int_0^{N_D(t)} |\phi_p^D|^2 \left(\mathbf{u} + \frac{\partial \mathbf{r}_D}{\partial t}\right)\,ds\right.\\
&+\hat{K}_p \int_0^{N_T(t)} |\phi_p^T|^2 \left(\mathbf{u} + \frac{\partial \mathbf{r}_T}{\partial t}\right)\,ds\\
&+\hat{K}_p \int_0^{N_{H_e}(t)} |\phi_{2p}^{H_e}|^2 \left(\mathbf{u} + \frac{\partial \mathbf{r}_{H_e}}{\partial t}\right)\,ds\\
&\left.+\,\hat{K}_e \int_0^{N_e(t)} \int_\Omega |\phi_e(x,y,t,s)|^2 \left(\mathbf{u}(y,t) + \frac{\partial \mathbf{r}_e(x,y,t)}{\partial t}\,dx\right)\,ds\right)\\
&\times(\text{ curl } \mathbf{A} - \mathbf{B}_0) - \frac{1}{c}\frac{\partial}{\partial t}(\text{ curl } \mathbf{A} - \mathbf{B}_0) = \mathbf{0},
\end{aligned} \tag{102}$$

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:

$$\begin{aligned}
\text{div } \mathbf{E} \;=\; & 4\pi\left(K_p\left(\int_0^{N_D(t)} |\phi_p^D|^2\,ds + \int_0^{N_T(t)} |\phi_p^T|^2\,ds + \int_0^{N_{H_e}(t)} |\phi_{2p}^{H_e}|^2\,ds\right)\right.\\
&\left.+K_e \int_0^{N_e(t)} \int_\Omega |\phi_e(x,y,t,s)|^2\,dx\,ds\right),
\end{aligned} \tag{103}$$

Preprints (www.preprints.org) | NOT PEER-REVIEWED | Posted: 21 August 2023 doi:10.20944/preprints202302.0051.v29

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

$$\begin{aligned} & J_3 = J_3(\phi, \mathbf{u}, \mathbf{r}, P, \mathbf{A}, \mathbf{B}, \mathbf{E}, \Lambda, E, \{N_D, N_T, N_{H_e}, N_N, N_e\}) \\ = \; & G(\nabla\phi) + F(\phi) + E_c(\phi, \mathbf{r}) + F_1 + F_2 + F_3 + F_4 \\ & + \left\langle \Lambda_k, \rho \left(\frac{\partial u_k}{\partial t} + u_j \frac{\partial u_k}{\partial x_j} \right) - \rho f_k + \frac{\partial P}{\partial x_k} - \tau_{kj,j} - (F_E)_k - (F_M)_k \right\rangle_{L^2} \\ & + \left\langle \Lambda_4, \frac{\partial \rho}{\partial t} + \text{ div } (\rho \mathbf{u}) \right\rangle_{L^2} + J_{Aux_1} + J_{Aux_2} + J_{Aux_3} + J_{Aux_4} + J_{Aux_5}, \end{aligned} \tag{104}$$

where,

$$\begin{aligned} J_{Aux_1} &= \left\langle \Lambda_5, \rho \frac{De}{Dt} + P(\text{ div } \mathbf{u}) - \frac{\partial Q}{\partial t} + \text{ div } \mathbf{q} \right\rangle_{L^2} \\ & + \langle \Lambda_6, P - F_7(\rho, T) \rangle_{L^2}, \end{aligned} \tag{105}$$

$$\begin{aligned} J_{Aux_2} &= \left\langle \Lambda_7, m_D(t) - \int_\Omega \rho_D(x,t)\, dx \right\rangle_{L^2} \\ & + \left\langle \Lambda_8, m_T(t) - \int_\Omega \rho_T(x,t)\, dx \right\rangle_{L^2} \\ & \left\langle \Lambda_9, m_{H_e}(t) - \int_\Omega \rho_{H_e}(x,t)\, dx \right\rangle_{L^2} \\ & \left\langle \Lambda_{10}, m_N(t) - \int_\Omega \rho_N(x,t)\, dx \right\rangle_{L^2} \\ & \left\langle \Lambda_{11}, m_e(t) - \int_\Omega \rho_e(x,t)\, dx \right\rangle_{L^2} \\ & \int_0^{t_f} E_{12}(t)(\alpha_N m_{H_e})_T(t) - \alpha_{H_e}(m_N)_T(t))\, dt, \end{aligned} \tag{106}$$

Preprints (www.preprints.org) | NOT PEER-REVIEWED | Posted: 21 August 2023 doi:10.20944/preprints202302.0051.v29

$$
\begin{aligned}
J_{Aux_3} &= -\int_0^{t_f}\int_\Omega (E_N^D)_5(y,t,s)\left(\int_\Omega |\phi_N^D(x,y,t,s)|^2\,dx - m_N\right)\,dy\,dt \\
&\quad -\int_0^{t_f}\int_\Omega (E_{N_1}^T)_6(y,t,s)\left(\int_\Omega |\phi_{N_1}^T(x,y,t,s)|^2\,dx - m_N\right)\,dy\,dt \\
&\quad -\int_0^{t_f}\int_\Omega (E_{N_2}^T)_7(y,t,s)\left(\int_\Omega |\phi_{N_2}^T(x,y,t,s)|^2\,dx - m_N\right)\,dy\,dt \\
&\quad -\int_0^{t_f}\int_\Omega (E_{N_1}^{H_e})_8(y,t,s)\left(\int_\Omega |\phi_{N_1}^{H_e}(x,y,t,s)|^2\,dx - m_N\right)\,dy\,dt \\
&\quad -\int_0^{t_f}\int_\Omega (E_{N_2}^{H_e})_9(y,t,s)\left(\int_\Omega |\phi_{N_2}^{H_e}(x,y,t,s)|^2\,dx - m_N\right)\,dy\,dt, \\
&\quad -\int_0^{t_f}\int_\Omega (E_p^D)(t,s)\left(\int_\Omega |\phi_p^D(y,t,s)|^2\,dy - m_p\right)\,ds\,dt, \\
&\quad -\int_0^{t_f}\int_\Omega (E_p^T)(t,s)\left(\int_\Omega |\phi_p^T(y,t,s)|^2\,dy - m_p\right)\,ds\,dt, \\
&\quad -\int_0^{t_f}\int_\Omega (E_{2p}^{H_e})(t,s)\left(\int_\Omega |\phi_{2p}^{H_e}(y,t,s)|^2\,dy - 2m_p\right)\,ds\,dt, \qquad (107)
\end{aligned}
$$

$$
\begin{aligned}
J_{Aux_4} &= \langle \Lambda_{12},\ \text{curl}\ \mathbf{E}_{ind} \\
&\quad +\frac{1}{c}\,\text{curl}\left(\hat{K}_p\int_0^{N_D(t)} |\phi_p^D|^2\left(\mathbf{u}+\frac{\partial \mathbf{r}_D}{\partial t}\right)\,ds\right. \\
&\quad +\hat{K}_p\int_0^{N_T(t)} |\phi_p^T|^2\left(\mathbf{u}+\frac{\partial \mathbf{r}_T}{\partial t}\right)\,ds \\
&\quad +\hat{K}_p\int_0^{N_{H_e}(t)} |\phi_{2p}^{H_e}|^2\left(\mathbf{u}+\frac{\partial \mathbf{r}_{H_e}}{\partial t}\right)\,ds \\
&\quad \left.+\,\hat{K}_e\int_0^{N_e(t)}\int_\Omega |\phi_e(x,y,t,s)|^2\left(\mathbf{u}(y,t)+\frac{\partial \mathbf{r}_e(x,y,t,s)}{\partial t}\,dx\right)\,ds\right) \\
&\quad \times(\,\text{curl}\ \mathbf{A}-\mathbf{B}_0) - \frac{1}{c}\frac{\partial}{\partial t}(\,\text{curl}\ \mathbf{A}-\mathbf{B}_0)\Big\rangle_{L^2} \\
&\quad +\langle \Lambda_{13},\ \text{div}\ \mathbf{B}\rangle_{L^2} \\
&\quad +\Big\langle \Lambda_{14},\ \text{div}\ \mathbf{E} - 4\pi\left(K_p\left(\int_0^{N_D(t)} |\phi_p^D|^2\,ds + \int_0^{N_T(t)} |\phi_p^T|^2\,ds + \int_0^{N_{H_e}(t)} |\phi_{2p}^{H_e}|^2\,ds\right)\right. \\
&\quad \left.\left.+K_e\int_\Omega |\phi_e|^2\,dx\,ds\right)\right\rangle_{L^2}. \qquad (108)
\end{aligned}
$$

$$
\begin{aligned}
J_{Aux_5} &= \langle \Lambda_{15},\ m_D(t) - (m_p\ N_D(t) + m_N\ N_D(t))\rangle_{L^2} \\
&\quad +\langle \Lambda_{16},\ m_T(t) - (m_p\ N_T(t) + m_N\ N_T(t))\rangle_{L^2} \\
&\quad +\langle \Lambda_{17},\ m_{H_e}(t) - (2m_p\ N_{H_e}(t) + 2m_N\ N_{H_e}(t))\rangle_{L^2} \\
&\quad +\langle \Lambda_{18},\ m_e(t) - (m_e\ N_D(t) + m_e\ N_T(t) + 2\ m_e\ N_{H_e}(t))\rangle_{L^2}. \qquad (109)
\end{aligned}
$$

Here we recall the following definitions and relations:

1. For the Deuterium field

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

Preprints (www.preprints.org) | NOT PEER-REVIEWED | Posted: 21 August 2023 doi:10.20944/preprints202302.0051.v29

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.
$$\rho_T(y,t) = \int_0^{N_T(t)} \int_\Omega |\phi_T(x,y,t,s)|^2 \, dx \, ds,$$
$$\rho_{H_e}(y,t) = \int_0^{N_{H_e}(t)} \int_\Omega |\phi_{H_e}(x,y,t,s)|^2 \, dx \, ds,$$
$$\rho_N(x,t) = \int_0^{N_N(t)} |\phi_N(x,t,s)|^2 \, ds,$$
$$\rho_e(y,t) = \int_0^{N_e(t)} \int_\Omega |\phi_e(x,y,t,s)|^2 \, dx \, ds.$$

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.
$$(m_{H_e})_T(t) = \int_\Omega \rho_{H_e}(x,t) \, dx + \int_0^t \int_{\partial\Omega_2} \rho_{H_e}(x,\tau)\mathbf{u}\cdot\mathbf{n} \, d\Gamma d\tau,$$

Preprints (www.preprints.org) | NOT PEER-REVIEWED | Posted: 21 August 2023 doi:10.20944/preprints202302.0051.v29

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.
$$\begin{aligned} m_e(t) &= \int_0^{N_D(t)} \int_\Omega |\phi_p^D(y,t,s)|^2\,dy\,dy\,ds\frac{m_e}{m_p} + \int_0^{N_T(t)} \int_\Omega |\phi_p^T(y,t,s)|^2\,dy\,ds\frac{m_e}{m_p} \\ &+ \int_0^{N_p(t)} \int_\Omega |\phi_{2p}^{H_e}(y,t,s)|^2\,dy\,ds\frac{m_e}{m_p}. \end{aligned} \tag{110}$$

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

$$\begin{aligned} J(u,v) &= \frac{\gamma_1}{2}\int_\Omega \nabla u\cdot\nabla u\,dx + \frac{\alpha_1}{2}\int_\Omega u^4\,dx \\ &\frac{\gamma_2}{2}\int_\Omega \nabla v\cdot\nabla v\,dx + \frac{\alpha_2}{2}\int_\Omega v^4\,dx \\ &-\frac{1}{2}\int_\Omega \omega^2(u^2+v^2)\,dx - \frac{E}{2}\left(\int_\Omega (u^2+v^2)\,dx - m_T\right). \end{aligned} \tag{111}$$

Here $\gamma_1 > 0,\ \gamma_2 > 0,\ \alpha_1 > 0,\ \alpha_2 > 0$ and $V = W^{1,2}(\Omega)$.

Preprints (www.preprints.org) | NOT PEER-REVIEWED | Posted: 21 August 2023 doi:10.20944/preprints202302.0051.v29

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 $v \approx 1$.

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.

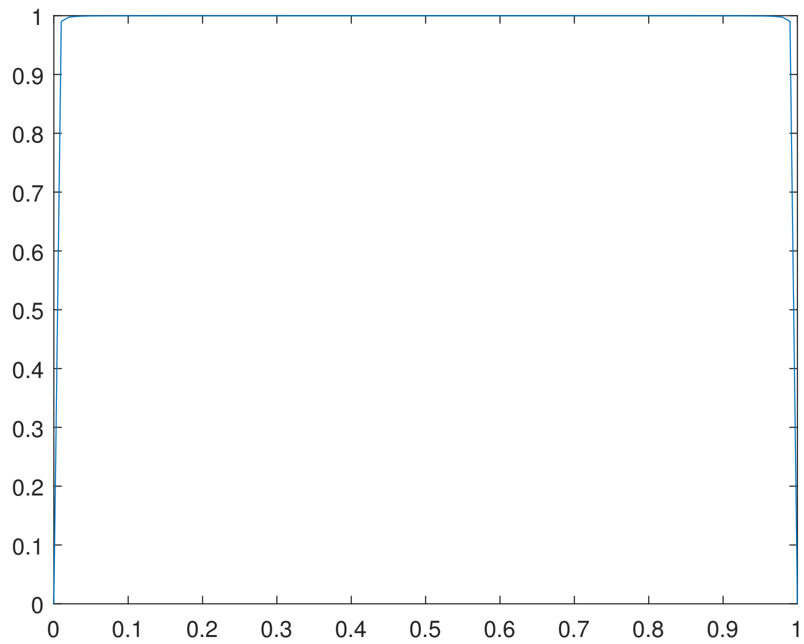

Figure 15. Solution $\phi_u(x)$ for $\omega = 1$.

Preprints (www.preprints.org) | NOT PEER-REVIEWED | Posted: 21 August 2023 doi:10.20944/preprints202302.0051.v29

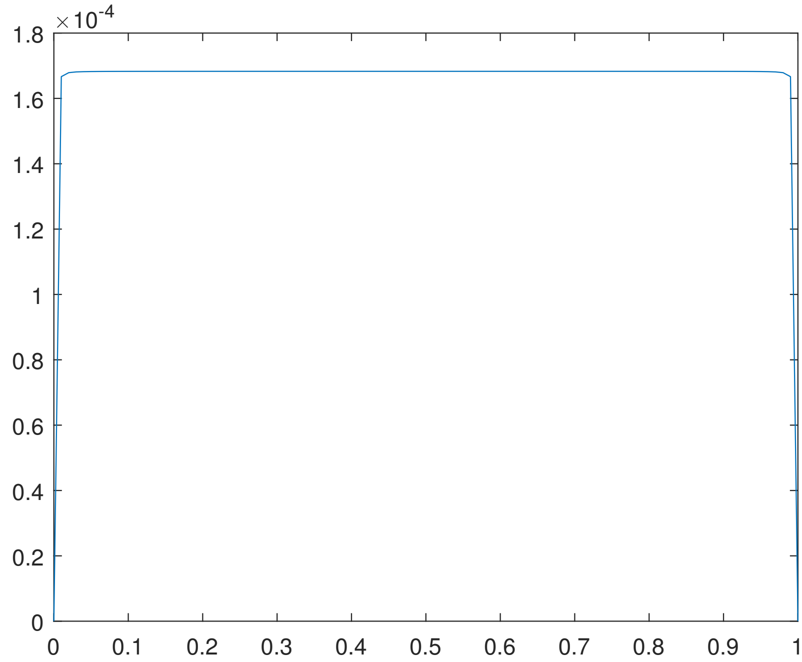

Figure 16. Solution $\phi_v(x)$ for $\omega = 1$.

For the corresponding solutions ϕ_u and ϕ_v, please see Figures 17 and 18, respectively.

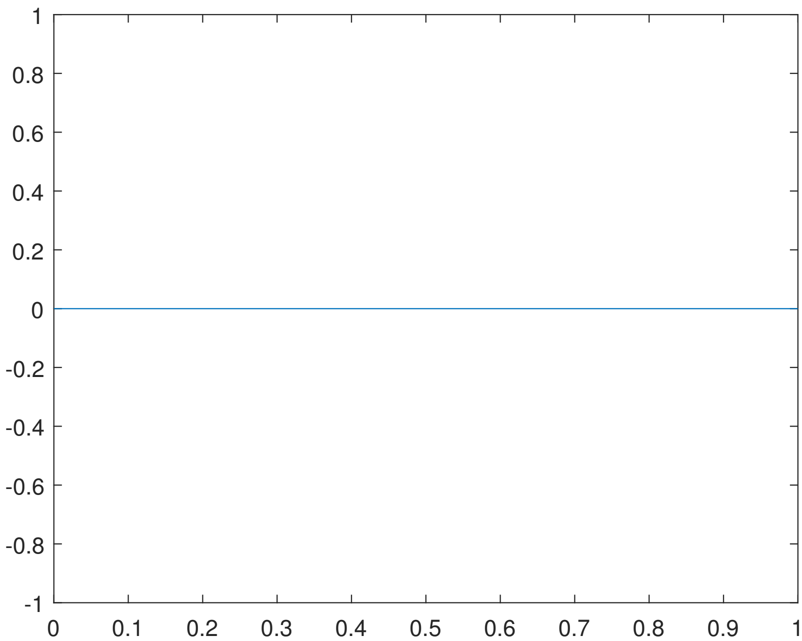

Figure 17. Solution $\phi_u(x)$ for $\omega = 15$.

Preprints (www.preprints.org) | NOT PEER-REVIEWED | Posted: 21 August 2023 doi:10.20944/preprints202302.0051.v29

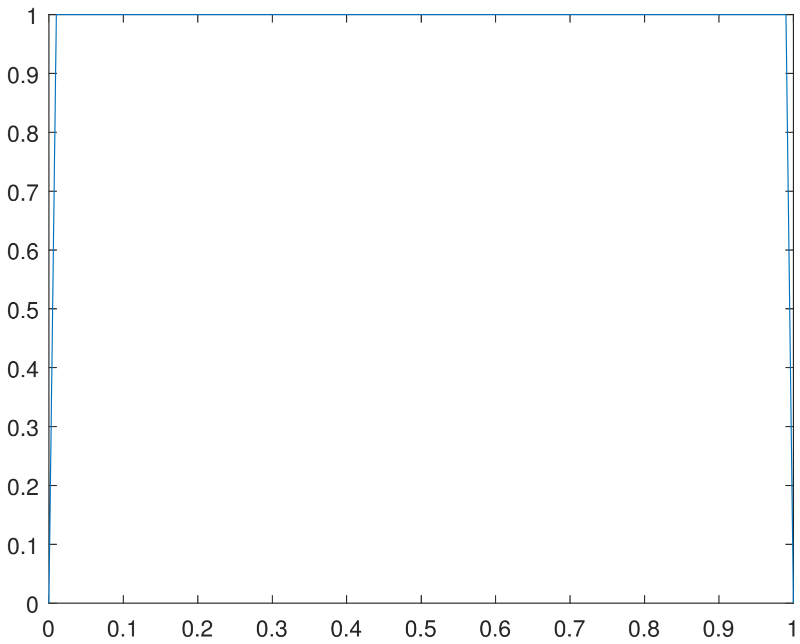

Figure 18. Solution $\phi_v(x)$ for $\omega = 15$.

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:

$$|\phi_{(p_{jkl})_T}(x, y, z, t)|^2 = \frac{|\phi_{p_{jkl}}(x, y, z, t)|^2 |\phi_{A_{kl}}(y, z, t)|^2 |\phi_{M_l}(z, t)|^2}{m_{A_{jk}} m_{M_l}}.$$

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:

 doi:10.20944/preprints202302.0051.v29

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

$$\begin{aligned} |\phi_{H_2}(x,y,z,t)|^2 &= \frac{|\phi_{p_1}(x,y,z,t)|^2|\phi_{A_1}(y,z,t)|^2|\phi_M(z,t)|^2}{m_{A_1}m_M} \\ &+ \frac{|\phi_{e_1}(x,y,z,t)|^2|\phi_{A_1}(y,z,t)|^2|\phi_M(z,t)|^2}{m_{A_1}m_M} \\ &+ \frac{|\phi_{p_2}(x,y,z,t)|^2|\phi_{A_2}(y,z,t)|^2|\phi_M(z,t)|^2}{m_{A_2}m_M} \\ &+ \frac{|\phi_{e_2}(x,y,z,t)|^2|\phi_{A_2}(y,z,t)|^2|\phi_M(z,t)|^2}{m_{A_2}m_M}. \end{aligned} \tag{112}$$

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:
$$\int_\Omega |\phi_{e_1}(x,y,z,t)|^2\,dx + \int_\Omega |\phi_{e_2}(x,y,z,t)|^2\,dx = 2m_e.$$
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

$$|(\phi_{p_j})_T|^2 = \frac{|\phi_{p_j}(x,y,z,t)|^2|\phi_{A_j}(y,z,t)|^2|\phi_M(z,t)|^2}{m_{A_j}m_M},$$

$$|(\phi_{e_j})_T|^2 = \frac{|\phi_{e_j}(x,y,z,t)|^2|\phi_{A_j}(y,z,t)|^2|\phi_M(z,t)|^2}{m_{A_j}m_M},\ \forall j \in \{1,2\}$$

Preprints (www.preprints.org) | NOT PEER-REVIEWED | Posted: 21 August 2023 doi:10.20944/preprints202302.0051.v29

we assume $\gamma_{(p_j)} > 0,\ \gamma_{e_j} > 0,\ \gamma_{A_j} > 0,\ \gamma_M > 0,\ \alpha_{(p_j)_T} > 0,\ \alpha_{(e_j)_T} > 0\ \alpha_{(p_j\, e_k)_T} < 0,\ \forall j,k \in \{1,2\},$

$$\begin{aligned} G(\nabla\phi) &= \frac{\gamma_{p_j}}{2}\int_0^{t_f}\int_\Omega (\nabla\phi_{p_j})\cdot(\nabla\phi_{p_j})\,dx\,dy\,dz\,dt \\ &+\frac{\gamma_{e_j}}{2}\int_0^{t_f}\int_\Omega (\nabla\phi_{e_j})\cdot(\nabla\phi_{e_j})\,dx\,dy\,dz\,dt \\ &\frac{\gamma_{A_j}}{2}\int_\Omega (\nabla\phi_{A_j})\cdot(\nabla\phi_{A_j})\,dy\,dz\,dt \\ &+\frac{\gamma_M}{2}\int_0^{t_f}\int_\Omega (\nabla\phi_M)\cdot(\nabla\phi_M)\,dz\,dt \end{aligned} \tag{113}$$

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,

$$\begin{aligned} J_{Aux}(\phi,E) &= \int_0^{t_f}\int_\Omega (E_p)_j(y,z,t)\left(\int_\Omega |\phi_{p_j}(x,y,z,t)|^2\,dx - m_p\right)dy\,dz\,dt \\ &\int_0^{t_f}\int_\Omega (E_e)(y,z,t)\left(\int_\Omega (|\phi_{e_1}(x,y,z,t)|^2+|\phi_{e_2}(x,y,z,t)|^2)\,dx - 2m_e\right)dy\,dz\,dt \\ &\int_0^{t_f}\int_\Omega (E_A)_j(z,t)\left(\int_\Omega |\phi_{A_j}(y,z,t)|^2\,dy - m_{A_j}\right)dz\,dt \\ &\int_0^{t_f}(E_M)(t)\left(\int_\Omega |\phi_M(z,t)|^2\,dz - m_M\right)dt. \end{aligned} \tag{114}$$

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.

Preprints (www.preprints.org) | NOT PEER-REVIEWED | Posted: 21 August 2023 doi:10.20944/preprints202302.0051.v29

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

$$\begin{aligned} |\phi_1(x,y,z,t)|^2 &= K_p \sum_{j=1}^{2} |(\phi_1^H)_{p_j}(x,y,z,t)|^2 \frac{|(\phi_1^H)_{A_j}(y,z,t)|^2 |(\phi_1)_M(z,t)|^2}{(m)_{A_j}^H \, (m_1)_M} \\ &+ K_e \sum_{j=1}^{2} |(\phi_1^H)_{e_j}(x,y,z,t)|^2 \frac{|(\phi_1^H)_{A_j}(y,z,t)|^2 |(\phi_1)_M(z,t)|^2}{(m_1)_{A_j}^H \, (m_1)_M} \\ &+ K_p \sum_{j=1}^{8} |(\phi_1^O)_{p_j}(x,y,z,t)|^2 \frac{|(\phi_1^O)_{A}(y,z,t)|^2 |(\phi_1)_M(z,t)|^2}{(m)_{A}^O \, (m_1)_M} \\ &+ K_e \sum_{j=1}^{8} |(\phi_1^O)_{e_j}(x,y,z,t)|^2 \frac{|(\phi_1^O)_{A}(y,z,t)|^2 |(\phi_1)_M(z,t)|^2}{(m)_{A}^O \, (m_1)_M} \end{aligned} \quad (115)$$

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.

2. For the OH^- density, denoted by $|\phi_2|^2$, we have

$$\begin{aligned} |\phi_2(x,y,z,t)|^2 &= K_p |(\phi_2^H)_p(x,y,z,t)|^2 \frac{|(\phi_2^H)_A(y,z,t)|^2 |(\phi_2)_M(z,t)|^2}{(m)_A^H \, (m_2)_M} \\ &+ K_e |(\phi_2^H)_{e_1}(x,y,z,t)|^2 \frac{|(\phi_2^H)_A(y,z,t)|^2 |(\phi_2)_M(z,t)|^2}{(m)_A^H \, (m_2)_M} \\ &+ K_e |(\phi_2^{OH^-})_{e_2}(x,z,t)|^2 \frac{|(\phi_2)_M(z,t)|^2}{(m_2)_M} \\ &+ K_p \sum_{j=1}^{8} |(\phi_2^O)_{p_j}(x,y,z,t)|^2 \frac{|(\phi_2^O)_A(y,z,t)|^2 |(\phi_2)_M(z,t)|^2}{(m)_A^O \, (m_2)_M} \\ &+ K_e \sum_{j=1}^{8} |(\phi_2^O)_{e_j}(x,y,z,t)|^2 \frac{|(\phi_2^O)_A(y,z,t)|^2 |(\phi_2)_M(z,t)|^2}{(m)_A^O \, (m_2)_M}, \end{aligned} \quad (116)$$

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:

Preprints (www.preprints.org) | NOT PEER-REVIEWED | Posted: 21 August 2023 doi:10.20944/preprints202302.0051.v29

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.
$$\int_\Omega |(\phi_3^H)_p(x,z,t)|^2\,dx = m_p,$$
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

$$J(\phi, E) = G(\nabla\phi) + F(\phi) + F_1(\phi) - J_{Aux}(\phi, E),$$

where

Preprints (www.preprints.org) | NOT PEER-REVIEWED | Posted: 21 August 2023 doi:10.20944/preprints202302.0051.v29

$$
\begin{aligned}
G(\nabla\phi) &= \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 $\gamma_p > 0$, $\gamma_e > 0$, $\gamma_A^H > 0$,, $\gamma_A^O > 0$, $\gamma_{M_1} > 0$, $\gamma_{M_2} > 0$, $\gamma_{A_3} > 0$.
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,

$$F_1(\phi) = \int_0^{t_f} \int_\Omega V(x,y,z,t)(|\phi_1|^2 + |\phi_2|^2 + |\phi_3|^2)\, dx\, dy\, dz\, dt, \quad (117)$$

where $V = V(x,y,z,t)$ is an electric potential originated from an external electric field $\mathbf{E}$ applied on Ω.

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. \quad (118)
\end{aligned}$$

References

1. R.A. Adams and J.F. Fournier, Sobolev Spaces, 2nd edn. (Elsevier, New York, 2003).
2. W.R. Bielski, A. Galka, J.J. Telega, The Complementary Energy Principle and Duality for Geometrically Nonlinear Elastic Shells. I. Simple case of moderate rotations around a tangent to the middle surface. Bulletin of the Polish Academy of Sciences, Technical Sciences, Vol. 38, No. 7-9, 1988.

3. W.R. Bielski and J.J. Telega, A Contribution to Contact Problems for a Class of Solids and Structures, Arch. Mech., 37, 4-5, pp. 303-320, Warszawa 1985.
4. J.F. Annet, Superconductivity, Superfluids and Condensates, 2nd edn. (Oxford Master Series in Condensed Matter Physics, Oxford University Press, Reprint, 2010)
5. F.S. Botelho, Functional Analysis, Calculus of Variations and Numerical Methods in Physics and Engineering, CRC Taylor and Francis, Florida, 2020.
6. F.S. Botelho, Advanced Calculus and its Applications in Variational Quantum Mechanics and Relativity Theory, CRC Taylor and Francis, Florida, 2021.
7. F.S. Botelho, *Variational Convex Analysis*, Ph.D. thesis, Virginia Tech, Blacksburg, VA -USA, (2009).
8. F. Botelho, *Topics on Functional Analysis, Calculus of Variations and Duality*, Academic Publications, Sofia, (2011).
9. F. Botelho, *Existence of solution for the Ginzburg-Landau system, a related optimal control problem and its computation by the generalized method of lines*, Applied Mathematics and Computation, 218, 11976-11989, (2012).
10. F. Botelho, Functional Analysis and Applied Optimization in Banach Spaces, Springer Switzerland, 2014.
11. P.Ciarlet, *Mathematical Elasticity*, Vol. II – Theory of Plates, North Holland Elsevier (1997).
12. J.C. Strikwerda, *Finite Difference Schemes and Partial Differential Equations*, SIAM, second edition (Philadelphia, 2004).
13. L.D. Landau and E.M. Lifschits, Course of Theoretical Physics, Vol. 5- Statistical Physics, part 1. (Butterworth-Heinemann, Elsevier, reprint 2008).
14. R.T. Rockafellar, Convex Analysis, Princeton Univ. Press, (1970).
15. J.J. Telega, *On the complementary energy principle in non-linear elasticity. Part I: Von Karman plates and three dimensional solids*, C.R. Acad. Sci. Paris, Serie II, 308, 1193-1198; Part II: Linear elastic solid and non-convex boundary condition. Minimax approach, ibid, pp. 1313-1317 (1989)
16. A.Galka and J.J.Telega *Duality and the complementary energy principle for a class of geometrically non-linear structures. Part I. Five parameter shell model; Part II. Anomalous dual variational priciples for compressed elastic beams*, Arch. Mech. 47 (1995) 677-698, 699-724.
17. J.F. Toland, A duality principle for non-convex optimisation and the calculus of variations, Arch. Rat. Mech. Anal., **71**, No. 1 (1979), 41-61.