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A BILINEAR OPTIMAL CONTROL PROBLEM APPLIED TO A TIME DEPENDENT HARTREE–FOCK EQUATION COUPLED WITH CLASSICAL NUCLEAR DYNAMICS

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Abstract: We study a problem of bilinear optimal control for the electronic wave function of an Helium atom by an external time dependent electric field. The behavior of the atom is modeled by the Hartree–Fock equation, whose solution is the wave function of the electrons, coupled with the classical Newtonian dynamics, corresponding to the motion of the nucleus. We prove the existence of a bilinear optimal control in the case when the position of the nucleus is known and also prove the corresponding optimality condition. Then, we detail the proof of the existence of an optimal control for the coupled system and complete the study giving a formal optimality condition to define the electric control.

1 – Introduction

We are interested in a bilinear optimal control problem applied to the mathematical model of the behavior of a simplified chemical system, in fact an Helium atom, controlled by an external electric field. We describe the chemical system in terms of ordinary and partial differential equations using very classical approximations of quantum chemistry.

On the one hand, since the nucleus is much heavier than the electrons, we consider it as a point particle which moves according to the Newton dynamics in the external electric field and in the electric potential created by the electronic

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density (nucleus-electron attraction of Hellman-Feynman type). We obtain a second order in time ordinary differential equation solved by the position $a(t)$ of the nucleus (of mass m). On the other hand, under the restricted Hartree–Fock formalism, we describe the behavior of the electrons by a wave function, solution of a time dependent Hartree–Fock equation. We can define it as a Schrödinger equation with a coulombian potential due to the nucleus, singular at finite distance, an electric potential corresponding to the external electric field, possibly unbounded, and a nonlinearity of Hartree type in the right hand side. We want precisely to study the optimal control of the wave function of the electrons only, the control being performed by the electric potential.

We are in fact considering the following coupled system:

$$
\begin{cases}
i\,\partial_t u + \Delta u + \dfrac{1}{|x-a(t)|}u + V_1 u = \left(|u|^2 \star \dfrac{1}{|x|}\right)u\,, & \text{in } \mathbb{R}^3\times(0,T)\\
u(0) = u_0\,, & \text{in } \mathbb{R}^3\\
m\,\dfrac{d^2a}{dt^2} = \displaystyle\int_{\mathbb{R}^3} -|u(x)|^2\,\nabla\frac{1}{|x-a|}\,dx - \nabla V_1(a)\,, & \text{in } (0,T)\\
a(0) = a_0\,, \quad \dfrac{da}{dt}(0) = v_0
\end{cases}
\tag{1}
$$

where V_1 is the external electric potential depending on space and time variables, which takes its values in $\mathbb{R}$ and satisfy the assumptions:

$$
\begin{aligned}
\left(1+|x|^2\right)^{-\frac{1}{2}} V_1 \;&\in L^\infty\big((0,T)\times\mathbb{R}^3\big)\,,\\
\left(1+|x|^2\right)^{-\frac{1}{2}} \partial_t V_1 \;&\in L^1\big(0,T;L^\infty(\mathbb{R}^3)\big)\,,\\
\left(1+|x|^2\right)^{-\frac{1}{2}} \nabla V_1 \;&\in L^1\big(0,T;L^\infty(\mathbb{R}^3)\big)\,,\\
\nabla V_1 \;&\in L^2\big(0,T;W^{1,\infty}_{\mathrm{loc}}(\mathbb{R}^3)\big)\,.
\end{aligned}
\tag{2}
$$

We will define later on the optimal control problem related to this system and recall the precise results of existence and regularity of the solution we need in the sequel. One can already find in reference [2] the study of existence and regularity of solutions to this coupled system.

The Cauchy problem for this kind of non-adiabatic approximation of the general chemical Schrödinger equation has also been studied in the particular case when the atom is subjected to a uniform external time-dependent electric field $I(t)$ such that in equation (1), one has $V_1 = -I(t)\cdot x$ as in reference [5]. The authors remove the electric potential from the equation using a change of unknown function and variables (gauge transformation given in [8]). From then on, they have to deal with the nonlinear Schrödinger equation with only a time dependent coulombian potential.

We work in $\mathbb{R}^3$ and throughout this paper, we use the following notations:

$$\nabla v = \left(\frac{\partial v}{\partial x_1}, \frac{\partial v}{\partial x_2}, \frac{\partial v}{\partial x_3}\right), \quad \Delta v = \sum_{i=1}^{3} \frac{\partial^2 v}{\partial x_i^2}, \quad \partial_t v = \frac{\partial v}{\partial t},$$

Re and Im are the real and the imaginary parts of a complex number,

$\langle\, .\,,\, .\,\rangle$ stands for the scalar product in an Hilbert space,

$W^{2,1}(0,T) = W^{2,1}(0,T;\mathbb{R}^3)$, for $p \geq 1$, $L^p = L^p(\mathbb{R}^3)$,

the usual Sobolev spaces are $H^1 = H^1(\mathbb{R}^3)$ and $H^2 = H^2(\mathbb{R}^3)$.

We also define

$$H_1 = \left\{ v \in L^2(\mathbb{R}^3),\ \int_{\mathbb{R}^3} \left(1+|x|^2\right) \left|v(x)\right|^2 dx < +\infty \right\},$$
$$H_2 = \left\{ v \in L^2(\mathbb{R}^3),\ \int_{\mathbb{R}^3} \left(1+|x|^2\right)^2 \left|v(x)\right|^2 dx < +\infty \right\}.$$

One can notice that H_1 and H_2 are respectively the images of H^1 and H^2 under the Fourier transform.

On a mathematical point of view, the optimal control problem consists in minimizing a cost functional depending on the solution of a state equation (here, a coupled system of partial differential equations) and to characterize the minimum of the functional by an optimality condition. One will see in the sequel that even if we can prove existence of an optimal control for system (1), we cannot justify the optimality condition we formally obtain. However, the process will be described and fully proved in the following section in the simpler situation where the position of the nucleus is known at every moment.

Let (u,a) be a solution of system (1) where the external electric field V_1 is the control, and $u_1 \in L^2$ be a given target. We define the cost functionnal J by

$$J(V_1,u) = \frac{1}{2}\int_{\mathbb{R}^3} \left|u(T) - u_1\right|^2 dx + \frac{r}{2}\,\|V_1\|^2_{\mathcal{H}}$$

where $r > 0$ is a weight affecting the control cost and

$$\mathcal{H} = \left\{ V,\ \left(1+|x|^2\right)^{-\frac{1}{2}} V \in H^1(0,T;\mathcal{W}) \text{ and } \nabla V \in L^2(0,T;W^{1,\infty}) \right\}$$

where $\mathcal{W}$ is an Hilbert space which satisfies $\mathcal{W} \hookrightarrow W^{1,\infty}(\mathbb{R}^3)$. The problem is:

Can one find a minimizer $V_1 \in \mathcal{H}$ for $\inf \left\{ J(V,u),\ V \in \mathcal{H} \right\}$?

Remarks. 1) For example, in the space $\mathcal{H}$, we can choose the Hilbert space

$$\mathcal{W} = H^3 \oplus \mathrm{Span}\{\psi_1, \psi_2, ..., \psi_m\}$$

where $m \in \mathbb{N}$, and for all $i \in [\![1, m]\!]$, $\psi_i \in W^{1,\infty}(\mathbb{R}^3)\backslash H^3(\mathbb{R}^3)$.

2) In $\mathcal{H}$, we can replace the hypothesis on ∇V by $\nabla V \in L^2\big(0,T; W^{1,\infty}_{\mathrm{loc}}\big)$ as in assumption (2). Indeed, since we do not use any hypothesis on ∇V_1 to prove that the solution a is bounded in $C([0,T])$ (see [2]), then we do not need any information on ∇V_1 at infinity in $\mathbb{R}^3$. We will give details later on. □

We can actually prove the following theorem:

Theorem 1. *There exists an optimal control* $V_1 \in \mathcal{H}$ *such that*

$$J(V_1, u) = \inf\big\{J(V,u),\ V \in \mathcal{H}\big\}\ .$$

One can notice that we first need an existence result for a solution of the coupled system (1) in order to be able to formulate the bilinear optimal control problem. We have already proved one, in reference [2] (also in [1]), actually with a more general hypothesis on V_1. Indeed, we have

Theorem 2. *We assume that* T *is a positive arbitrary time and*

$$(3)\qquad \begin{aligned} \big(1+|x|^2\big)^{-1}V_1 &\in L^\infty\big((0,T)\times\mathbb{R}^3\big)\ ,\\ \big(1+|x|^2\big)^{-1}\partial_t V_1 &\in L^1\big(0,T;L^\infty(\mathbb{R}^3)\big)\ ,\\ \big(1+|x|^2\big)^{-1}\nabla V_1 &\in L^1\big(0,T;L^\infty(\mathbb{R}^3)\big)\ ,\\ \nabla V_1 &\in L^2\big(0,T;W^{1,\infty}_{\mathrm{loc}}(\mathbb{R}^3)\big)\ . \end{aligned}$$

If $u_0 \in H^2 \cap H_2$, $a_0, v_0 \in \mathbb{R}$, *then system* (1) *has at least a solution*

$$(u,a)\ \in\ \Big(W^{1,\infty}(0,T;L^2)\cap L^\infty(0,T;H^2\cap H_2)\Big)\times W^{2,1}(0,T)\ .$$

Moreover, for any solution of (1) *in this class, if* $\rho_0 > 0$ *is such that*

$$\big\|\big(1+|x|^2\big)^{-1}V_1\big\|_{W^{1,1}(0,T,L^\infty)} \le\ \rho_0\ ,$$

then there exists $R > 0$ *depending on* ρ_0 *such that* $\|a\|_{C([0,T])} \le R$ *and if* $\rho_1 > 0$ *is such that*

$$\left\|\frac{V_1}{1+|x|^2}\right\|_{W^{1,1}(0,T,L^\infty)} + \left\|\frac{\nabla V_1}{1+|x|^2}\right\|_{L^1(0,T,L^\infty)} + \big\|\nabla V_1\big\|_{L^2(0,T;W^{1,\infty}(B_R))}\ \le\ \rho_1$$

then there exists a non-negative constant K^0_{T,ρ_1} depending on the time T, on ρ_1, on $\|u_0\|_{H^2\cap H_2}$ and on $|a_0|$, $|v_0|$, such that:

$$\|u\|_{L^\infty(0,T;H^2\cap H_2)} + \|\partial_t u\|_{L^\infty(0,T;L^2)} + m\left\|\frac{da}{dt}\right\|_{L^\infty(0,T)} + m\left\|\frac{d^2a}{dt^2}\right\|_{L^1(0,T)} + \\ + \sup_{t\in[0,T]}\left(\int_{\mathbb{R}^3}\left(\left|u(t,x)\right|^2 \star \frac{1}{|x|}\right)\left|u(t,x)\right|^2\right)^{\frac{1}{2}} \leq K^0_{T,\rho_1} . \blacksquare \tag{4}$$

One can notice that if $V_1 \in \mathcal{H}$ then it satisfies assumptions (2) and (3), and we have at least a solution to equation (1) with Theorem 2. The optimal control problem is then well defined.

The reader may also notice that we do not give any uniqueness result for the coupled system (1) in Theorem 2. Indeed, even if we are convinced that the solution in this class is unique, we do not have a proof of this result up to now. Actually, E. Cancès and C. Le Bris give a proof of existence and uniqueness of solutions for the analogous system without electric potential in [5]. Of course, the method for proving uniqueness used in this article cannot be applied here because the Marcinkiewicz spaces which are used do not suit the general electric potential V_1 satisfying (3).

We underline that the lack of proof for uniqueness of the solution has no effects on the proof of existence of an optimal control (Theorem 1) but of course it is a main obstruction to the obtention of an optimality condition.

The next section presents the study of the situation where the position of the nucleus is known, instead of being the solution of an ordinary differential equation coupled to the Hartree–Fock equation. Without any coupling, the problem comes down to the difficulty of dealing with a nonlinear Schrödinger equation. In section 3, we give the proof of Theorem 1 and a formal optimality condition.

2 – Nonlinear Schrödinger equation

Before studying the optimal control problem linked with the coupled situation described in the introduction, we will consider the position $a(t)$ of the nucleus as known at any time $t \in [0,T]$ and forget the second equation in (1). Of course, this is too restrictive for the study of the control of chemical reactions by an external electric potential, but this section is only a first step in the study of the more realistic coupled situation. Moreover, in this present case, we will give a full result for the optimal control problem described further, from the existence of an optimal control to the proof of a necessary optimality condition.

2.1. Existence, uniqueness and regularity of solution

We consider the following nonlinear Schrödinger equation:

$$\text{(5)}\qquad \begin{cases} i\,\partial_t u + \Delta u + \dfrac{1}{|x-a|}u + V_1 u \;=\; \left(|u|^2 \star \dfrac{1}{|x|}\right)u\,, & \mathbb{R}^3\times(0,T) \\ u(0) = u_0\,, & \mathbb{R}^3 \end{cases}$$

where V_1 takes its values in $\mathbb{R}$ and we make the following assumptions:

$$\text{(6)}\qquad \begin{aligned} a \;&\in\; W^{2,1}(0,T) \ \text{ is known}\ , \\ \big(1+|x|^2\big)^{-1}V_1 \;&\in\; L^\infty\big((0,T)\times\mathbb{R}^3\big)\ , \\ \big(1+|x|^2\big)^{-1}\partial_t V_1 \;&\in\; L^1\big(0,T;L^\infty\big)\ , \\ \big(1+|x|^2\big)^{-1}\nabla V_1 \;&\in\; L^1\big(0,T;L^\infty(\mathbb{R}^3)\big)\ . \end{aligned}$$

We have to underline that one can find in reference [7] the proof of existence, uniqueness and regularity for the analogous equation without the electric potential V_1. This paper also deals with the more general case of an atom with more than two electrons. We draw the reader's attention on the fact that one of the main difficulty we encounter in the situation we are interested in is the coexistence of two potentials whose singularities are non-comparable.

Before describing the optimal control problem we will consider here, we first give two regularity results, very useful in the sequel. The first one is a theorem about the linear Schrödinger equation, given in [4] and proved in reference [3] (also in [1]). The next one gives existence and regularity of the unique solution to equation (5) and its proof is given in reference [2].

We first consider the linear Schrödinger equation

$$\begin{cases} i\,\partial_t u + \Delta u + \dfrac{1}{|x-a|}u + V_1 u = 0, & \mathbb{R}^3\times(0,T) \\ u(0) = u_0\,, & \mathbb{R}^3\ , \end{cases}$$

we set $\rho > 0$ and $\alpha > 0$ such that

$$\text{(7)}\qquad \left\|\frac{V_1}{1+|x|^2}\right\|_{W^{1,1}(0,T,L^\infty)} + \left\|\frac{\nabla V_1}{1+|x|^2}\right\|_{L^1(0,T,L^\infty)} \le \rho \quad\text{and}\quad \left\|\frac{d^2a}{dt^2}\right\|_{L^1(0,T)} \le \alpha$$

and we have the following result:

Theorem 3. *Let the initial data u_0 belongs to $H^2 \cap H_2$ and the electric potential V_1 and the position a of the nucleus satisfy assumption* (6)*. We define the family of Hamiltonians $\{H(t),\, t \in [0,T]\}$ by $H(t) = -\Delta - \dfrac{1}{|x-a(t)|} - V_1(t)$. Then, there exists a unique family of evolution operators $\{U(t,s),\ s,t \in [0,T]\}$ (the so called propagator associated with $H(t)$) on $H^2 \cap H_2$ such that for $u_0 \in H^2 \cap H_2$ we have*

- **(i)** *$U(t,s)U(s,r)u_0 = U(t,r)u_0$ and $U(t,t)u_0 = u_0$ for all $s,t,r \in [0,T]$;*
- **(ii)** *$(t,s) \mapsto U(t,s)u_0$ is strongly continuous in L^2 on $[0,T]^2$ and $U(t,s)$ is an isometry on L^2, that is $\|U(t,s)u_0\|_{L^2} = \|u_0\|_{L^2}$;*
- **(iii)** *$U(t,s) \in \mathcal{L}(H^2 \cap H_2)$ for all $(s,t) \in [0,T]^2$ and $(t,s) \mapsto U(t,s)u_0$ is weakly continuous from $[0,T]^2$ to $H^2 \cap H_2$; moreover, there exists $M_{T,\alpha,\rho} > 0$ such that: $\forall\, t,s \in [0,T]$, $\forall f \in H^2 \cap H_2$, $\|U(t,s)f\|_{H^2\cap H_2} \leq M_{T,\alpha,\rho}\|f\|_{H^2\cap H_2}$.*
- **(iv)** *Equalities $i\,\partial_t U(t,s)u_0 = H(t)U(t,s)u_0$ and $i\,\partial_s U(t,s)u_0 = -U(t,s)H(s)u_0$ hold in L^2.* ∎

Now, Theorem 3 is the main ingredient to prove the following result of existence along with a Picard fixed point theorem.

Theorem 4. *Let T be a positive arbitrary time and α and ρ satisfy* (7)*. Under assumption* (6)*, and if we also assume $u_0 \in H^2 \cap H_2$, then equation* (5) *has a unique solution*

$$u \in L^\infty(0,T; H^2 \cap H_2) \quad \text{with } \ \partial_t u \in L^\infty(0,T; L^2)$$

and there exists a real constant $C > 0$ depending on T, u_0, α and ρ such that:

$$\|u\|_{L^\infty(0,T;H^2\cap H_2)} + \|\partial_t u\|_{L^\infty(0,T;L^2)} \leq C\|u_0\|_{H^2\cap H_2}\,. \ \blacksquare$$

We draw the reader's attention to the uniqueness of the solution of (5) in this result. Thus, we can correctly define an optimal control problem on equation (5), the control being the external electric potential V_1 and the solution u.

From now on, we may denote $\dfrac{1}{|x-a|}$ by V_0 and we mean $a \in W^{2,1}(0,T)$. Theorem 3 is also useful to give a meaning to the equations we will encounter in the sequel. More precisely, we consider the general equation

$$\text{(8)} \qquad \begin{cases} i\,\partial_t v + \Delta v + V_0 v + V_1 v = f(v)\,, & \mathbb{R}^3 \times (0,T) \\ v(0) = v_0\,, & \mathbb{R}^3 \end{cases}$$

and we give the following result:

Proposition 5. *Let T be a positive arbitrary time. Under assumption* (6), *if we assume $v_0 \in L^2$ and if we also assume that there exists $C, C_M > 0$ such that for all $u, v \in C([0,T]; L^2)$,*

$$\|f(u)\|_{L^1(0,T,L^2)} \leq C\,T\big(\|u\|_{C([0,T];L^2)} + 1\big)$$

and when $\|u\|_{C([0,T];L^2)} \leq M$ and $\|v\|_{C([0,T];L^2)} \leq M$,

$$\|f(u) - f(v)\|_{L^1(0,T,L^2)} \leq C_M\,T\|u - v\|_{C([0,T];L^2)} \ ,$$

then equation (8) *has a unique solution $v \in C([0,T]; L^2)$.* ∎

The proof uses a Picard fixed point theorem on the functional Φ defined on the space $C([0,T]; L^2)$ by $\Phi\colon v \mapsto v_0 - i\displaystyle\int_0^{\cdot} U(\cdot, s) f(v(s))\, ds$ where U is the propagator of Theorem 3.

2.2. Optimal control problem

On the evolution system (5), we define an optimal control problem which reads as follows: if $u_1 \in L^2$ is a given target, find a minimizer $V_1 \in H$ for

$$\inf\big\{J(V),\ V \in H\big\} \tag{9}$$

where the cost functionnal J is defined by

$$J(V_1) = \frac{1}{2}\int_{\mathbb{R}^3} \big|u(T) - u_1\big|^2\, dx + \frac{r}{2}\,\|V_1\|_H^2 \ , \qquad r > 0 \ . \tag{10}$$

There,

$$H = \Big\{V,\ \big(1 + |x|^2\big)^{-\frac{1}{2}}\, V \in H^1(0,T;W)\Big\}$$

where W is an Hilbert space such that $W \hookrightarrow W^{1,\infty}(\mathbb{R}^3)$ and in (10), u is the solution of equation (5).

Remarks. 1) One can notice that if V_1 belongs to H, then it satisfies (6) and we can apply Theorem 4 that gives a unique solution u.

2) This space H has been chosen here as an Hilbert space in order to have a differentiable norm.

3) This optimal control problem is a so-called "bilinear optimal control problem" and the mapping *control* → *state* ($V_1 \mapsto u$) is strongly nonlinear. □

Let us now formulate the result on the bilinear optimal control problem.

Theorem 6. *There exists an optimal control $V_1 \in H$ such that*

$$J(V_1) \;=\; \inf\left\{J(V),\;\; V\!\in H\right\}$$

and for all δV in H, V_1 satisfies

$$r\langle V_1, \delta V\rangle_H \;=\; \mathrm{Im}\int_0^T\!\!\int_{\mathbb{R}^3} \delta\, V(x,t)\, u(x,t)\, \bar{p}(x,t)\; dx\, dt \tag{11}$$

where u is solution of (5) *and p is solution of the following adjoint problem, set in $\mathbb{R}^3\!\times\!(0,T)$.*

$$\begin{cases} i\,\partial_t p + \Delta p + V_0 p + V_1 p \;=\; \left(|u|^2 \star \dfrac{1}{|x|}\right)p + 2\,i\left(\mathrm{Im}(u\overline{p}) \star \dfrac{1}{|x|}\right)u \\ p(T) = u(T) - u_1\ . \end{cases} \tag{12}$$

Remark. If we substitute the Hilbert space H by a reflexive space satisfying assumption (6) in the definition of J and in (9), the existence of an optimal control can also be proved. Nevertheless, the proof of an optimality condition needs an Hilbert space. □

A result of existence for a bilinear optimal control problem, governed by a Schrödinger equation with the same Hartree nonlinearity $\left(|u|^2 \star \frac{1}{|x|}\right)u$, has also been given by E. Cancès, C. Le Bris and M. Pilot in [6]. The authors deal with an electric potential homogeneous in space $V_1 = -I(t)\cdot x$ with $I \in L^2(0,T)$, while we take into account here a more general electric potential optimal control. For instance, in the definition of H, we can consider the Hilbert space $W\!= H^3 \oplus \mathrm{Span}\{\psi_1, \psi_2, ..., \psi_m\}$ with $m \in \mathbb{N}$, and for all $i \in [\![1,m]\!]$, $\psi_i \in W^{1,\infty}(\mathbb{R}^3)\backslash H^3(\mathbb{R}^3)$. Then $W \hookrightarrow W^{1,\infty}$ and this example enables us to deal both with the particular case of [6] where $V_1(x,t) = -I(t)\cdot x$ but for $I \in H^1(0,T)$ and with general electric potentials $(1+|x|^2)^{-\frac{1}{2}}V_1(t) \in H^2(\mathbb{R}^3)$ which are non-homogeneous in space.

We can also specify the optimality condition in the particular case where $W\!= H^3(\mathbb{R}^3) \oplus \mathrm{Span}\{\psi_1\}$ by an optimality system. We choose for instance $\psi_1 = \mathbb{1}$ where $\psi_1(x) = 1$, for all $x \in \mathbb{R}^3$. Therefore, from the optimality condition (11), we can get an optimality system that reads:

$$\begin{cases} r\,(I-\partial_t^2)\,(I-\Delta)\,Y_1 \;=\; (I-\Delta)^{-1}\Big(\mathrm{Im}(u\overline{p})\,\sqrt{1+|x|^2}\Big) & \text{in } \mathbb{R}^3\times D(0,T) \\ \partial_t(Y_1-\Delta Y_1)(T) \;=\; \partial_t(Y_1-\Delta Y_1)(0) \;=\; 0 & \text{in } \mathbb{R}^3 \\ r\Big(E-\dfrac{d^2E}{dt^2}\Big) \;=\; \mathrm{Im}\displaystyle\int_{\mathbb{R}^3} u\overline{p}\,\sqrt{1+|x|^2}\;dx & \text{in } (0,T) \\ \dfrac{dE}{dt}(T) = \dfrac{dE}{dt}(0) = 0 \end{cases}$$

where $V_1(x,t) = \big(1+|x|^2\big)^{\frac{1}{2}}\,\big[(I-\Delta)^{-1}\;Y_1(x,t)+E(t)\big]$ and p is the solution of the adjoint equation (12). The proof when $W = H^3$ can be read for the problem of optimal control for the linear Schrödinger equation in reference [3], the only changes being the adjoint equation solved by p and the absence of E.

The proof of Theorem 6 is divided in two steps. Existence of an optimal control can be treated first while the optimality condition requires the proof of the continuity and the differentiability of J. The regularity result of Theorem 4 is strongly needed for proving this differentiability result.

2.2.1. Existence of an optimal control

We will prove here the existence of an electric optimal control minimizing the cost functional. Indeed, we are going to prove:

$$\exists\; V_1 \in H \quad \text{ such that } \; J(V_1) = \inf\big\{J(V),\; V\in H\big\}\;.$$

Remark. The structure of the proof given in reference [3], for a bilinear optimal control problem defined on the linear Schrödinger equation, is analogous to the one we will follow here. ▫

We consider a minimizing sequence $(V_1^n)_{n\geq 0}$ in H for the functional J:

$$\inf_H J(V) = \lim_{n\to\infty} J(V_1^n)\;.$$

Since

$$J(V_1^n) \;=\; \frac{1}{2}\int_{\mathbb{R}^3}\big|u_n(T)-u_1\big|^2\,dx \;+\; \frac{r}{2}\,\|V_1^n\|_H^2$$

where u_n is solution of (5) with potential $V_1 = V_1^n$, we then obtain that $(V_1^n)_{n\geq 0}$ is bounded in H, independently of n. Up to a subsequence, we have $V_1^n \rightharpoonup V_1$ weakly in H and

$$\|V_1\|_H \;\leq\; \underline{\lim}\,\|V_1^n\|_H\;. \tag{13}$$

The difficulty comes from the term $\|u_n(T)-u_1\|^2_{L^2}$. More precisely, the point is to prove the weak convergence of $u_n(T)$ toward $u(T)$ in L^2 and this is not obvious. It will imply $\underline{\lim}\|u_n(T)-u_1\|^2_{L^2} \geq \|u(T)-u_1\|^2_{L^2}$ but actually, we are going to prove the strong convergence of $u_n(T)$ toward $u(T)$ in L^2. Indeed, if for all t in $[0,T]$, $u_n(t) \longrightarrow u(t)$ in L^2, where u is the solution associated with V_1, then

$$\lim_{n\to+\infty} \big\|u_n(T) - u_1\big\|^2_{L^2} = \big\|u(T) - u_1\big\|^2_{L^2} , \tag{14}$$

and from (13) and (14) we obtain

$$J(V_1) \leq \underline{\lim}\, J(V_1^n) = \inf_{V\in H} J(V) .$$

As $V_1 \in H$, we get $J(V_1) = \inf\limits_{H} J$ and the existence of an optimal control is proved.

We set $F(u) = \big(|u|^2 \star \frac{1}{|x|}\big)u$ and we consider $w_n = u_n - u$ solution of the following equation:

$$\begin{cases} i\,\partial_t w_n + \Delta w_n + V_0 w_n + V_1^n w_n = F(u_n) - F(u) + u(V_1 - V_1^n)\,, & \mathbb{R}^3\times(0,T) \\ w_n(0) = 0\,, & \mathbb{R}^3 . \end{cases} \tag{15}$$

We are going to prove that for all t in $[0,T]$, $\|w_n(t)\|_{L^2} \longrightarrow 0$.

In order to deal with the nonlinearity, we observe that we have, from Cauchy–Schwarz and Hardy's inequality,

$$\begin{aligned} \big\|F(u) - F(u_n)\big\|_{L^2} &\leq \left\|\left(|u|^2 \star \frac{1}{|x|}\right)u - \left(|u_n|^2 \star \frac{1}{|x|}\right)u_n\right\|_{L^2} \\ &\leq \left\|\left(|u|^2 \star \frac{1}{|x|}\right)(u-u_n)\right\|_{L^2} + \left\|\left(\left(|u|^2 - |u_n|^2\right) \star \frac{1}{|x|}\right)u_n\right\|_{L^2} \\ &\leq 2\,\|u\|_{L^2}\,\|\nabla u\|_{L^2}\,\|u-u_n\|_{L^2} \\ &\quad + 2\,\|u_n\|_{L^2}\Big(\|\nabla u\|_{L^2} + \|\nabla u_n\|_{L^2}\Big)\,\|u-u_n\|_{L^2} \\ &\leq C\Big(\|u\|^2_{H^1} + \|u_n\|^2_{H^1}\Big)\,\|u-u_n\|_{L^2} . \end{aligned} \tag{16}$$

Therefore, if we multiply equation (15) by $\overline{w_n}$ integrate on $\mathbb{R}^3$ and take the imaginary part, which means we calculate $\operatorname{Im}\displaystyle\int_{\mathbb{R}^3}(15)\,.\,\overline{w_n}(x)\,dx$, we obtain:

$$\begin{aligned} \frac{d}{dt}\left(\int_{\mathbb{R}^3}|w_n|^2\,dx\right) &\leq C\,\big\|F(u) - F(u_n)\big\|_{L^2}\,\|w_n\|_{L^2} + C\int_{\mathbb{R}^3}|V_1^n - V_1|\,|u|\,|w_n|\,dx \\ &\leq C\,\big(\|u_n\|^2_{H^1} + \|u\|^2_{H^1}\big)\,\|w_n\|^2_{L^2} \\ &\quad + C\,\big\|V_1^n - V_1\big\|_H \int_{\mathbb{R}^3}|u|\,\big(1+|x|^2\big)^{\frac{1}{2}}\,|w_n|\,dx . \end{aligned}$$

From Theorem 4, we have:

$$\|u_n\|_{L^\infty(0,T;H^2\cap H_2)} + \|\partial_t u_n\|_{L^\infty(0,T;L^2)} \le C\,\|u_0\|_{H^2\cap H_2}$$

where C is independent of n since $(V_1^n)_{n\ge 0}$ is bounded in H. Then,

$$\forall\, t\in[0,T]\ , \qquad \|u_n(t)\|^2_{H^1} + \|u(t)\|^2_{H^1} \le C$$

and we actually obtain (C denoting a generic constant depending on T),

$$\frac{d}{dt}\big(\|w_n(t)\|^2_{L^2}\big) \le C\,\|w_n(t)\|^2_{L^2} + C\int_{\mathbb{R}^3} |u(t)|\,\big(1+|x|^2\big)^{\frac12}\,|w_n(t)|\,dx \tag{17}$$

Moreover, we will need the following compactness lemma (see reference [9] for its proof).

Lemma 7. *Let X, B and Y be Banach spaces and $p\in[1,\infty]$.*

We assume that $X\hookrightarrow B\hookrightarrow Y$ with compact embedding $X\hookrightarrow B$.

If $\{f_n,\, n\in\mathbb{N}\}$ is bounded in $L^p(0,T;X)$ and if $\{\partial_t f_n,\, n\in\mathbb{N}\}$ is bounded in $L^p(0,T;Y)$ then $\{f_n,\, n\in\mathbb{N}\}$ is relatively compact in $L^p(0,T;B)$ (and in $C([0,T];B)$ if $p=\infty$). ∎

Then, it has to be noticed that up to a subsequence we also have $u_n \longrightarrow u$ in $C([0,T];H^1_{\rm loc})$. Indeed, we can use Lemma 7 since $(u_n)_{n\ge 0}$ is bounded in $L^\infty(H^2\cap H_2)$ and $(\partial_t u_n)_{n\ge0}$ is bounded in $L^\infty(L^2)$. Then for all $R>0$,

$$\big\|w_n\big\|_{C([0,T];L^2(B(0,R)))} \overset{n\to\infty}{\longrightarrow} 0 \tag{18}$$

and on the other hand, for all t in $[0,T]$,

$$\left(\int_{B(0,R)^c} \frac{|w_n(t)|^2}{1+|x|^2}\,dx\right)^{\frac12} \le \left(\frac{1}{1+R^2}\right)^{\frac12} \|w_n(t)\|_{L^2}\ .$$

Thus, using Cauchy–Schwarz inequality, we can write

$$\begin{aligned}
&\int_{\mathbb{R}^3} |u(t)|\,\big(1+|x|^2\big)^{\frac12}\,|w_n(t)|\,dx \le \\
&\qquad \le \int_{B(0,R)} |u(t)|\,\big(1+|x|^2\big)^{\frac12}\big|w_n(t)\big|\,dx \\
&\qquad\quad + \int_{B(0,R)^c} |u(t)|\,\big(1+|x|^2\big)\,\frac{|w_n(t)|}{\big(1+|x|^2\big)^{\frac12}}\,dx \\
&\qquad \le \|u(t)\|_{H_1}\,\|w_n(t)\|_{L^2(B(0,R))} + \frac{1}{\sqrt{1+R^2}}\,\|u(t)\|_{H_2}\,\|w_n(t)\|_{L^2} \\
&\qquad \le C\left(\|w_n\|_{C([0,T];L^2(B(0,R)))} + \frac{1}{\sqrt{1+R^2}}\,\|w_n(t)\|_{L^2}\right).
\end{aligned} \tag{19}$$

We set $E_n(t) = \|w_n(t)\|_{L^2}^2 + \|w_n\|_{C([0,T];L^2(B(0,R))}$, where one can notice that $\|w_n\|_{C([0,T];L^2(B(0,R))}$ does not depend on t. From (17) and (19), it satisfies

$$\frac{dE_n}{dt}(t) \le CE_n(t) + \frac{C}{\sqrt{1+R^2}}\sqrt{E_n(t)}\ .$$

Since $E_n(0) = \|w_n\|_{C([0,T];L^2(B(0,R))}$ and since we have actually

$$\frac{d\sqrt{E_n}}{dt}(t) \le C\sqrt{E_n(t)} + \frac{C}{\sqrt{1+R^2}}\ ,$$

then, from Gronwall lemma, we obtain that for all t in $[0,T]$,

$$\sqrt{E_n(t)} \le C\,T\,\frac{e^{CT}}{\sqrt{1+R^2}} + e^{CT}\|w_n\|_{C([0,T];L^2(B(0,R))}^{\frac{1}{2}}\ .$$

It means that since T is fixed and since we have (18), then for any $\varepsilon > 0$, there exists $R > 0$ and n_0 large enough in $\mathbb{N}$ such that

$$C\,T\,\frac{e^{CT}}{\sqrt{1+R^2}} \le \frac{\varepsilon}{2} \qquad \text{and} \qquad \forall\, n \ge n_0,\ \ e^{CT}\|w_n\|_{C([0,T];L^2(B(0,R))}^{\frac{1}{2}} \le \frac{\varepsilon}{2}\ .$$

We finally obtain that for all t in $[0,T]$, $\|w_n(t)\|_{L^2} \overset{n\to\infty}{\longrightarrow} 0$ and therefore, u is the solution of (5) in the sense of distributions and we have proved the existence of an optimal control V_1 associated with the functionnal J. We then have to write an optimality condition for V_1.

2.2.2. Optimality condition

The usual way to obtain an optimality condition is to prove that the cost functional J is differentiable and to translate the necessary condition

$$DJ(V_1)[\delta V_1] = 0\ , \qquad \forall\,\delta V_1 \in H$$

in terms of the adjoint state. Since $J(V_1) = \frac{1}{2}\|u(T)-u_1\|_{L^2}^2 + \frac{r}{2}\|V_1\|_H^2$, as announced in the introduction, the main difficulty comes from the necessity to differentiate the state variable u with respect to the control V_1, in order to calculate the gradient $DJ(V_1)$. We postpone the proof of the following lemma.

Lemma 8. *Let u be the solution of* (5). *The functional ϕ defined by*

$$\begin{aligned} \phi\colon\ H &\to L^2(\mathbb{R}^3) \\ V_1 &\mapsto u(T) \end{aligned}$$

is differentiable and if z is the solution of the following equation, set in $\mathbb{R}^3 \times (0,T)$*:*

$$\begin{cases} i\,\partial_t z + \Delta z + V_0 z + V_1 z \;=\; -\delta V_1 u + \left(|u|^2 \star \dfrac{1}{|x|}\right) z + 2\,\mathrm{Re}\left(u\overline{z} \star \dfrac{1}{|x|}\right) u\ , \\ z(t{=}0) = 0 \end{cases} \tag{20}$$

we have $z \in C([0,T];L^2)$ *and* $D\phi(V_1)[\delta V_1] = z(T)$*.*

We deduce from Lemma 8 that J is differentiable with respect to V_1. Thereafter, since $D\phi(V_1)[\delta V_1] = z(T)$, the condition

$$DJ(V_1)[\delta V_1] = 0\ , \qquad \forall\, \delta V_1 \in H$$

reads

$$\mathrm{Re} \int_{\mathbb{R}^3} \Big(u(T,x) - u_1(x) \Big)\, \overline{z(T,x)}\; dx \;+\; r\langle V_1, \delta V_1\rangle_H \;=\; 0\ . \tag{21}$$

Remarks. 1) As for the study of the same bilinear optimal control problem for the linear Schrödinger equation one has read in reference [3], we can prove the differentiability of $V_1 \mapsto u(T)$ with values in L^2 but we don't know whether this remains true if we consider the same mapping with values in H^1 for example. We think that the differentiability is not true anymore. Therefore, in the functional J, the first term cannot be replaced by a stronger norm of $u(T) - u_1$.

2) We can also underline the choice of H we made on purpose. As it is an Hilbert space, we can easily take the derivative of the norm $\|\cdot\|_H$ in the functional J. □

Now, we consider the adjoint system (12):

$$\begin{cases} i\,\partial_t p + \Delta p + V_0 p + V_1 p \;=\; \left(|u|^2 \star \dfrac{1}{|x|}\right) p + 2\,i \left(\mathrm{Im}(u\overline{p}) \star \dfrac{1}{|x|}\right)\overline{u} & \text{in } \mathbb{R}^3 \times (0,T) \\ p(T) \;=\; u(T) - u_1 & \text{in } \mathbb{R}^3\ . \end{cases}$$

Using Proposition 5, one can prove that the equivalent integral equation has a unique solution $p \in C([0,T];L^2)$ since we have

$$\left\| \left(|u|^2 \star \frac{1}{|x|}\right) p + 2\,i \left(\mathrm{Im}(u\overline{p}) \star \frac{1}{|x|}\right)\overline{u} \right\|_{L^1(0,T;L^2)} \leq\; C\,T\,\|p\|_{C([0,T];L^2)}\ .$$

We then multiply equation (20) by $\overline{p}$, integrate on $[0,T]\times\mathbb{R}^3$ and take the imaginary part. We obtain:

$$\begin{aligned}
&\operatorname{Im}\int_0^T\!\!\int_{\mathbb{R}^3} \big(i\,\partial_t z + \Delta z + V_0 z + V_1 z\big)\overline{p} \;= \\
&\quad= \operatorname{Im}\int_0^T\!\!\int_{\mathbb{R}^3} -\delta V_1 u\overline{p} \,+\, \operatorname{Im}\int_0^T\!\!\int_{\mathbb{R}^3}\Big(|u|^2\star\frac{1}{|x|}\Big)z\overline{p} \,+\, 2\operatorname{Im}\int_0^T\!\!\int_{\mathbb{R}^3}\operatorname{Re}\Big(u\overline{z}\star\frac{1}{|x|}\Big)u\overline{p}\;.
\end{aligned}$$

Then $z(0)=0$ implies

$$\begin{aligned}
&\operatorname{Im}\int_0^T\!\!\int_{\mathbb{R}^3} z\Big(\overline{i\,\partial_t p} + \overline{\Delta p} + \overline{(V_0{+}V_1)p}\Big) \,+\, \operatorname{Im}\, i\int_{\mathbb{R}^3} z(T)\,\overline{p(T)} \;= \\
&\quad= -\operatorname{Im}\int_0^T\!\!\int_{\mathbb{R}^3}\delta V_1 u\overline{p} \,+\, \operatorname{Im}\int_0^T\!\!\int_{\mathbb{R}^3} z\,\overline{\Big(|u|^2\star\frac{1}{|x|}\Big)p} \,+\, 2\int_0^T\!\!\int_{\mathbb{R}^3}\Big(\operatorname{Im}(u\overline{p})\star\frac{1}{|x|}\Big)\operatorname{Re}(u\overline{z})
\end{aligned}$$

and since p satisfies equation (12), we get

$$\operatorname{Im}\; i\int_{\mathbb{R}^3} z(T)\,.\,\overline{\big(u(T)-u_1\big)} \;=\; -\operatorname{Im}\int_0^T\!\!\int_{\mathbb{R}^3}\delta V_1 u\overline{p}$$

which gives

$$\operatorname{Re}\int_{\mathbb{R}^3}\overline{z(T)}\,\big(u(T)-u_1\big) \;=\; -\operatorname{Im}\int_0^T\!\!\int_{\mathbb{R}^3}\delta V_1 u\overline{p}\;. \tag{22}$$

Using (22), the optimality condition (21) can be written:

$$r\langle V_1,\delta V_1\rangle_H \;=\; \operatorname{Im}\int_0^T\!\!\int_{\mathbb{R}^3}\delta V_1 u\overline{p}\;dx\,dt\;, \qquad \forall\,\delta V_1\in H\;.$$

The proof of Theorem 6 will be complete with the proof of Lemma 8. ∎

Proof of Lemma 8: Actually, we will first study the continuity of ϕ and then the differentiability. We recall the definition of the functional ϕ: if u is the solution of (5) with electric potential V_1 in H, then

$$\begin{aligned}
\phi\colon\; H &\;\to\; L^2(\mathbb{R}^3)\\
V_1 &\;\mapsto\; u(T)\;.
\end{aligned}$$

According to Proposition 5 and to the properties of F, we consider the solution $\delta u\in C([0,T];L^2)$ of the following equation set in $\mathbb{R}^3\times(0,T)$:

$$\left\{\begin{array}{l} i\,\partial_t\delta u + \Delta\delta u + V_0\delta u + (V_1{+}\delta V_1)\delta u \;=\; -\delta V_1 u + F(u{+}\delta u) - F(u)\\[2ex] \delta u(0)=0\;. \end{array}\right. \tag{23}$$

In order to prove the continuity of ϕ, we will prove that

$$\|\delta u\|_{L^\infty(0,T;L^2)} = O\big(\|\delta V_1\|_H\big)\,.$$

Let us calculate $\operatorname{Im}\displaystyle\int_{\mathbb{R}^3}(23)\,.\,\overline{\delta u}(x)\,dx$. Using the property (16) of F, we obtain

$$\begin{aligned}
\frac{d}{dt}\left(\int_{\mathbb{R}^3}|\delta u|^2\,dx\right) &\leq C\,\|\delta V_1\|_H\,\|u\|_{H_1}\,\|\delta u\|_{L^2} + C\big\|F(u{+}\delta u) - F(u)\big\|_{L^2}\,\|\delta u\|_{L^2}\\
&\leq C\,\|\delta V_1\|_H\,\|u\|_{H_1}\,\|\delta u\|_{L^2} + C\Big(\|\delta u{+}u\|^2_{L^2} + \|\delta u\|^2_{L^2}\Big)\,\|\delta u\|^2_{L^2}\\
&\leq C\,\|\delta V_1\|_H\,\|\delta u\|_{L^2} + C\,\|\delta u\|^2_{L^2}\,.
\end{aligned}$$

Indeed, the solution u of equation (5) and the solution $u{+}\delta u$ of the same equation but with potential $V_1{+}\delta V_1$, are bounded in L^2. As $\delta u(0) = 0$ and using Gronwall's lemma, it follows

$$\|\delta u(t)\|_{L^2} \leq C\,T\,e^{Ct}\|\delta V_1\|_H\,, \qquad \forall\, t\in[0,T]\,.$$

Eventually, we get $\|\delta u\|_{C([0,T];L^2)} = O(\|\delta V_1\|_H)$, the continuity of ϕ is proved and we will now prove the differentiability.

We first have to prove that $z(T)$ is well defined in L^2 where z is solution of (20) and then, if we set $w = \delta u - z$, we will prove that

$$\|w(T)\|_{L^2} = o\big(\|\delta V_1\|_H\big)$$

which means that $D\phi(V_1)[\delta V_1] = z(T)$ and completes the proof of Lemma 8.

Since we can prove the right hand side of equation (20) satisfies

$$\left\|\left(|u|^2\star\frac{1}{|x|}\right)z + 2\operatorname{Re}\left(u\overline{z}\star\frac{1}{|x|}\right)u - \delta V_1 u\right\|_{L^1(0,T;L^2)} \leq C\,T\Big(\|z\|_{C([0,T],L^2)} + 1\Big)\,,$$

then Proposition 5 gives a unique solution $z\in C([0,T];L^2)$ to equation (20). Moreover, if we calculate $\operatorname{Im}\displaystyle\int_{\mathbb{R}^3}(20)\,.\,\overline{z}(x)\,dx$, we obtain from Hardy's inequality:

$$\begin{aligned}
\frac{d}{dt}\left(\int_{\mathbb{R}^3}|z|^2\,dx\right) &= -2\operatorname{Im}\int_{\mathbb{R}^3}\delta V_1 u\overline{z}\;dx \;+\; 2\int_{\mathbb{R}^3}\left(\operatorname{Re}(u\overline{z})\star\frac{1}{|x|}\right)\operatorname{Im}(u\overline{z})\;dx\\
&\leq C\,\|\delta V_1\|_H\,\|u\|_{H_1}\|z\|_{L^2} + C\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\frac{|u(x)||z(x)|}{|x-y|}\,|u(y)|\,|z(y)|\;dx\,dy\\
&\leq C\,\|\delta V_1\|_H\,\|z\|_{L^2} + C\,\|\nabla u\|_{L^2}\,\|z\|_{L^2}\int_{\mathbb{R}^3}|u(x)|\,|z(x)|\,dx\\
&\leq C\,\|\delta V_1\|_H\,\|z\|_{L^2} + C\,\|z\|^2_{L^2}\,.
\end{aligned}$$

It implies

$$\|z(t)\|_{L^2}^2 \le C\,\|\delta V_1\|_H \int_0^t \|z(s)\|_{L^2}\,ds \,+\, C\int_0^t \|z(s)\|_{L^2}^2\,ds \tag{24}$$

and a Gronwall argument leads us easily to deduce that there exists a constants $C_T > 0$ such that

$$\|z(t)\|_{L^2} \le C_T \|\delta V_1\|_H\ , \qquad \forall\, t\in[0,T]\ . \tag{25}$$

In order to simplify the right hand side of the equation solved by $w = \delta u - z$, we consider the source terms of equation (23) solved by δu:

$$\begin{aligned}
&F(u+\delta u) - F(u) - \delta V_1 u \ = \\
&\quad = \left(|u+\delta u|^2 \star \frac{1}{|x|}\right)(u+\delta u) - \left(|u|^2\star\frac{1}{|x|}\right)u - \delta V_1 u\\
&\quad = \left(|u|^2\star\frac{1}{|x|}\right)\delta u + 2\,\mathrm{Re}\left(u\overline{\delta u}\star\frac{1}{|x|}\right)(u+\delta u) + \left(|\delta u|^2\star\frac{1}{|x|}\right)(u+\delta u) - \delta V_1 u
\end{aligned}$$

and since z satisfies (20), we have finally the following right hand side

$$\begin{aligned}
F(u+\delta u) - F(u) - \delta V_1 u - \left(-\delta V_1 u + \left(|u|^2\star\frac{1}{|x|}\right)z + 2\,\mathrm{Re}\left(u\overline{z}\star\frac{1}{|x|}\right)u\right) \ = \\
= \left(|u|^2\star\frac{1}{|x|}\right)\delta u + 2\,\mathrm{Re}\left(u\overline{\delta u}\star\frac{1}{|x|}\right)(u+\delta u)\\
+ \left(|\delta u|^2\star\frac{1}{|x|}\right)(u+\delta u) - \left(|u|^2\star\frac{1}{|x|}\right)z - 2\,\mathrm{Re}\left(u\overline{z}\star\frac{1}{|x|}\right)u\\
= \left(|u|^2\star\frac{1}{|x|}\right)w + 2\,\mathrm{Re}\left(u\overline{w}\star\frac{1}{|x|}\right)u + 2\,\mathrm{Re}\left(u\overline{\delta u}\star\frac{1}{|x|}\right)\delta u\\
+ \left(|\delta u|^2\star\frac{1}{|x|}\right)(u+w+z)\ .
\end{aligned}$$

Therefore, the equation satisfied by w in $\mathbb{R}^3\times(0,T)$ is:

$$\begin{cases}
i\,\partial_t w + \Delta w + V_0 w + (V_1 + \delta V_1)w \ = \\
\quad = -\delta V_1 z + \left(|u|^2\star\frac{1}{|x|}\right)w + 2\,\mathrm{Re}\left(u\overline{w}\star\frac{1}{|x|}\right)u + 2\,\mathrm{Re}\left(u\overline{\delta u}\star\frac{1}{|x|}\right)\delta u\\
\qquad + \left(|\delta u|^2\star\frac{1}{|x|}\right)(u+w+z)\\
w(t{=}0) = 0\ .
\end{cases} \tag{26}$$

Using Proposition 5, since the right hand side of equation (26) belongs to $L^1(0,T;L^2)$ and has the good properties, we can prove that there exists a unique solution $w \in C([0,T];L^2)$. We can also formally calculate $\mathrm{Im}\int_{\mathbb{R}^3}(26)\,.\,\overline{w}(x)\,dx$ in the same way we did to prove (25). Since we have $\|\delta u\|_{L^\infty(L^2)} = O(\|\delta V_1\|_H)$, we obtain:

$$\begin{aligned}
\frac{d}{dt}\big(\|w\|_{L^2}^2\big) \;\le\; & C\int_{\mathbb{R}^3}|\delta V_1|\,|z|\,|w|\,dx \;+\; C\int_{\mathbb{R}^3}\left|\left(\mathrm{Re}(u\overline{w})\star\frac{1}{|x|}\right)\mathrm{Im}(u\overline{w})\right|dx \\
& + C\int_{\mathbb{R}^3}\left|\mathrm{Re}\left(u\overline{\delta u}\star\frac{1}{|x|}\right)\mathrm{Im}(\delta u\,\overline{w})\right|dx \\
& + C\int_{\mathbb{R}^3}\left|\left(|\delta u|^2\star\frac{1}{|x|}\right)\mathrm{Im}\,\big((u+z)\overline{w}\big)\right|dx \\
\le\; & C\,\|\delta V_1\|_H\,\|z\|_{H_1}\|w\|_{L^2} + C\,\|\nabla u\|_{L^2}\,\|u\|_{L^2}\,\|w\|_{L^2}^2 \\
& + C\Big(\|\nabla u\|_{L^2} + \|\nabla z\|_{L^2}\Big)\,\|\delta u\|_{L^2}^2\,\|w\|_{L^2} \\
\le\; & C\,\|\delta V_1\|_H\,\|z\|_{H_1}\|w\|_{L^2} + C\,\|w\|_{L^2}^2 + C\,\|\delta V_1\|_H^2\,\|w\|_{L^2} \\
& + C\,\|z\|_{H^1}\|\delta V_1\|_H^2\,\|w\|_{L^2}
\end{aligned}$$

which means that for all t in $[0,T]$,

$$\frac{d}{dt}\big(\|w(t)\|_{L^2}\big) \;\le\; C\,\|\delta V_1\|_H\Big(\|z(t)\|_{H^1\cap H_1} + \|\delta V_1\|_H\Big) + C\|w(t)\|_{L^2}\;. \tag{27}$$

Since we want to prove that $\|w\|_{L^\infty(0,T;L^2)} \le C\|\delta V_1\|_H^2$, we have to work more on equation (20) in order to obtain an $H^1\cap H_1$ estimate on z. Actually, we could have directly proved with Theorem 3 and a Picard fixed point theorem that $z\in C([0,T];H^1\cap H_1)$. If we calculate $\mathrm{Im}\int_{\mathbb{R}^3}(20)\,.\,|x|^2\,\overline{z}(x)\,dx$, we obtain the following estimate in the usual way:

$$\begin{aligned}
\frac{d}{dt}\Big(\big\||x|\,z(t)\big\|_{L^2}^2\Big) \;\le\; & C\,\|\nabla z(t)\|_{L^2}\,\||x|\,z(t)\|_{L^2} + C\,\|\delta V_1\|_H\,\|u(t)\|_{H_1}\||x|z(t)\|_{L^2} \\
& + C\,\|\nabla u(t)\|_{L^2}\,\|u(t)\|_{H_2}\,\|z(t)\|_{H_1}^2 \\
\le\; & C\,\|\nabla z(t)\|_{L^2}^2 + C\,\|z(t)\|_{H_1}^2 + C\,\|\delta V_1\|_H\,\||x|z(t)\|_{L^2}\;.
\end{aligned}$$

Therefore, an integration on $[0,t]$ and $z(0)=0$ give

$$\begin{aligned}
\big\||x|\,z(t)\big\|_{L^2}^2 \;\le\; & C\int_0^t\|\nabla z(s)\|_{L^2}^2\,ds \;+\; C\int_0^t\|z(t)\|_{H_1}^2\,ds \\
& + C\int_0^t\|\delta V_1\|_H\,\||x|\,z(t)\|_{L^2}\,ds\;.
\end{aligned} \tag{28}$$

Now, as we need to estimate ∇z, we will calculate $\mathrm{Re}\displaystyle\int_{\mathbb{R}^3}(20)\,.\,\partial_t\overline{z}(x)\,dx$. Before, we can notice that:

$$\mathrm{Re}\int_{\mathbb{R}^3}\left(|u|^2\star\frac{1}{|x|}\right)z\,\partial_t\overline{z} \;=\; \frac{1}{2}\,\frac{d}{dt}\left(\int_{\mathbb{R}^3}\left(|u|^2\star\frac{1}{|x|}\right)|z|^2\right)-\int_{\mathbb{R}^3}\left(\mathrm{Re}(u\partial_t\overline{u})\star\frac{1}{|x|}\right)|z|^2$$

and

$$\begin{aligned}
2\,\mathrm{Re}\int_{\mathbb{R}^3}&\left(\mathrm{Re}(u\overline{z})\star\frac{1}{|x|}\right)u\,\partial_t\overline{z} \;= \\
&= \frac{d}{dt}\left(\int_{\mathbb{R}^3}\left(\mathrm{Re}(u\overline{z})\star\frac{1}{|x|}\right)\mathrm{Re}(u\overline{z})\right) \;-\; 2\int_{\mathbb{R}^3}\left(\mathrm{Re}(u\overline{z})\star\frac{1}{|x|}\right)\mathrm{Re}(\overline{z}\,\partial_t u)\;.
\end{aligned}$$

After some calculations and integrations by parts, we obtain

$$\begin{aligned}
\frac{d}{dt}&\left(\int_{\mathbb{R}^3}V_0|z|^2+\int_{\mathbb{R}^3}V_1|z|^2-\int_{\mathbb{R}^3}|\nabla z|^2\right) \;= \\
&= \int_{\mathbb{R}^3}\partial_t V_0|z|^2+\int_{\mathbb{R}^3}\partial_t V_1|z|^2 \;-\; 2\,\frac{d}{dt}\left(\int_{\mathbb{R}^3}\delta V_1\,\mathrm{Re}(u\overline{z})\right) \\
&\quad + 2\int_{\mathbb{R}^3}\partial_t(\delta V_1)\,\mathrm{Re}(u\overline{z}) \;+\; 2\int_{\mathbb{R}^3}\delta V_1\,\mathrm{Re}(\partial_t u\;\overline{z}) \;+\; \frac{d}{dt}\left(\int_{\mathbb{R}^3}\left(|u|^2\star\frac{1}{|x|}\right)|z|^2\right) \\
&\quad - 2\int_{\mathbb{R}^3}\left(\mathrm{Re}(u\partial_t\overline{u})\star\frac{1}{|x|}\right)|z|^2 \;+\; 2\,\frac{d}{dt}\left(\int_{\mathbb{R}^3}\left(\mathrm{Re}(u\overline{z})\star\frac{1}{|x|}\right)\mathrm{Re}(u\overline{z})\right) \\
&\quad - 4\int_{\mathbb{R}^3}\left(\mathrm{Re}(u\overline{z})\star\frac{1}{|x|}\right)\mathrm{Re}(\overline{z}\,\partial_t u)\;.
\end{aligned}$$

We recall here that $V_0(x,t)=\dfrac{1}{|x-a(t)|}$ with $a\in W^{2,1}(0,T;\mathbb{R}^3)$ thus we have $|\partial_t V_0(x,t)|=\dfrac{|\partial_t a(t)|}{|x-a(t)|^2}$. We also remind Hardy's inequality for $u\in H^1(\mathbb{R}^3)$:

$$\int_{\mathbb{R}^3}\frac{|u(x)|^2}{|x|^2}\,dx \;\leq\; 4\int_{\mathbb{R}^3}|\nabla u(x)|^2\,dx\;.$$

Therefore we obtain

$$\begin{aligned}
\frac{d}{dt}\left(\int_{\mathbb{R}^3}|\nabla z(t)|\right) \;\leq\; &\frac{d}{dt}\left(\int_{\mathbb{R}^3}\big(V_0(t)+V_1(t)\big)\,|z(t)|^2 \;+\; 2\,\mathrm{Re}\int_{\mathbb{R}^3}\delta V_1(t)\,u(t)\,\overline{z}(t)\right) \\
&+\frac{d}{dt}\left(2\int_{\mathbb{R}^3}\left(\mathrm{Re}\,\big(u(t)\,\overline{z}(t)\big)\star\frac{1}{|x|}\right)\mathrm{Re}\,\big(u(t)\,\overline{z}(t)\big)\right) \\
&+\frac{d}{dt}\left(\int_{\mathbb{R}^3}\left(|u(t)|^2\star\frac{1}{|x|}\right)|z(t)|^2\right) \\
&+C\,\|\nabla z(t)\|_{L^1}^2+C\,\|V_1\|_H\,\||x|\,z(t)\|_{L^2}^2 \\
&+C\,\|\partial_t u(t)\|_{L^2}\,\|\nabla u(t)\|_{L^2}\,\|z(t)\|_{L^2} \\
&+C\,\|\delta V_1\|_H\Big(\|u(t)\|_{L^2}+\|\partial_t u(t)\|_{L^2}\Big)\,\||x|\,z(t)\|_{L^2}\;.
\end{aligned}$$

We integrate this, between 0 and $t \in [0,T]$, using $z(0)=0$, $u \in L^\infty(0,T;H^2\cap H_2)$ and $\partial_t u \in L^\infty(0,T;L^2)$. We obtain:

$$\begin{aligned}\|\nabla z(t)\|_{L^2}^2 \le &\int_{\mathbb{R}^3} \big(V_0(t)+V_1(t)\big)\,|z(t)|^2 \,+\, 2\int_{\mathbb{R}^3} |\delta V_1(t)|\,|u(t)|\,|z(t)| \\ &+ 2\int_{\mathbb{R}^3}\left(|u(t)|\,|z(t)| \star \frac{1}{|x|}\right)|u(t)|\,|z(t)| \,+\, \int_{\mathbb{R}^3}\left(|u(t)|^2 \star \frac{1}{|x|}\right)|z(t)|^2 \\ &+ C\int_0^t \Big(\|\nabla z(s)\|_{L^2}^2 + \|z(s)\|_{H_1}^2\Big)\,ds \,+\, C\,\|\delta V_1\|_H \int_0^t \|z(s)\|_{H_1}\,ds\ .\end{aligned}$$

We set

$$E(t) \,=\, \|z(t)\|_{H^1}^2 + \|z(t)\|_{H_1}^2 \,=\, \int_{\mathbb{R}^3}\big(1+|x|^2\big)\,|z(t,x)|^2\,dx \,+\, \int_{\mathbb{R}^3}\big|\nabla z(t,x)\big|^2\,dx\ .$$

Moreover, we remind that we have (24) and (28) and adding this to (29), we get, for all t in $[0,T]$,

$$\begin{aligned}E(t) \,\le\, &C\,\|\delta V_1\|_H \int_0^t \sqrt{E(s)}\;ds \,+\, C\int_0^t E(s)\,ds \\ &+ \int_{\mathbb{R}^3}\big(V_0(t)+V_1(t)\big)\,|z(t)|^2 \,+\, C\,\|\delta V_1\|_H\,\|u(t)\|_{H_1}\|z(t)\|_{L^2} \\ &+ C\,\|u(t)\|_{L^2}\,\|u(t)\|_{H^1}\|z(t)\|_{L^2}^2\ .\end{aligned}$$

Then, we can prove that for all $\eta>0$ there exists a constant $C_\eta>0$ such that

$$\int_{\mathbb{R}^3}\big(V_0(t)+V_1(t)\big)\,|z(t)|^2 \,\le\, C_\eta\|z(t)\|_{L^2}^2 + \eta\|z(t)\|_{H^1\cap H_1}^2\ . \tag{29}$$

Indeed, from Cauchy–Schwarz and Hardy's inequalities, we have

$$\int_{\mathbb{R}^3} V_0(t)\,|z(t)|^2 \,\le\, \int_{\mathbb{R}^3}\frac{|z(t)|^2}{|x-a(t)|} \,\le\, C\,\|z(t)\|_{H^1}\|z(t)\|_{L^2}\ ,$$

$$\int_{\mathbb{R}^3} V_1(t)\,|z(t)|^2 \,\le\, \|V_1\|_H \int_{\mathbb{R}^3}\big(1+|x|^2\big)^{\frac12}\,|z(t)|^2 \,\le\, \|V_1\|_H\,\|z(t)\|_{L^2}\,\|z(t)\|_{H_1}$$

and we obtain (29) from Young's inequality. Consequently, if we choose η small enough, we obtain

$$E(t) \,\le\, C\,\|\delta V_1\|_H \int_0^t \sqrt{E(s)}\,ds \,+\, C\int_0^t E(s)\,ds \,+\, C_\eta\|z(t)\|_{L^2}^2 + C\,\|\delta V_1\|_H\,\|z(t)\|_{L^2}$$

and using (25), we get

$$E(t) \,\le\, C\,\|\delta V_1\|_H \int_0^t \sqrt{E(s)}\,ds \,+\, C\int_0^t E(s)\,ds \,+\, C\,\|\delta V_1\|_H^2\ .$$

We recall that here again, C denotes various positive constants, depending only on the time T. We set

$$F(t) \;=\; \|\delta V_1\|_H \int_0^t \sqrt{E(s)}\, ds \;+\; \int_0^t E(s)\, ds \;+\; \|\delta V_1\|_H^2 \;.$$

We have both

$$\begin{aligned} E(t) \;&\leq\; C\, F(t) \quad \text{ and} \\ \frac{dF}{dt}(t) \;&=\; E(t) + \|\delta V_1\|_H \sqrt{E(t)} \\ &\leq\; C\, F(t) + C\, \|\delta V_1\|_H \sqrt{F(t)} \;. \end{aligned}$$

Then, $\dfrac{d}{dt}\left(e^{-Ct}\sqrt{F(t)}\right) \leq e^{-Ct}\, C\, \|\delta V_1\|_H$ and we obtain after an integration in time:

$$\forall\, t \in (0,T)\,, \qquad F(t) \leq C\, \|\delta V_1\|_H^2 \;.$$

This implies that there exists a constant $C_T > 0$ such that

$$\forall\, t \in (0,T)\,, \qquad E(t) = \|z(t)\|^2_{H^1 \cap H_1} \leq C_T \|\delta V_1\|_H^2 \;.$$

Eventually, we have proved that,

$$\sup_{t\in[0,T]} \Big(\big\| \big(1+|x|\big)\, z(t) \big\|_{L^2} + \|\nabla z(t)\|_{L^2} \Big) \xrightarrow{\|\delta V_1\|_H \to 0} 0 \;.$$

Now, using this in (27), we obtain

$$\frac{d}{dt}\big(\|w(t)\|_{L^2}\big) \;\leq\; C\, \|\delta V_1\|_H^2 + C\, \|w(t)\|_{L^2}$$

and applying Gronwall lemma we get: $\forall\, t \in [0,T]$, $\|w(t)\|_{L^2} \leq C_T \|\delta V_1\|_H^2$. Therefore, we have

$$\|w(T)\|_{L^2} = o\big(\|\delta V_1\|_H\big)$$

and the proof of Lemma 8 is complete. ∎

3 – Optimal control of the coupled system

We recall the coupled system (1) we are considering:

$$\begin{cases} i\,\partial_t u + \Delta u + \dfrac{u}{|x-a|} + V_1 u \;=\; \left(|u|^2 \star \dfrac{1}{|x|}\right) u\,, & \text{in } \mathbb{R}^3\times(0,T) \\ u(0) = u_0\,, & \text{in } \mathbb{R}^3 \\ m\,\dfrac{d^2a}{dt^2} \;=\; \displaystyle\int_{\mathbb{R}^3} -|u(x)|^2\,\nabla\frac{1}{|x-a|}\,dx \;-\; \nabla V_1(a)\,, & \text{on } (0,T) \\ a(0) = a_0\,, \quad \dfrac{da}{dt}(0) = v_0\;. \end{cases}$$

The electric potential V_1 takes its values in $\mathbb{R}$ and satisfy assumption (2):

$$\begin{aligned} \big(1+|x|^2\big)^{-\frac12} V_1 \;&\in\; L^\infty\big((0,T)\times\mathbb{R}^3\big)\;, \\ \big(1+|x|^2\big)^{-\frac12} \partial_t V_1 \;&\in\; L^1(0,T;L^\infty)\;, \\ \big(1+|x|^2\big)^{-\frac12} \nabla V_1 \;&\in\; L^1(0,T;L^\infty)\;, \\ \nabla V_1 \;&\in\; L^2\big(0,T;W^{1,\infty}_{\text{loc}}\big)\;. \end{aligned} \tag{30}$$

On this evolution system we define the following optimal control problem:

If (u,a) is a solution of system (1) and if $u_1 \in L^2$ is a given target, find a minimizer $V_1 \in \mathcal{H}$ for

$$\inf\Big\{J(V,u),\;\; V\in\mathcal{H}\Big\}$$

where the cost functionnal J is defined by

$$J(V_1,u) \;=\; \frac12\int_{\mathbb{R}^3} \big|u(T,x) - u_1(x)\big|^2\,dx \;+\; \frac{r}{2}\,\|V_1\|^2_{\mathcal{H}}$$

and

$$\mathcal{H} \;=\; \Big\{V,\;\; \big(1{+}|x|^2\big)^{-\frac12} V \in H^1(0,T;\mathcal{W}) \;\text{ and }\; \nabla V \in L^2\left(0,T;W^{1,\infty}\right)\Big\}$$

where $\mathcal{W}$ is an Hilbert space which satisfies $\mathcal{W} \hookrightarrow W^{1,\infty}(\mathbb{R}^3)$.

We are now going to prove Theorem 1 and we will make, at the end of the proof, a remark about the obtaining an optimality condition.

Proof of Theorem 1: We consider a minimizing sequence $(V_1^n)_{n\ge0}$ in $\mathcal{H}$ for the functional J. It means that

$$\inf\Big\{J(V,u),\;\; V\in\mathcal{H}\Big\} \;=\; \lim_{n\to\infty} J(V_1^n,u_n)$$

where $(u_n, a_n) \in \big(W^{1,\infty}(0,T;L^2) \cap L^\infty(0,T;H^2 \cap H_2)\big) \times W^{2,1}(0,T)$ is solution of

$$
(31) \qquad \begin{cases}
i\,\partial_t u_n + \Delta u_n + \dfrac{u_n}{|x-a_n|} + V_1^n u_n = \left(|u_n|^2 \star \dfrac{1}{|x|}\right) u_n \,, & \text{in } \mathbb{R}^3\times(0,T) \\
u_n(0) = u_0 \,, & \text{in } \mathbb{R}^3 \\
m\,\dfrac{d^2 a_n}{dt^2} = \displaystyle\int_{\mathbb{R}^3} -|u_n(x)|^2\, \nabla \frac{1}{|x-a_n|}\; dx \;-\; \nabla V_1^n(a_n)\,, & \text{on } (0,T) \\
a_n(0) = a_0\,, \qquad \dfrac{da_n}{dt}(0) = v_0\;.
\end{cases}
$$

Since

$$
J(V_1^n, u_n) \;=\; \frac{1}{2}\int_{\mathbb{R}^3} \big|u_n(T,x) - u_1(x)\big|^2\, dx \;+\; \frac{r}{2}\,\|V_1^n\|_{\mathcal{H}}^2\;,
$$

we then obtain that $(V_1^n)_{n\geq 0}$ is bounded in $\mathcal{H}$, independently of n. Up to a subsequence, we have $V_1^n \rightharpoonup V_1$ weakly in $\mathcal{H}$ and

$$
\|V_1\|_{\mathcal{H}} \;\leq\; \underline{\lim}\, \|V_1^n\|_{\mathcal{H}}\;.
$$

The difficulty comes again from the term $\|u_n(T) - u_1\|_{L^2}^2$. We will prove that the limit (u,a) of $(u_n,a_n)_{n\in\mathbb{N}}$ is a solution of system (1) associated with V_1. If we consider a solution (u_n,a_n) of system (31), since the sequence of the electric potentials (V_1^n) is bounded in $\mathcal{H}$, we can apply Theorem 2 and obtain that the sequence (u_n,a_n) is bounded in

$$
\Big(W^{1,\infty}(0,T;L^2) \cap L^\infty(0,T;H^2 \cap H_2)\Big) \times W^{2,1}(0,T)
$$

independently of n. We get $a_n \to a$ in $L^\infty(0,T)$ strongly and $u_n \rightharpoonup u$ weak in $C([0,T],L^2)$.

Therefore, since the application $u \mapsto \|u(T)-u_1\|_{L^2}^2$ is lower semi-continuous, then $u_n(T) \rightharpoonup u(T)$ weak in $L^2(\mathbb{R}^3)$ implies

$$
\|u(T)-u_1\|_{L^2}^2 \;\leq\; \underline{\lim}\, \|u_n(T)-u_1\|_{L^2}^2
$$

and we finally obtain

$$
J(V_1,u) \;\leq\; \underline{\lim}\, J(V_1^n,u_n) \;=\; \inf_{V\in\mathcal{H}} J(V,u)\;.
$$

Since $V_1 \in \mathcal{H}$, that leads to $J(V_1,u) = \inf_{V\in\mathcal{H}} J(V,u)$ and the existence of an optimal control is proved.

Remark. As mentioned in the introduction, we can replace $\nabla V \in L^2(0,T;W^{1,\infty})$ by $\nabla V \in L^2\big(0,T;W^{1,\infty}_{\rm loc}\big)$ in the definition of $\mathcal{H}$. Then, in the cost functional J, $\|V_1\|_{\mathcal{H}}$ has to be replaced by $\big\|(1+|x|^2)^{-\frac{1}{2}}V_1\big\|_{H^1(0,T;\mathcal{W})} + \|\nabla V_1\|_{L^2(0,T;W^{1,\infty}(B_\rho))}$ where $B_\rho = B(0,\rho) \subset \mathbb{R}^3$ and the point is to choose $\rho > 0$ conveniently. From reference [2], and as one can read in Theorem 2, we know that without any hypothesis on ∇V_1, we can bound a in $C([0,T])$. In fact, we only need $(1+|x|^2)^{-\frac{1}{2}}\, V_1 \in H^1(0,T;\mathcal{W})$. Moreover, when we consider a minimizing sequence $(V_1^n)_{n\geq 0}$ in $\mathcal{H}$, as soon as $J(V_1^n,u_n)$ is then bounded, for instance by $J(0,u_n)$, we obtain an a priori bound for $\|(1+|x|^2)^{-\frac{1}{2}}V_1\|_{H^1(0,T;\mathcal{W})}$ and then for $\|a_n\|_{C([0,T])}$. Thus, if ρ is chosen large enough to satisfy $\|a_n\|_{C([0,T])} \leq \rho$ for all $n \in \mathbb{N}$, we will be able to proceed to the same proof as follows. □

For clarity, we denote by (32) and (33) the two equations solved by u and a:

$$i\,\partial_t u + \Delta u + \frac{u}{|x-a|} + V_1 u \;=\; \left(|u|^2 \star \frac{1}{|x|}\right)u, \qquad \text{in } \; \mathbb{R}^3 \times (0,T)\;, \tag{32}$$

$$m\,\frac{d^2a}{dt^2} \;=\; -\int_{\mathbb{R}^3} |u(x)|^2\, \nabla \frac{1}{|x-a|}\, dx \;+\; \nabla V_1(a), \qquad \text{in } \; (0,T) \tag{33}$$

and we want to prove that the limit (u,a) of $(u_n,a_n)_{n\in\mathbb{N}}$ is a solution of (1).

Up to a subsequence, we have $\partial_t u_n \to \partial_t u$ and $\Delta u_n \to \Delta u$ in $\mathcal{D}'((0,T)\times\mathbb{R}^3)$. Moreover, on the one hand, since V_1 is bounded in $\mathcal{H}$, we have $\left(\dfrac{V_1^n}{(1+|x|^2)^{\frac{1}{2}}}\right)_{n\geq 0}$ bounded in $H^1(0,T;\mathcal{W})$. Since the embedding $W^{1,\infty}(\mathbb{R}^3) \hookrightarrow L^2_{\rm loc}(\mathbb{R}^3)$ is compact and since $\mathcal{W} \hookrightarrow W^{1,\infty}(\mathbb{R}^3)$, then from Lemma 7, we get the local strong convergence

$$\frac{V_1^n}{\big(1+|x|^2\big)^{\frac{1}{2}}} \xrightarrow{n\to+\infty} \frac{V_1}{\big(1+|x|^2\big)^{\frac{1}{2}}} \qquad \text{in } \; L^2(0,T;L^2_{\rm loc})\;.$$

On the other hand, $(u_n)_{n\geq 0}$ is bounded in $L^\infty(0,T;H_2)$ and since $(u_n)_{n\geq 0}$ is bounded in $L^\infty(0,T;H^2)\cap W^{1,\infty}(0,T;L^2)$, we have the local strong convergence

$$u_n \xrightarrow{n\to+\infty} u \qquad \text{in } \; L^\infty(0,T;L^2_{\rm loc})\;.$$

We have, for all $R>0$,

$$\int_0^T\!\!\int_{\mathbb{R}^3} |V_1^n u_n - V_1 u| \;\leq\; \int_0^T\!\!\int_{B_R} |V_1^n u_n - V_1 u| \;+\; \int_0^T\!\!\int_{B_R^c} |V_1^n u_n - V_1 u| \;\leq$$

$$\leq \int_0^T\!\!\int_{B_R} \left| \frac{V_1^n - V_1}{\big(1+|x|^2\big)^{\frac{1}{2}}}\ u_n\big(1+|x|^2\big)^{\frac{1}{2}} \right|$$

$$+ \ (1+R^2)^{\frac{1}{2}} \int_0^T\!\!\int_{B_R} \left| \frac{V_1}{\big(1+|x|^2\big)^{\frac{1}{2}}}\ (u_n - u) \right|$$

$$+ \ \frac{1}{\big(1+R^2\big)^{\frac{1}{2}}} \int_0^T\!\!\int_{B_R^c} \frac{|V_1^n u_n| + |V_1 u|}{\big(1+|x|^2\big)^{\frac{1}{2}}}\ \big(1+|x|^2\big)\ .$$

Then, using Cauchy–Schwarz inequality, we can prove:

$$\int_0^T\!\!\int_{B_R} \left| \frac{V_1^n - V_1}{\big(1+|x|^2\big)^{\frac{1}{2}}}\ u_n\big(1+|x|^2\big)^{\frac{1}{2}} \right| \ \leq$$

$$\leq \int_0^T \left(\int_{B_R} \frac{|V_1^n - V_1|^2}{\big(1+|x|^2\big)} \right)^{\frac{1}{2}} \left(\int_{B_R} |u_n|^2 \big(1+|x|^2\big) \right)^{\frac{1}{2}}$$

$$\leq \sqrt{T}\ \left\| (V_1^n - V_1)\big(1+|x|^2\big)^{-\frac{1}{2}} \right\|_{L^2(0,T;L^2(B_R))} \|u_n\|_{L^\infty(0,T;H_2)}$$

$$\leq C_T \left\| (V_1^n - V_1)\big(1+|x|^2\big)^{-\frac{1}{2}} \right\|_{L^2(0,T;L^2(B_R))} \xrightarrow{n\to+\infty} 0$$

and

$$(1+R^2)^{\frac{1}{2}} \int_0^T\!\!\int_{B_R} \left| \frac{V_1}{\big(1+|x|^2\big)^{\frac{1}{2}}}\ (u_n - u) \right| \ \leq$$

$$\leq C_T \left\| V_1\big(1+|x|^2\big)^{-\frac{1}{2}} \right\|_{L^2(0,T;L^2)} \|u_n - u\|_{L^\infty(0,T;L^2(B_R))}$$

$$\leq C_T \|u_n - u\|_{L^\infty(0,T;L^2(B_R))} \xrightarrow{n\to+\infty} 0$$

and for all $\varepsilon > 0$, there exists $R > 0$ such that

$$\frac{1}{(1+R^2)^{\frac{1}{2}}} \int_0^T\!\!\int_{B_R^c} \frac{|V_1^n u_n| + |V_1 u|}{\big(1+|x|^2\big)^{\frac{1}{2}}} \big(1+|x|^2\big) \ \leq$$

$$\leq \frac{2\sqrt{T}}{(1+R^2)^{\frac{1}{2}}} \left\| V_1^n\big(1+|x|^2\big)^{-\frac{1}{2}} \right\|_{L^2(0,T;L^2)} \|u_n\|_{L^\infty(0,T;H_2)}$$

$$\leq \frac{C_T}{(1+R^2)^{\frac{1}{2}}} \ \leq \ \varepsilon\ .$$

Eventually, we obtain $V_1^n u_n \to V_1 u$ in $L^1((0,T)\times\mathbb{R}^3)$.

Then, we have to work on the terms $\dfrac{u_n}{|x-a_n|}$ and $\left(|u_n|^2 \star \dfrac{1}{|x|}\right) u_n$ of system (31). One can notice that $(a_n)_{n\geq 0}$ is bounded in $W^{2,1}(0,T)$. We then have, up to a subsequence, the strong convergence $a_n \xrightarrow{n\to+\infty} a$ in $L^\infty(0,T)$. We will check later that a, together with u, is a solution of coupled system (1). We set $\varphi \in \mathcal{D}((0,T)\times\mathbb{R}^3)$ which means in particular that $\operatorname{Supp}\varphi$ is a compact set of $(0,T)\times\mathbb{R}^3$.

We have

$$\frac{u_n}{|x-a_n|} = \left(\frac{1}{|x-a_n|} - \frac{1}{|x-a|}\right) u_n + \frac{u_n}{|x-a|}$$

and we will prove that in $\mathcal{D}'((0,T)\times\mathbb{R}^3)$, we have the following convergences

$$\frac{u_n}{|x-a|} \xrightarrow{n\to+\infty} \frac{u}{|x-a|} \quad \text{and} \quad \left(\frac{1}{|x-a_n|} - \frac{1}{|x-a|}\right) u_n \xrightarrow{n\to+\infty} 0\ .$$

On the one hand, since $\operatorname{Supp}\varphi$ is compact, from Hardy's inequality we have

$$\left| \int_{[0,T]\times\mathbb{R}^3} \frac{\big(u_n(t,x) - u(t,x)\big)\,\varphi(t,x)}{\big|x-a(t)\big|}\ dt\,dx \right| \leq C\, \|u_n - u\|_{L^\infty(0,T;H^1(B_R))}$$

where $\operatorname{Supp}\varphi \subset (0,T)\times B_R$ and $(u_n)_{n\geq 0}$ being bounded in the space $L^\infty(0,T;H^2) \cap W^{1,\infty}(0,T;L^2)$ gives the local strong convergence

$$u_n \xrightarrow{n\to+\infty} u \qquad \text{in } C\big([0,T];H^1_{\text{loc}}\big)\,.$$

Then $\|u_n - u\|_{L^\infty(0,T;H^1(B_R))} \to 0$ and we get $\dfrac{u_n}{|x-a|} \xrightarrow{n\to+\infty} \dfrac{u}{|x-a|}$ in $\mathcal{D}'$.

On the other hand, for the same reasons, we have

$$\begin{aligned}
&\left| \int_{[0,T]\times\mathbb{R}^3} \left(\frac{1}{|x-a_n(t)|} - \frac{1}{|x-a(t)|}\right) u_n(t,x)\,\varphi(t,x)\ dt\,dx \right| \leq \\
&\qquad \leq \int_{[0,T]\times\mathbb{R}^3} \frac{|u_n(t,x)|\,|\varphi(t,x)|\,|a_n(t)-a(t)|}{|x-a_n(t)|\,|x-a(t)|}\ dt\,dx \\
&\qquad \leq \|u_n\|_{L^\infty(0,T;H^1(B_R))}\ |a_n - a|_{L^\infty(0,T)} \left(\int_{\operatorname{Supp}\varphi} \frac{|\varphi(t,x)|^2}{|x-a(t)|^2}\ dt\,dx\right)^{\frac{1}{2}} \\
&\qquad \leq C\,|a_n - a|_{L^\infty(0,T)} \xrightarrow{n\to+\infty} 0
\end{aligned}$$

which means $\left(\dfrac{1}{|x-a_n|} - \dfrac{1}{|x-a|}\right) u_n \xrightarrow{n\to+\infty} 0$ in $\mathcal{D}'$.

Finally, we are going to prove that $\left(|u_n|^2 \star \frac{1}{|x|}\right)u_n - \left(|u|^2 \star \frac{1}{|x|}\right)u \xrightarrow{n\to+\infty} 0$ in $\mathcal{D}'((0,T)\times\mathbb{R}^3)$. We have

$$\left(|u_n|^2\star\frac{1}{|x|}\right)u_n-\left(|u|^2\star\frac{1}{|x|}\right)u \;=\; \left(|u_n|^2\star\frac{1}{|x|}\right)(u_n-u)+\left(\left(|u_n|^2-|u|^2\right)\star\frac{1}{|x|}\right)u\,.$$

First of all, using Cauchy–Schwarz inequality and omitting the time t fixed in $[0,T]$, we can write

$$\begin{aligned}
&\int_{\mathbb{R}^3}|\varphi|\left|\left(|u_n|^2\star\frac{1}{|x|}\right)u_n-\left(|u|^2\star\frac{1}{|x|}\right)u\right|\,dx \;\le\\
&\quad\le \int_{\mathbb{R}^3}|\varphi|\,|u_n-u|\left(|u_n|^2\star\frac{1}{|x|}\right)dx + \int_{\mathbb{R}^3}|\varphi|\,|u|\left(\left(|u_n|+|u|\right)|u_n-u|\star\frac{1}{|x|}\right)dx\\
&\quad\le \left(\int_{\mathbb{R}^3}|\varphi|\,|u_n-u|^2\,dx\right)^{\frac12}\left(\int_{\mathbb{R}^3}|\varphi|\left(|u_n|^2\star\frac{1}{|x|}\right)^2dx\right)^{\frac12}\\
&\qquad+\left(\int_{\mathbb{R}^3}|u|^2\,dx\right)^{\frac12}\left(\int_{\mathbb{R}^3}|\varphi|^2\left(\left(|u_n|+|u|\right)|u_n-u|\star\frac{1}{|x|}\right)^2dx\right)^{\frac12}
\end{aligned}$$

which gives

$$\begin{aligned}
&\int_{\mathbb{R}^3}|\varphi|\left|\left(|u_n|^2\star\frac{1}{|x|}\right)u_n-\left(|u|^2\star\frac{1}{|x|}\right)u\right|\,dx \;\le\\
&\qquad\le \|u_n-u\|_{L^2(B_R)}\left(\int_{\mathbb{R}^3}|\varphi|\left(|u_n|^2\star\frac{1}{|x|}\right)^2dx\right)^{\frac12}\\
&\qquad\quad+\|u\|_{L^2}\left(\int_{\mathbb{R}^3}|\varphi|^2\left(\left(|u_n|+|u|\right)|u_n-u|\star\frac{1}{|x|}\right)^2dx\right)^{\frac12}.
\end{aligned}\tag{34}$$

Next, from Hardy's inequality, we have

$$\left(|u_n|^2\star\frac{1}{|x|}\right)(x)\;\le\;\|u_n\|_{L^2}\,\|\nabla u_n\|_{L^2}\,,\qquad \forall\, x\in\mathbb{R}^3$$

and since $\varphi\in\mathcal{D}((0,T)\times\mathbb{R}^3)$,

$$\left(\int_{\mathbb{R}^3}\varphi(x)\left(|u_n|^2\star\frac{1}{|x|}\right)^2(x)\;dx\right)^{\frac12}\;\le\; C\,\|u_n\|_{H^1}^2\,.\tag{35}$$

We will also need the following:

Lemma 9. *Let $r>0$, $v\in H^1$ and $v_n\in L^2$. If we assume that $v_n \xrightarrow{n\to+\infty} 0$ in $L^2_{\rm loc}$, then*

$$\forall\,|x|<r\ ,\qquad \int_{\mathbb{R}^3}\frac{v(y)\,v_n(y)}{|x-y|}\,dy \ \xrightarrow{n\to+\infty}\ 0\ .$$

Proof: We set $R>r$ and $B_R=\{y\in\mathbb{R}^3,\ |y|<R\}$. From Cauchy–Schwarz and Hardy's inequalities, we obtain for all x such that $|x|<r$,

$$\begin{aligned}\left|\int_{\mathbb{R}^3}\frac{v(y)\,v_n(y)}{|x-y|}\,dy\right| &\le \int_{B_R}\frac{|v(y)|\,|v_n(y)|}{|x-y|}\,dy+\int_{B_R^c}\frac{|v(y)|\,|v_n(y)|}{|y-x|}\,dy\\ &\le \|v\|_{H^1}\|v_n\|_{L^2(B_R)}+\frac{1}{R-|x|}\,\|v\|_{L^2}\,\|v_n\|_{L^2}\\ &\le C\left(\|v_n\|_{L^2(B_R)}+\frac{1}{R-r}\right).\end{aligned}$$

Moreover, if we set $\varepsilon>0$, then there exists $n_0\in\mathbb{N}$ and $R_0>0$ such that

$$\frac{C}{R_0-r}\le\frac{\varepsilon}{2}\qquad\text{and}\qquad \forall\,n>n_0,\quad C\,\|v_n\|_{L^2(B_{R_0})}\le\frac{\varepsilon}{2}\ .$$

Thus, for all $\varepsilon>0$ there exists $n_0\in\mathbb{N}$ such that for all $n>n_0$,

$$\left|\int_{\mathbb{R}^3}\frac{v(y)\,v_n(y)}{|x-y|}\,dy\right|\ \le\ \varepsilon$$

and the lemma has been proved. ∎

We use this result to deal with the term $\displaystyle\int_{\mathbb{R}^3}\varphi^2\left(\big(|u_n|+|u|\big)\,|u_n-u|\star\frac{1}{|x|}\right)^2$. Let $t\in(0,T)$ be fixed. Since $\operatorname{Supp}\varphi$ is compact, we apply Lebesgue's theorem on a bounded domain to the sequence $\big(f_n(t)\big)_{n\in\mathbb{N}}$ defined by

$$f_n(x,t)\ =\ \left(\Big(|u_n(t)|+|u(t)|\Big)\,\big|u_n(t)-u(t)\big|\star\frac{1}{|x|}\right)^2(x)\ .$$

Indeed, since $u_n-u\xrightarrow{n\to+\infty}0$ in $C([0,T];L^2_{\rm loc})$, $u\in L^\infty(0,T;H^1)$ and u_n is bounded in $L^\infty(0,T;H^1)$ independently of n, using Lemma 9 we obtain that for all t in $[0,T]$ and for all x in $\operatorname{Supp}\varphi$, $f_n(x,t)\to0$. Then, from usual estimates we prove that $|f_n(t)|\le C\in L^1_{\rm loc}(\mathbb{R}^3)$ and we finally get: $\forall\,t\in[0,T]$,

$$\int_{\mathbb{R}^3}\varphi^2(t,x)\,f_n(x,t)\ dx\ =\ I_n(t)\ \xrightarrow{n\to+\infty}\ 0\ . \tag{36}$$

Now, plugging (35) and (36) in (34) we obtain, for all t in $[0,T]$,

$$\int_{\mathbb{R}^3} \varphi(t) \left| \left(|u_n(t)|^2 \star \frac{1}{|x|} \right) u_n(t) - \left(|u(t)|^2 \star \frac{1}{|x|} \right) u(t) \right| \le$$

$$\le C \, \|u_n\|^2_{L^\infty(0,T;H^1)} \, \|u_n - u\|_{L^\infty(0,T;L^2(B_R))} + \|u\|_{L^\infty(0,T;L^2)} \sqrt{I_n(t)}$$

$$\le C \left(\|u_n - u\|_{L^\infty(0,T;L^2(B_R))} + \sqrt{I_n(t)} \right) \xrightarrow{n \to +\infty} 0 \, .$$

Thus we have proved

$$\left(|u_n|^2 \star \frac{1}{|x|} \right) u_n - \left(|u|^2 \star \frac{1}{|x|} \right) u \xrightarrow{n \to +\infty} 0 \quad \text{ in } \mathcal{D}'\big((0,T) \times \mathbb{R}^3\big) \, .$$

Therefore, we have all the elements to insure that (u_n) is converging in a weak sense towards u which is a solution of (32) in the sense of distributions. We finally have to prove that the limit a of the sequence (a_n) is a solution of (33). We already know that $(a_n)_{n \ge 0}$ is bounded in $W^{2,1}(0,T)$ and that $a_n \to a$ in $L^\infty(0,T)$ and we have in [0,T],

$$m \frac{d^2 a_n}{dt^2} = \int_{\mathbb{R}^3} -|u_n(x)|^2 \, \nabla \frac{1}{|x - a_n|} \, dx + \nabla V_1^n(a_n) \, .$$

On the one hand, omitting again the fixed time t in $[0,T]$, we have

$$\nabla V_1^n(a_n) - \nabla V_1(a) = \Big(\nabla V_1^n(a_n) - \nabla V_1^n(a) \Big) + \Big(\nabla V_1^n(a) - \nabla V_1(a) \Big)$$

and of course, since V_1^n is bounded in $\mathcal{H}$ and $V_1^n \rightharpoonup V_1$ weakly in $\mathcal{H}$, we get

$$\nabla V_1^n(a) - \nabla V_1(a) \xrightarrow{n \to +\infty} 0 \quad \text{ in } \mathcal{D}'(0,T) \, ,$$

$$\big\| \nabla V_1^n(a_n) - \nabla V_1^n(a) \big\|_{L^2(0,T)} \le \|\nabla V_1^n\|_{L^2(0,T;W^{1,\infty})} \, |a_n - a|_{L^\infty(0,T)} \xrightarrow{n \to +\infty} 0 \, .$$

Therefore we obtain

$$\nabla V_1^n(a_n) \to \nabla V_1(a) \quad \text{ in } \mathcal{D}'(0,T) \, .$$

On the other hand, using the idea of the proof of Lemma 9 we will prove

$$\int_{\mathbb{R}^3} |u_n(x)|^2 \, \nabla \frac{1}{|x - a_n|} \, dx \xrightarrow{n \to +\infty} \int_{\mathbb{R}^3} |u(x)|^2 \, \nabla \frac{1}{|x - a|} \, dx \quad \text{ in } \mathcal{D}'(0,T) \, .$$

Actually for all t in $[0,T]$, we can prove that an integration by parts gives

$$\left|\int_{\mathbb{R}^3} |u_n(t,x)|^2 \, \nabla \frac{1}{|x-a_n(t)|} \, dx - \int_{\mathbb{R}^3} |u(t,x)|^2 \, \nabla \frac{1}{|x-a(t)|} \, dx\right| \le$$

$$\le \left|\int_{\mathbb{R}^3} |u_n|^2 \, \nabla \left(\frac{1}{|x-a_n|} - \frac{1}{|x-a|}\right) dx\right| + \left|\int_{\mathbb{R}^3} \left(|u_n|^2 - |u|^2\right) \nabla \frac{1}{|x-a|} \, dx\right| \tag{37}$$

$$\le C \int_{\mathbb{R}^3} \left(|u_n| \, |\nabla u_n| \left| \frac{1}{|x-a_n|} - \frac{1}{|x-a|}\right| + \frac{\left(|u_n| + |u|\right) |u_n - u|}{|x-a|^2} \right) dx \,.$$

Since u_n is bounded in $L^\infty(0,T;H^2)$, using Cauchy–Schwarz and Hardy's inequality we are able to deal with the first right hand side term. Indeed,

$$\begin{aligned}
\int_{\mathbb{R}^3} |u_n(t)| \, |\nabla u_n(t)| \left| \frac{1}{|x-a_n(t)|} - \frac{1}{|x-a(t)|}\right| \le& \\
&\le \int_{\mathbb{R}^3} \frac{|u_n| \, |\nabla u_n|}{|x-a_n| \, |x-a|} \, |a_n - a| \\
&\le \|u_n\|_{L^2(0,T;H^1)} \, \|\nabla u_n\|_{L^2(0,T;H^1)} \, |a_n - a|_{L^\infty(0,T)} \\
&\le \|u_n\|^2_{L^\infty(0,T;H^2)} \, |a_n - a|_{L^\infty(0,T)} \\
&\le C \, |a_n - a|_{L^\infty(0,T)} \xrightarrow{n\to+\infty} 0 \,.
\end{aligned} \tag{38}$$

Now, since a is bounded on $(0,T)$, $u_n - u \xrightarrow{n\to+\infty} 0$ in $C([0,T];H^1_{\mathrm{loc}})$, u belongs to $L^\infty(0,T;H^1)$ and u_n is bounded in $L^\infty(0,T;H^1)$ independently of n, then we obtain in an analogous way as in the proof of Lemma 9 that for all t in $[0,T]$,

$$\int_{\mathbb{R}^3} \frac{\Big(|u_n(t)| + |u(t)|\Big) \, |u_n(t) - u(t)|}{\big|x - a(t)\big|^2} \, dx = J_n(t) \xrightarrow{n\to+\infty} 0 \,. \tag{39}$$

In fact, omitting the time t, we have from Hardy's inequality

$$\begin{aligned}
J_n &\le \int_{B_R} \frac{\left(|u_n| + |u|\right) |u_n - u|}{|x-a|^2} \, dx + \int_{B_R^c} \frac{\left(|u_n| + |u|\right)^2}{|x-a|^2} \, dx \\
&\le \Big(\|u\|_{H^1} + \|u_n\|_{H^1} \Big) \, \|u_n - u\|_{H^1(B_R)} + \frac{2}{R - |a(t)|} \Big(\|u\|^2_{L^2} + \|u_n\|^2_{L^2} \Big) \\
&\le C \left(\|u_n - u\|_{H^1(B_R)} + \frac{1}{R - \|a\|_{L^\infty(0,T)}} \right)
\end{aligned}$$

and we can prove (see Lemma 9) that for all t in $[0,T]$ and for all $\varepsilon > 0$, there exists $n_0 \in \mathbb{N}$ such that for all $n > n_0$, $J_n(t) \le \varepsilon$.

Thus, using (38) and (39) together with (37), we get, for all t in $[0,T]$,

$$\left| \int_{\mathbb{R}^3} |u_n(t,x)|^2 \, \nabla \frac{1}{|x-a_n(t)|} \, dx - \int_{\mathbb{R}^3} |u(t,x)|^2 \, \nabla \frac{1}{|x-a(t)|} \, dx \right| \leq$$
$$\leq \; C \, |a_n - a|_{L^\infty(0,T)} + J_n(t) \; \xrightarrow{n\to+\infty} \; 0$$

and we finally obtain the awaited result.

We then have proved that a is a solution of (33). As a consequence, the limit (u,a) of (u_n,a_n) is a solution in the sense of distribution of system (1). Moreover, since (u,a) belongs to the class $\big(W^{1,\infty}(0,T;L^2) \cap L^\infty(0,T;H^2 \cap H_2)\big) \times W^{2,1}(0,T)$, then it satisfies the estimate (4) of Theorem 2 and is in fact a strong solution of system (1).

Hence the proof of Theorem 1. ∎

Remark. First order optimality condition. As we did in the case when the position a of the nucleus is known (Section 2.2.2), we would like to give an optimality condition for the optimal control V_1. A first step is to study the differentiability of the functional

$$\begin{aligned} \Phi\colon\; \widetilde{\mathcal{H}} &\longrightarrow L^\infty\big(0,T;L^2(\mathbb{R}^3)\big) \times L^\infty(0,T) \\ V_1 &\longmapsto \big(u(V_1), a(V_1)\big) \;, \end{aligned}$$

where $\widetilde{\mathcal{H}}$ is an appropriate Hilbert space. One can notice that the lack of proof for the uniqueness of the solution (u,a) of system (1) makes the study of optimality conditions completely formal. It is a first and main obstacle to prove the differentiability with respect to V_1 of Φ and of the cost functional

$$J\colon\; (V_1,u) \;\mapsto\; \frac{1}{2} \left\|u(T) - u_1\right\|^2_{L^2} + \frac{r}{2} \left\|V_1\right\|^2_{\widetilde{\mathcal{H}}} \,.$$

Nevertheless, one can obtain a formal derivative of J and an optimal system. We present these following formal results in order to make completely explicit the difficulty encountered in trying to show the differentiability of the mapping Φ: *control* $\to$ *state* and to give the possibility to make direct computations on approximations of the optimality system after regularization of the singularities.

Thus, assuming that we have uniqueness of the solution of system (1) and assuming that Φ is differentiable, if we set $D\Phi(\delta V_1) = (z,b)$, then one can prove that $\big(z(t,x),b(t)\big)$ has to satisfy the following coupled system set in $\mathbb{R}^3\times(0,T)$

$$\begin{cases} i\,\partial_t z+\Delta z+V_0 z+V_1 z \;=\; -\dfrac{\partial V_0}{\partial a}\cdot b\,u-\delta V_1 u+\left(|u|^2\star\dfrac{1}{|x|}\right)z+2\left(\mathrm{Re}(u\overline{z})\star\dfrac{1}{|x|}\right)u\\ z(0)=0\,,\quad b(0)=0\,,\quad \dfrac{db}{dt}(0)=0\\ m\,\dfrac{d^2b}{dt^2}\;=\;-\displaystyle\int_{\mathbb{R}^3}|u|^2\,\nabla\frac{\partial V_0}{\partial a}\cdot b\;-\;2\int_{\mathbb{R}^3}\mathrm{Re}(u\overline{z})\,\nabla V_0-\nabla\delta V_1(a)-\nabla(\nabla V_1)\cdot b(a)\end{cases}$$

where $V_0=\dfrac{1}{|x-a|}$. Thereafter, if J is differentiable with respect to V_1, we obtain that the condition $DJ(V_1,u)[\delta V_1]=0,\ \forall\,\delta V_1\in\widetilde{\mathcal{H}}$ now reads

$$\mathrm{Re}\int_{\mathbb{R}^3}\Big(u(T,x)-u_1(x)\Big)\,\overline{z}(T,x)\;dx\;+\;r\langle V_1,\delta V_1\rangle_{\widetilde{\mathcal{H}}}\;=\;0\,. \tag{40}$$

The main difficulty we encounter when trying to give a meaning to the system of equations satisfied by the couple (z,b) is of same nature than the one we had when we studied the equations solved by the difference of two solutions of system (1). Indeed, as for the proof of uniqueness which misses in Theorem 2, even in a formal study of the solutions, we have to deal with singularities of type $\frac{u}{|x|^2}$ that we cannot bound with Hardy's inequality. Moreover, the use of Marcinkiewicz (or Lorentz) spaces as in reference [5] is not directly appropriate here because of the properties of V_1. □

At last, the following formal adjoint system

$$\begin{cases} i\,\partial_t p+\Delta p+V_0 p+V_1 p \;=\; \left(|u|^2\star\dfrac{1}{|x|}\right)p+2i\,\left(\mathrm{Im}(u\overline{p})\star\dfrac{1}{|x|}\right)\overline{u}-2\,i\,\overline{u}\;\nabla V_0\cdot\varrho\\ p(T)\;=\;u(T)-u_1\\ m\,\dfrac{d^2\varrho}{dt^2}\;=\;-\displaystyle\int_{\mathbb{R}^3}\frac{\partial V_0}{\partial a}\;\mathrm{Im}(u\overline{p})\;-\;2\int_{\mathbb{R}^3}\mathrm{Re}(\overline{u}\nabla u)\,\frac{\partial V_0}{\partial a}\cdot\varrho\;-\;\nabla(\nabla V_1)(a)\cdot\varrho\\ \varrho(T)=0\,,\quad \dfrac{d\varrho}{dt}(T)=0\end{cases}$$

is such that we have

$$\mathrm{Re}\int_{\mathbb{R}^3}\overline{z(T)}\;\big(u(T)-u_1\big)\;=\;-\,\mathrm{Im}\int_0^T\!\!\int_{\mathbb{R}^3}\delta V_1 u\overline{p}\;-\;\int_0^T\varrho\cdot\nabla\delta V_1(a)\;. \tag{41}$$

Eventually, if δ_a denotes the Dirac mass at point $a\in\mathbb{R}^3$, and using (40) and (41), we prove that the bilinear optimal control V_1 is the solution of a partial differential equation defined by variational formulation: $\forall\,\delta V_1\in\widetilde{\mathcal{H}}$

$$r\langle V_1,\delta V_1\rangle_{\widetilde{\mathcal{H}}}\;=\;\int_0^T\!\!\int_{\mathbb{R}^3}\mathrm{Im}\Big(u(t,x)\,\overline{p}(t,x)\Big)\delta V_1(t,x)\;dx\,dt-\int_0^T\Big\langle\varrho(t)\cdot\nabla\delta_{a(t)},\delta V_1(t)\Big\rangle\,dt\,.$$

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