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► **To cite this version:**

Lucie Baudouin, Otared Kavian, Jean-Pierre Puel. Regularity for a Schrödinger equation with singular potentials and application to bilinear optimal control. *Journal of Differential Equations*, 2005, 216 (1), pp.188-222. hal-00145710

**HAL Id: hal-00145710**

**<https://hal.science/hal-00145710>**

Submitted on 11 May 2007

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# Regularity for a Schrödinger equation with singular potentials and application to bilinear optimal control

Lucie BAUDOUIN, Otared KAVIAN and Jean-Pierre PUEL \*

ABSTRACT : We study the Schrödinger equation  $i\partial_t u + \Delta u + V_0 u + V_1 u = 0$  on  $\mathbb{R}^3 \times (0, T)$ , where  $V_0(x, t) = |x - a(t)|^{-1}$ , with  $a \in W^{2,1}(0, T; \mathbb{R}^3)$ , is a coulombian potential, singular at finite distance, and  $V_1$  is an electric potential, possibly unbounded. The initial condition  $u_0 \in H^2(\mathbb{R}^3)$  is such that  $\int_{\mathbb{R}^3} (1 + |x|^2)^2 |u_0(x)|^2 dx < \infty$ . The potential  $V_1$  is also real valued and may depend on space and time variables. We prove that if  $V_1$  is regular enough and at most quadratic at infinity, this problem is well-posed and the regularity of the initial data is conserved for the solution. We also give an application to the bilinear optimal control of the solution through the electric potential.

*Keywords* : Schrödinger equation, singular potential, regularity, existence, bilinear optimal control, optimality condition.

*AMS Classification* : 35B65, 49J20

## 1 Introduction

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,

$\langle \cdot, \cdot \rangle_H$  stands for the scalar product in the space  $H$ ;

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

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

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We also define

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

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

We consider the following linear Schrödinger equation

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

where the potential  $V_1$  takes its values in  $\mathbb{R}$ .

Actually, this equation could correspond to the linear modelling of a hydrogen atom subjected to an external electric field, where  $u$  is the wave function of the electron. Indeed,  $V_0 = |x - a(t)|^{-1}$  is a coulombian potential, where  $a(t)$  is the position of the nucleus at instant  $t$  and  $V_1$  is the electric potential (which may be unbounded at infinity) such that  $E(t, x) = \nabla V_1(x, t)$  where  $E$  is the electric field created by a laser beam.

Our main result is the following:

**Theorem 1.** *Let  $T > 0$  be an arbitrary time and assume that the function  $a : [0, T] \longrightarrow \mathbb{R}^3$  and the potential  $V_1$  satisfy*

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

Let for some  $\alpha > 0$  and  $\rho > 0$ ,

$$\begin{aligned} \|a\|_{W^{2,1}(0, T)} &\leq \alpha \text{ and} \\ \|(1 + |x|^2)^{-1}V_1\|_{W^{1,1}(0, T, L^\infty)} + \|(1 + |x|^2)^{-1}\nabla V_1\|_{L^1(0, T, L^\infty)} &\leq \rho. \end{aligned}$$

Then there exists a positive constant  $C_{T, \alpha, \rho}$  depending on  $T$ ,  $\alpha$  and  $\rho$  such that for any  $u_0 \in H^2 \cap H_2$ , equation (1) has a unique solution  $u$  with

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

which satisfies the estimate

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

This type of result has already been obtained in the particular case when the atom is subjected to an external uniform time-dependent electric field  $I(t)$

such that in equation (1), one has  $V_1 = -I(t) \cdot x$  as in reference [4] and [7]. They both use a change of unknown function and variables (gauge transformation) to remove the electric potential from the equation such that they only have to deal with the usual Schrödinger equation with a time dependent potential like  $V_0$ . Of course, we cannot use this technique here because of the generality of the potential  $V_1$  we are considering. In the case  $V_1 = 0$ , K. YAJIMA [10] proved the  $H^2(\mathbb{R}^d)$  regularity of the solution of equation (1) considered in  $\mathbb{R}^d \times (0, T)$ , using strongly T. KATO's results in reference [8]. We can also mention that K. YAJIMA and G. ZHANG prove in [11] a smoothing property for one dimensional time dependent Schrödinger equation with potentials superquadratic at infinity, like  $V_1$ .

In order to prove Theorem 1, we will first prove an existence and regularity result for the solution of equation (1) in the space  $H^1 \cap H_1$ , actually under weaker hypothesis on  $V_1$  and  $a$ . In both proofs of the two theorems, we will regularize  $V_0$  and  $V_1$  by  $V_0^\varepsilon$  and  $V_1^\varepsilon$  and obtain accurate estimates, independent of  $\varepsilon$ . The key point in the proof of Theorem 1 is to find an  $L^2$ -estimate for the time derivative of the solution  $u^\varepsilon$ . Thus, we will use a change of variable  $y = x - a(t)$  to get rid of the time derivative of the coulombian potential which appears in the time derivative of equation (1). We finally obtain the awaited estimate which is independent of  $\varepsilon$ .

We also prove in this paper continuity results for the solution  $u$ . Indeed, under the same hypothesis, we prove the weak continuity of the solution in  $H^2 \cap H_2$  and the strong continuity in  $H_1 \cap H^1$ :

**Theorem 2.** *Under assumption (2), the solution  $u$  to equation (1) with initial condition  $u_0 \in H^2 \cap H_2$  satisfies*

$$u \in C([0, T]; H_1 \cap H^1) \quad \text{and} \quad u \in C_w([0, T]; H_2 \cap H^2).$$

(Here  $u \in C_w([0, T], H^2 \cap H_2)$  means that  $u$  is weakly continuous from  $[0, T]$  into  $H^2 \cap H_2$ ).

## 2 Preliminary estimates

As we just explained, we are going to regularize the potential of the Schrödinger equation we consider. Therefore, we need a first classical proposition to ensure the existence of smooth solution when the potential is more regular. A first step is to show that the free Schrödinger semi-group acts continuously in the space  $H^2 \cap H_2$  (resp.  $H^1 \cap H_1$ ). To be more precise, consider the equation:

$$\begin{cases} i\partial_t u(x, t) + \Delta u(x, t) = 0, & x \in \mathbb{R}^3, t \in [0, T] \\ u(x, 0) = u_0(x), & x \in \mathbb{R}^3 \end{cases} \quad (3)$$

**Lemma 3.** *Let us denote by  $(S(t))_{t \in \mathbb{R}}$  the free Schrödinger semi-group  $e^{it\Delta}$ . Then for any  $T > 0$  there exists a positive constant  $C_T$  such that if  $u_0 \in$*

$H^2 \cap H_2$ , then  $u(t) = S(t)u_0$  is the unique solution of equation (3) and satisfies  $u \in C([0, T]; H^2 \cap H_2) \cap C^1([0, T]; L^2)$  and for all  $t \in [0, T]$  we have

$$\|u(t)\|_{H^2 \cap H_2} \leq C_T \|u_0\|_{H^2 \cap H_2}.$$

**Proof.** This is a well-known result as far as the continuity in  $H^2$  is concerned (see [6]), but obtaining the continuity in  $H_2$  is not more difficult. Indeed denoting by  $\widehat{u}$  the Fourier transform of  $u$ , it is clear that  $u(t)$  satisfies equation (3) if and only if

$$\widehat{u}(t, \xi) = e^{it|\xi|^2} \widehat{u}_0(\xi).$$

From this relation, Parseval's identity and the fact that

$$\|\Delta u(t)\|_{L^2}^2 = \|\xi|^2 \widehat{u}(t)\|_{L^2}^2 = \|\xi|^2 \widehat{u}_0\|_{L^2}^2,$$

we infer that  $t \mapsto S(t)u_0$  is continuous on  $H^2$ : more precisely we have that  $u \in C(\mathbb{R}, H^2) \cap C^1(\mathbb{R}, L^2)$  (in fact for any  $s \in \mathbb{R}$  the group  $S(t)$  is an isometry on  $H^s$ ). On the other hand it is clear that

$$\| |x|^2 u(t) \|_{L^2}^2 = \|\Delta \widehat{u}(t)\|_{L^2}^2.$$

Since  $u_0 \in H^2 \cap H_2$  and

$$\Delta \widehat{u}(\xi, t) = [(6it - 4t^2|\xi|^2)\widehat{u}_0(\xi) + 4it\xi \cdot \nabla \widehat{u}_0(\xi) + \Delta \widehat{u}_0(\xi)] e^{it|\xi|^2},$$

one sees that  $t \mapsto |x|^2 u(t)$  is continuous as a mapping from  $\mathbb{R}$  into  $L^2$ . Therefore  $u \in C(\mathbb{R}, H^2 \cap H_2)$  and the lemma is proved.  $\square$

**Remark.** The same result can be proved in the same way when  $H^2 \cap H_2$  is replaced by  $H^1 \cap H_1$ .  $\square$

Next we prove that when the potential  $V \in L^\infty(0, T, C_b^2(\mathbb{R}^3))$  the following result holds (here  $C_b^2(\mathbb{R}^3)$  denotes the space of bounded  $C^2$  functions with bounded first and second derivatives):

**Proposition 4.** *If  $V \in L^\infty(0, T; C_b^2(\mathbb{R}^3))$  is real valued and if  $u_0 \in H^2 \cap H_2$  then there exists a unique solution  $u \in C([0, T]; H^2 \cap H_2)$  of*

$$\begin{cases} i\partial_t u(x, t) + \Delta u(x, t) + V(x, t)u(x, t) = 0, & x \in \mathbb{R}^3, t \in (0, T) \\ u(x, 0) = u_0(x), & x \in \mathbb{R}^3. \end{cases} \quad (4)$$

Let  $\rho > 0$  be such that  $\|V\|_{L^\infty(0, T, C_b^2(\mathbb{R}^3))} \leq \rho$ . Then there exists a positive constant  $C_{T, \rho}$  such that

$$\|u\|_{C([0, T], H^2 \cap H_2)} \leq C_{T, \rho} \|u_0\|_{H^2 \cap H_2}.$$

**Proof.** Denote by  $Y = C([0, T], H^2 \cap H_2)$  endowed with the norm

$$\|u\|_Y = \sup_{t \in [0, T]} e^{-\lambda t} \|u(t)\|_{H^2 \cap H_2}$$

for  $u \in Y$ ; here  $\lambda > 0$  is a given positive number which will be fixed hereafter. The solution of equation (4) is obtained as a mild solution, that is a solution to the integral equation

$$u(t) = S(t)u_0 + i \int_0^t S(t-s)V(s)u(s) ds.$$

We are going to show that this equation has a unique solution in  $Y$ , by proving that the operator  $\Phi$  defined as being

$$\Phi(u)(t) = S(t)u_0 + i \int_0^t S(t-s)V(s)u(s) ds$$

has a unique fixed point in a closed ball  $B_R = \{u \in Y ; \|u\|_Y \leq R\}$  for  $R$  suitably chosen.

Note that if  $V \in L^\infty(0, T; C_b^2(\mathbb{R}^3))$  with  $\|V\|_{L^\infty(0, T; C_b^2(\mathbb{R}^3))} \leq \rho$  and  $\varphi \in H^2 \cap H_2$ , there exists a positive constant  $c_0(\rho)$  such that

$$\|V(t)\varphi\|_{H^2 \cap H_2} \leq c_0(\rho)\|\varphi\|_{H^2 \cap H_2}.$$

Next we choose  $\lambda > 2c_0(\rho)C_T$  where  $C_T$  is given by Lemma 3. Then for  $u \in B_R$ , since we have

$$\|u(s)\|_{H^2 \cap H_2} \leq e^{\lambda s}\|u\|_Y \leq Re^{\lambda s},$$

by using twice Lemma 3 we obtain

$$\begin{aligned} \|\Phi(u)(t)\|_{H^2 \cap H_2} &\leq C_T \int_0^t \|V(s)u(s)\|_{H^2 \cap H_2} ds + C_T\|u_0\|_{H^2 \cap H_2} \\ &\leq C_T c_0(\rho)R \int_0^t e^{\lambda s} ds + C_T\|u_0\|_{H^2 \cap H_2}. \end{aligned}$$

It follows that if  $R > 0$  is large enough so that  $C_T\|u_0\|_{H^2 \cap H_2} \leq \frac{R}{2}$ , then

$$\|\Phi(u)\|_Y \leq \frac{c_0(\rho)C_T R}{\lambda} + C_T\|u_0\|_{H^2 \cap H_2} \leq R.$$

This means that  $\Phi$  maps  $B_R$  into itself. Also for  $u_1, u_2 \in B_R$  it is clear that

$$\begin{aligned} \|(\Phi(u_1) - \Phi(u_2))(t)\|_{H^2 \cap H_2} &\leq C_T \int_0^t \|V(s)(u_1 - u_2)(s)\|_{H^2 \cap H_2} ds \\ &\leq C_T c_0(\rho) \int_0^t e^{\lambda s} ds \|u_1 - u_2\|_Y \\ &\leq \lambda^{-1} c_0(\rho) C_T e^{\lambda t} \|u_1 - u_2\|_Y, \end{aligned}$$

and since  $\lambda$  has been appropriately chosen, this shows that  $\Phi$  is a strict contraction from  $B_R$  into itself as

$$\|(\Phi(u_1) - \Phi(u_2))\|_Y \leq \frac{c_0(\rho)C_T}{\lambda} \|u_1 - u_2\|_Y \leq \frac{1}{2} \|u_1 - u_2\|_Y,$$

and therefore  $\Phi$  has a unique fixed point, yielding the solution of equation (4). One can notice that uniqueness is not only true in  $B_R$  but also easily proved using the norm in  $C([0, T], L^2)$ .  $\square$

**Remarks.** 1) Following the same kind of arguments and the results in reference [10] of K. YAJIMA, we could also consider this proposition for potentials in  $C^1([0, T]; L^\infty(\mathbb{R}^3))$ .

2) Again, the same result can be proved in the same way when  $H^2 \cap H_2$  is replaced by  $H^1 \cap H_1$ .  $\square$

### 3 Existence and regularity result in $H^1 \cap H_1$

In this section, we will prove the following theorem, which first allows us to consider an electric potential with a growth at infinity in  $(1 + |x|^2)$ .

**Theorem 5.** *Let  $T > 0$  be an arbitrary time and let  $a$  and the potential  $V_1$  satisfy*

$$\begin{aligned} a &\in W^{1,1}(0, T), \\ (1 + |x|^2)^{-1}V_1 &\in L^\infty((0, T) \times \mathbb{R}^3) \quad \text{and} \\ (1 + |x|^2)^{-1}\partial_t V_1 &\in L^1(0, T; L^\infty) \end{aligned} \quad (5)$$

and for some  $\alpha_0 > 0$  and  $\rho_0 > 0$ :

$$\begin{aligned} \|a\|_{W^{1,1}(0, T)} &\leq \alpha_0 \quad \text{and} \\ \|(1 + |x|^2)^{-1}V_1\|_{W^{1,1}(0, T; L^\infty)} &\leq \rho_0. \end{aligned}$$

Then there exists a positive constant  $C_{T, \alpha_0, \rho_0}$  depending on  $T$ ,  $\alpha_0$  and  $\rho_0$  such that for any  $u_0 \in H^1 \cap H_1$  equation (1) has a unique solution

$$u \in L^\infty(0, T; H^1 \cap H_1)$$

which satisfies the estimate

$$\|u\|_{L^\infty(0, T; H^1 \cap H_1)} \leq C_{T, \alpha_0, \rho_0} \|u_0\|_{H^1 \cap H_1}.$$

**Proof.** First of all, we approach the potentials  $V_1$  and  $V_0 = |x - a(t)|^{-1}$  by appropriate real valued potentials  $V_0^\varepsilon$  and  $V_1^\varepsilon \in C([0, T]; C_b^2(\mathbb{R}^3))$ . More precisely:

— on the one hand, we set  $V_0^\varepsilon = \frac{1}{(\varepsilon^2 + |x - a(t)|^2)^{\frac{1}{2}}}$  and we have

$$|V_0^\varepsilon(x, t)| \leq \frac{1}{|x - a(t)|} \quad \text{and} \quad |\partial_t V_0^\varepsilon(x, t)| \leq \left| \frac{da}{dt}(t) \right| \frac{1}{|x - a(t)|^2}$$

— on the other hand, we choose  $\varrho_0 \in C_c^\infty(\mathbb{R}^3)$  and  $\chi \in C_c^\infty(\mathbb{R})$  such that for all  $x$  in  $\mathbb{R}^3$ ,  $\varrho_0(x) \geq 0$ , for all  $t$  in  $\mathbb{R}$ ,  $\chi(t) \geq 0$  and  $\int_{\mathbb{R}^3} \varrho_0(x) dx = \int_{\mathbb{R}} \chi(t) dt = 1$  and we define the truncation function

$$\begin{aligned} T_\varepsilon : \mathbb{R} &\longrightarrow \mathbb{R} \\ s &\longmapsto T_\varepsilon(s) = \frac{|s|}{s} \min(|s|, \frac{1}{\varepsilon}). \end{aligned}$$

Then, we set

$$\zeta_\varepsilon(x, t) := \frac{1}{\varepsilon^4} \chi\left(\frac{t}{\varepsilon}\right) \varrho_0\left(\frac{x}{\varepsilon}\right)$$

and we define  $V_1^\varepsilon := T_\varepsilon(V_1) \star \zeta_\varepsilon$ , where the convolution is meant in  $\mathbb{R}^3 \times \mathbb{R}$ . We have actually

$$V_1^\varepsilon(x, t) = \int_{\mathbb{R}^3 \times \mathbb{R}} T_\varepsilon(V_1(x + \varepsilon y, t + \varepsilon s)) \chi(s) \varrho_0(y) ds dy$$

and we point out that the norm of  $V_1^\varepsilon$  is bounded by the norm of  $V_1$  in the space where it is defined.

Next for  $\varepsilon > 0$ , we consider the solution  $u_\varepsilon$  of

$$\begin{cases} i\partial_t u_\varepsilon + \Delta u_\varepsilon + V_0^\varepsilon u_\varepsilon + V_1^\varepsilon u_\varepsilon = 0, & \text{in } \mathbb{R}^3 \times (0, T) \\ u_\varepsilon(0) = u_0, & \text{in } \mathbb{R}^3. \end{cases} \quad (6)$$

Thanks to Proposition 4 and the remark at the end of its proof, we know that there exists a unique solution  $u_\varepsilon \in C([0, T]; H^1 \cap H_1)$ . In the sequel,  $C > 0$  denotes various constants which may depend on  $T$  but are independent of  $\varepsilon$ .

In order to get an  $H_1$ -estimate of  $u_\varepsilon$ , we calculate the imaginary part of the product of equation (1) by  $(1 + |x|^2)\bar{u}_\varepsilon(x)$ , integrated on  $\mathbb{R}^3$ . This gives

$$\frac{d}{dt} \left( \int_{\mathbb{R}^3} (1 + |x|^2) |u_\varepsilon|^2 \right) \leq \int_{\mathbb{R}^3} |\nabla u_\varepsilon|^2 + \int_{\mathbb{R}^3} |x|^2 |u_\varepsilon|^2.$$

Then, we have to obtain an  $H^1$ -estimate of  $u_\varepsilon$ . On the one hand, we multiply equation (1) by  $\partial_t \bar{u}_\varepsilon$ , integrate on  $\mathbb{R}^3$  and take the real part. After an integration by parts we obtain:

$$-\frac{1}{2} \frac{d}{dt} \int_{\mathbb{R}^3} |\nabla u_\varepsilon|^2 + \operatorname{Re} \int_{\mathbb{R}^3} V_0^\varepsilon u_\varepsilon \partial_t \bar{u}_\varepsilon + \operatorname{Re} \int_{\mathbb{R}^3} V_1^\varepsilon u_\varepsilon \partial_t \bar{u}_\varepsilon = 0$$

which is equivalent to

$$\frac{d}{dt} \int_{\mathbb{R}^3} |\nabla u_\varepsilon|^2 - \int_{\mathbb{R}^3} (V_0^\varepsilon + V_1^\varepsilon) \partial_t (|u_\varepsilon|^2) = 0.$$



Then,

$$\begin{aligned} \frac{d}{dt} \left( \int_{\mathbb{R}^3} |\nabla u_\varepsilon|^2 - \int_{\mathbb{R}^3} (V_0^\varepsilon + V_1^\varepsilon) |u_\varepsilon|^2 \right) \\ = - \int_{\mathbb{R}^3} (\partial_t V_0^\varepsilon + \partial_t V_1^\varepsilon) |u_\varepsilon|^2. \end{aligned} \quad (7)$$

On the other hand, since  $V_1$  satisfies assumption (5), we have

$$- \int_{\mathbb{R}^3} \partial_t V_1^\varepsilon |u_\varepsilon|^2 \leq C \left\| \frac{\partial_t V_1(t)}{1 + |x|^2} \right\|_{L^\infty} \|u_\varepsilon(t)\|_{H^1}^2$$

and from Hardy's inequality asserting that for  $\varphi \in H^1$  and any  $a \in \mathbb{R}^3$  we have

$$\int_{\mathbb{R}^3} \frac{|\varphi(x)|^2}{|x - a|^2} dx \leq 4 \int_{\mathbb{R}^3} |\nabla \varphi(x)|^2 dx,$$

we conclude that

$$- \int_{\mathbb{R}^3} \partial_t V_0^\varepsilon |u_\varepsilon|^2 \leq \int_{\mathbb{R}^3} \left| \frac{da}{dt} \right| \frac{|u_\varepsilon|^2}{|x - a|^2} \leq 4 \left| \frac{da}{dt}(t) \right| \|u_\varepsilon(t)\|_{H^1}^2.$$

We define  $E_\lambda^\varepsilon$  at time  $t \in [0, T]$  by

$$E_\lambda^\varepsilon(t) = \int_{\mathbb{R}^3} |\nabla u_\varepsilon(t, x)|^2 dx + \lambda \int_{\mathbb{R}^3} (1 + |x|^2) |u_\varepsilon(t, x)|^2 dx, \quad (8)$$

where  $\lambda$  is a positive constant to be chosen later. From now on,  $C$  denotes various positive constants, depending only on  $\lambda$  and  $T$ . We obviously have:

$$\begin{aligned} \frac{dE_\lambda^\varepsilon(t)}{dt} &\leq \frac{d}{dt} \left( \int_{\mathbb{R}^3} (V_0^\varepsilon(t) + V_1^\varepsilon(t)) |u_\varepsilon(t)|^2 \right) \\ &\quad + C \left( 1 + \left| \frac{da}{dt}(t) \right| + \left\| \frac{\partial_t V_1(t)}{1 + |x|^2} \right\|_{L^\infty} \right) E_\lambda^\varepsilon(t) \end{aligned}$$

and if we integrate on  $(0, t)$ , we obtain

$$\begin{aligned} E_\lambda^\varepsilon(t) &\leq \int_{\mathbb{R}^3} (|V_0^\varepsilon(0)| + |V_1^\varepsilon(0)|) |u_0|^2 + \int_{\mathbb{R}^3} (V_0^\varepsilon(t) + V_1^\varepsilon(t)) |u_\varepsilon(t)|^2 \\ &\quad + C \int_0^t \left( 1 + \left| \frac{da}{dt}(s) \right| + \left\| \frac{\partial_t V_1(s)}{1 + |x|^2} \right\|_{L^\infty} \right) E_\lambda^\varepsilon(s) ds + E_\lambda^\varepsilon(0). \end{aligned} \quad (9)$$

Using Cauchy-Schwarz, Hardy and Young's inequalities, and since it is easy to show the conservation of the  $L^2$ -norm of  $u_\varepsilon$ , we prove that for all  $\eta > 0$ ,

$$\begin{aligned} \int_{\mathbb{R}^3} |V_0^\varepsilon(t)| |u_\varepsilon(t)|^2 &\leq \int_{\mathbb{R}^3} \frac{|u_\varepsilon(t)|^2}{|x - a(t)|} \\ &\leq 2 \left( \int_{\mathbb{R}^3} |\nabla u_\varepsilon(t)|^2 \right)^{\frac{1}{2}} \left( \int_{\mathbb{R}^3} |u_\varepsilon(t)|^2 \right)^{\frac{1}{2}} \\ &\leq \eta \|\nabla u_\varepsilon(t)\|_{L^2}^2 + \frac{1}{\eta} \|u_0\|_{L^2}^2. \end{aligned} \quad (10)$$

and we have also

$$\int_{\mathbb{R}^3} V_1^\varepsilon(t) |u_\varepsilon(t)|^2 \leq C \left\| \frac{V_1}{1+|x|^2} \right\|_{L^\infty((0,T) \times \mathbb{R}^3)} \|u_\varepsilon(t)\|_{H_1}^2. \quad (11)$$

Moreover,  $(1+|x|^2)^{-1}V_1 \in W^{1,1}(0,T, L^\infty)$  and  $W^{1,1}(0,T) \hookrightarrow C([0,T])$ , then we have  $(1+|x|^2)^{-1}V_1(0) \in L^\infty$  and we have for the same reasons as above,

$$\begin{aligned} \int_{\mathbb{R}^3} (|V_0^\varepsilon(0)| + |V_1^\varepsilon(0)|) |u_0|^2 &\leq \int_{\mathbb{R}^3} \left( \frac{1}{|x-a(0)|} + \left\| \frac{V_1(0)}{1+|x|^2} \right\|_{L^\infty} \right) |u_0|^2 \\ &\leq C_{\rho_0} \|u_0\|_{H^1 \cap H_1}^2. \end{aligned} \quad (12)$$

We also notice that clearly

$$E_\lambda^\varepsilon(0) \leq C \|u_0\|_{H^1 \cap H_1}^2.$$

Then, if we set

$$\eta = \frac{1}{2} \quad \text{and} \quad \lambda = \frac{1}{2} + \left\| \frac{V_1}{1+|x|^2} \right\|_{L^\infty((0,T) \times \mathbb{R}^3)},$$

reporting the estimates (10)–(12) into (9) we get

$$\begin{aligned} E_\lambda^\varepsilon(t) &\leq C_{\rho_0} \|u_0\|_{H^1 \cap H_1}^2 + \frac{1}{2} \|u_\varepsilon(t)\|_{H^1}^2 + \left( \lambda - \frac{1}{2} \right) \|u_\varepsilon(t)\|_{H_1}^2 \\ &\quad + C \int_0^t \left( 1 + \left| \frac{da}{dt}(t) \right| + \left\| \frac{\partial_t V_1(s)}{1+|x|^2} \right\|_{L^\infty} \right) E_\lambda^\varepsilon(s) ds. \end{aligned} \quad (13)$$

We define  $F^\varepsilon$  at time  $t \in [0, T]$  by

$$F^\varepsilon(t) = \int_{\mathbb{R}^3} |\nabla u_\varepsilon(t, x)|^2 dx + \int_{\mathbb{R}^3} (1+|x|^2) |u_\varepsilon(t, x)|^2 dx = \|u_\varepsilon(t)\|_{H^1 \cap H_1}^2$$

and it is easy to see that we have, for all  $t$  in  $[0, T]$ ,

$$F^\varepsilon(t) \leq C_{\rho_0} \|u_0\|_{H^1 \cap H_1}^2 + C \int_0^t \left( 1 + \left| \frac{da}{dt}(t) \right| + \left\| \frac{\partial_t V_1(s)}{1+|x|^2} \right\|_{L^\infty} \right) F^\varepsilon(s) ds.$$

We obtain from Gronwall's lemma:

$$F^\varepsilon(t) \leq C_{T, \rho_0} \exp \left( \int_0^t \beta(s) ds \right) \|u_0\|_{H^1 \cap H_1}^2.$$

where

$$\beta = 1 + \left| \frac{da}{dt} \right| + \left\| \frac{\partial_t V_1}{1+|x|^2} \right\|_{L^\infty} \in L^1(0, T).$$

Therefore, there exists a positive constant  $C_{T, \alpha_0, \rho_0}$ , independent of  $\varepsilon$  and depending on the time  $T$ , on  $\alpha_0$  and on  $\rho_0$  such that for all  $t$  in  $[0, T]$ ,

$$\|u_\varepsilon(t)\|_{H^1 \cap H_1}^2 \leq C_{T, \alpha_0, \rho_0} \|u_0\|_{H^1 \cap H_1}^2.$$

Then we can make  $\varepsilon$  tend to 0 and pass to the limit in the distributions sense in equation (6). Indeed, this last estimate implies the convergence of a subsequence  $(u_{\varepsilon'})$  in the following way:

$$u_{\varepsilon'} \rightharpoonup u \quad \text{in } L^\infty(0, T; H^1 \cap H_1) \text{ w } \star .$$

We also have these other convergences:

$$\begin{aligned} V_0^\varepsilon &\rightarrow \frac{1}{|x - a(t)|} \quad \text{in } L^\infty(0, T; L^p + L^\infty), p \in [2, 3[ \\ V_1^\varepsilon &\rightarrow V_1 \quad \text{in } L^\infty(0, T; L^r_{\text{loc}}), r > 1 \end{aligned}$$

Thus,  $u$  is the solution of equation (1) in the sense of distributions and satisfies  $u \in L^\infty(0, T; H^1 \cap H_1)$  and we obtain

$$\|u(t)\|_{H^1 \cap H_1}^2 \leq C_{T, \alpha_0, \rho_0} \|u_0\|_{H^1 \cap H_1}^2.$$

We will end the proof of Theorem 5 by the study of the uniqueness of the solution of equation (1).

Let  $u_1$  and  $u_2$  be two solutions of equation (1). We set  $v = u_2 - u_1$  and it satisfies the following :

$$\begin{cases} i\partial_t v + \Delta v + \frac{v}{|x - a(t)|} + V_1(x, t)v = 0, & (x, t) \in \mathbb{R}^3 \times (0, T) \\ v(x, 0) = 0, & x \in \mathbb{R}^3. \end{cases} \quad (14)$$

We then consider a function  $\theta \in C_c^\infty(\mathbb{R})$ ,  $0 \leq \theta \leq 1$ , such that for  $s \in \mathbb{R}$

$$\theta(s) = \begin{cases} 1 & \text{for } |s| \leq 1 \\ 0 & \text{for } |s| \geq 2, \end{cases}$$

and we set

$$\theta_R(x) = \theta\left(\frac{|x|}{R}\right)$$

which is such that  $|\nabla \theta_R(x)| \leq CR^{-1}$  for all  $x$  in  $\mathbb{R}^3$ , where  $C$  is a constant independent of  $R$ .

First, multiplying (14) by  $\theta_R^2(x)\bar{v}$  we integrate over  $\mathbb{R}^3$  and taking the imaginary part, we obtain, using Cauchy-Schwarz inequality:

$$\begin{aligned} \frac{d}{dt} \left( \int_{\mathbb{R}^3} \theta_R^2(x) |v(x, t)|^2 dx \right) &= -2 \operatorname{Im} \int_{\mathbb{R}^3} \nabla v(x, t) \nabla(\theta_R^2)(x) \bar{v}(x, t) dx \\ &\leq C \int_{\mathbb{R}^3} |\nabla v(x, t)| |\theta_R(x)| |\nabla \theta_R(x)| |v(x, t)| dx \\ &\leq \frac{C}{R} \|\nabla v\|_{L^\infty(0, T; L^2)} \left( \int_{\mathbb{R}^3} \theta_R^2(x) |v(x, t)|^2 dx \right)^{\frac{1}{2}}. \end{aligned}$$

Next, as we know that  $v \in L^\infty(0, T; H^1 \cap H_1)$ , from this we get, for all  $R > 0$  and for all  $t$  in  $(0, T)$ ,

$$\int_{\mathbb{R}^3} \theta_R^2(x) |v(x, t)|^2 dx \leq \frac{C}{R} \int_0^t \left( \int_{\mathbb{R}^3} \theta_R^2(x) |v(x, s)|^2 dx \right)^{\frac{1}{2}} ds.$$

Thus, from Gronwall's inequality, since  $v(0) = 0$  we finally obtain

$$\int_{\mathbb{R}^3} \theta_R^2(x) |v(x, t)|^2 dx = 0, \quad \forall t \in (0, T), \quad \forall R > 0.$$

Hence  $v = 0$  and the proof of Theorem 5 is complete.  $\square$

## 4 Proof of Theorem 1

We use the same regularization as in the preceding section. Then for  $\varepsilon > 0$  we consider the solution  $u_\varepsilon$  of (6) :

$$\begin{cases} i\partial_t u_\varepsilon + \Delta u_\varepsilon + V_0^\varepsilon u_\varepsilon + V_1^\varepsilon u_\varepsilon = 0, & \text{in } \mathbb{R}^3 \times (0, T) \\ u_\varepsilon(0) = u_0, & \text{in } \mathbb{R}^3 \end{cases}$$

Thanks to Proposition 4, we know that  $u_\varepsilon$  is unique in  $C([0, T]; H^2 \cap H_2)$ . We also recall that  $\alpha > 0$  and  $\rho > 0$  are such that:

$$\begin{aligned} \|a\|_{W^{2,1}(0,T)} &\leq \alpha \\ \|(1 + |x|^2)^{-1} V_1\|_{W^{1,1}(0,T,L^\infty)} + \|(1 + |x|^2)^{-1} \nabla V_1\|_{L^1(0,T,L^\infty)} &\leq \rho. \end{aligned}$$

### 4.1 First Step: Energy estimates

Again here,  $C$  denotes various constants independent of  $\varepsilon$ . We first show the following estimate:

**Lemma 6.** *Let  $V_0$  and  $V_1$  satisfy assumption (2) and let  $V_0^\varepsilon$ ,  $V_1^\varepsilon$  and  $u_0$  be defined as above. There exists  $C > 0$  depending only on  $\rho$  such that the solution  $u_\varepsilon$  of (6) satisfies for all  $t \in [0, T]$ :*

$$\|u_\varepsilon(t)\|_{H^2} \leq C \|\partial_t u_\varepsilon(t)\|_{L^2} + C \|u_\varepsilon(t)\|_{H_2}.$$

**Proof.** Since  $u_\varepsilon$  is the solution of (6), we have for all  $t \in [0, T]$ ,

$$\begin{aligned} \|u_\varepsilon(t)\|_{H^2} &\leq \|\Delta u_\varepsilon(t)\|_{L^2} + \|u_\varepsilon(t)\|_{L^2} \\ &\leq \|\partial_t u_\varepsilon(t)\|_{L^2} + \|V_0^\varepsilon(t) u_\varepsilon(t)\|_{L^2} \\ &\quad + \|V_1^\varepsilon(t) u_\varepsilon(t)\|_{L^2} + \|u_\varepsilon(t)\|_{L^2}. \end{aligned} \tag{15}$$

It is clear that

$$\|V_1^\varepsilon(t)u_\varepsilon(t)\|_{L^2} \leq C \left\| \frac{V_1(t)}{1+|x|^2} \right\|_{L^\infty} \|u_\varepsilon(t)\|_{H_2}. \quad (16)$$

Next, from Hardy's and then Young's inequalities, we can prove that for all  $\eta > 0$ , there exists  $C_\eta > 0$  such that

$$\begin{aligned} \|V_0^\varepsilon(t)u_\varepsilon(t)\|_{L^2} &\leq \left\| \frac{u_\varepsilon(t)}{|x-a(t)|} \right\|_{L^2} \leq 2\|\nabla u_\varepsilon(t)\|_{L^2} \\ &\leq \eta\|u_\varepsilon(t)\|_{H^2} + C_\eta\|u_\varepsilon(t)\|_{L^2}. \end{aligned} \quad (17)$$

Then, reporting the estimates (16) and (17) into (15), we have

$$\begin{aligned} \|u_\varepsilon(t)\|_{H^2} &\leq \eta\|u_\varepsilon(t)\|_{H^2} + (C_\eta + 1)\|u_\varepsilon(t)\|_{L^2} \\ &\quad + \|\partial_t u_\varepsilon(t)\|_{L^2} + C \left\| \frac{V_1(t)}{1+|x|^2} \right\|_{L^\infty} \|u_\varepsilon(t)\|_{H_2} \end{aligned}$$

and if we choose  $\eta$  small enough, we finally obtain that for all  $t \in [0, T]$ ,

$$\|u_\varepsilon(t)\|_{H^2} \leq C\|\partial_t u_\varepsilon(t)\|_{L^2} + C_\rho\|u_\varepsilon(t)\|_{H_2},$$

where  $C$  and  $C_\rho$  are independent of  $\varepsilon$ .  $\square$

**Lemma 7.** *With the above notations let  $E_\varepsilon(t)$  be defined as being*

$$E_\varepsilon(t) = \|u_\varepsilon(t)\|_{H_2}^2 + \|\partial_t u_\varepsilon(t)\|_{L^2}^2.$$

*Then there exists  $C > 0$  depending only on  $T$ ,  $\alpha$  and  $\rho$  such that for all  $t \in [0, T]$  we have:*

$$\|u_\varepsilon(t)\|_{H_2}^2 \leq C\|u_0\|_{H_2}^2 + C \int_0^t E_\varepsilon(s) ds. \quad (18)$$

**Proof.** Note that all the integrations by parts and all the calculations we are going to do are justified because of the regularity of the data we are manipulating.

Multiplying (6) by  $|x|^4 \bar{u}_\varepsilon(x)$ , integrating by parts on  $\mathbb{R}^3$  and taking imaginary parts, we obtain

$$\operatorname{Re} \int_{\mathbb{R}^3} |x|^4 \bar{u}_\varepsilon \partial_t u_\varepsilon = \operatorname{Im} \int_{\mathbb{R}^3} i|x|^4 \bar{u}_\varepsilon \partial_t u_\varepsilon = 4 \int_{\mathbb{R}^3} x \cdot \nabla u_\varepsilon |x|^2 \bar{u}_\varepsilon$$

and we deduce that

$$\frac{d}{dt} \left( \int_{\mathbb{R}^3} |x|^4 |u_\varepsilon|^2 \right) \leq C \int_{\mathbb{R}^3} |x|^2 |\nabla u_\varepsilon|^2 + C \int_{\mathbb{R}^3} |x|^4 |u_\varepsilon|^2. \quad (19)$$

Besides, if we calculate the real part of equation (6) multiplied by  $|x|^2\bar{u}_\varepsilon$  and integrated on  $\mathbb{R}^3$ , we get

$$\begin{aligned}
\int_{\mathbb{R}^3} |x|^2 |\nabla u_\varepsilon|^2 &\leq \int_{\mathbb{R}^3} |x| |\nabla u_\varepsilon| |u_\varepsilon| + \int_{\mathbb{R}^3} |V_1^\varepsilon| |x|^2 |u_\varepsilon|^2 \\
&\quad + \int_{\mathbb{R}^3} |V_0^\varepsilon| |x|^2 |u_\varepsilon|^2 + \int_{\mathbb{R}^3} |\partial_t u_\varepsilon| |x|^2 |u_\varepsilon| \\
&\leq C \int_{\mathbb{R}^3} |\nabla u_\varepsilon|^2 + C \int_{\mathbb{R}^3} (1 + |x|^4) |u_\varepsilon|^2 + C \int_{\mathbb{R}^3} |\partial_t u_\varepsilon|^2 \\
&\quad + C \int_{\mathbb{R}^3} |V_1^\varepsilon|^2 |u_\varepsilon|^2 + C \int_{\mathbb{R}^3} |V_0^\varepsilon|^2 |u_\varepsilon|^2 \tag{20}
\end{aligned}$$

Also, from (16) and Hardy's inequalities, we have

$$\int_{\mathbb{R}^3} |V_0^\varepsilon|^2 |u_\varepsilon|^2 + \int_{\mathbb{R}^3} |V_1^\varepsilon|^2 |u_\varepsilon|^2 \leq C \int_{\mathbb{R}^3} |\nabla u_\varepsilon|^2 + C_\rho \int_{\mathbb{R}^3} (1 + |x|^4) |u_\varepsilon|^2,$$

and therefore, according to (20), we get

$$\int_{\mathbb{R}^3} |x|^2 |\nabla u_\varepsilon|^2 \leq C \int_{\mathbb{R}^3} |\nabla u_\varepsilon|^2 + C \int_{\mathbb{R}^3} |\partial_t u_\varepsilon|^2 + C_\rho \int_{\mathbb{R}^3} (1 + |x|^4) |u_\varepsilon|^2. \tag{21}$$

Now if we calculate the real part of equation (6) multiplied by  $\bar{u}_\varepsilon$  and integrated on  $\mathbb{R}^3$ , from the same kind of arguments we used to prove (16) and (17), we have

$$\begin{aligned}
\int_{\mathbb{R}^3} |\nabla u_\varepsilon|^2 &\leq C \int_{\mathbb{R}^3} |\partial_t u_\varepsilon| |u_\varepsilon| + C \int_{\mathbb{R}^3} (|V_0^\varepsilon| + |V_1^\varepsilon|) |u_\varepsilon|^2 \\
&\leq C \int_{\mathbb{R}^3} |\partial_t u_\varepsilon|^2 + C \int_{\mathbb{R}^3} |u_\varepsilon|^2 + C \int_{\mathbb{R}^3} \left( \frac{|u_\varepsilon|^2}{|x - a(t)|} + |V_1^\varepsilon| |u_\varepsilon|^2 \right) \\
&\leq C \int_{\mathbb{R}^3} |\partial_t u_\varepsilon|^2 + \eta \int_{\mathbb{R}^3} |\nabla u_\varepsilon|^2 + C_{\eta, \rho} \int_{\mathbb{R}^3} (1 + |x|^2) |u_\varepsilon|^2. \tag{22}
\end{aligned}$$

Then, if we choose  $\eta$  small enough, we finally deduce from (22) that for all  $t \in [0, T]$  we have

$$\int_{\mathbb{R}^3} |\nabla u_\varepsilon|^2 \leq C \int_{\mathbb{R}^3} |\partial_t u_\varepsilon|^2 + C_\rho \int_{\mathbb{R}^3} (1 + |x|^2) |u_\varepsilon|^2. \tag{23}$$

Plugging estimates (21) and (23) into (19) we can finally conclude that there exists  $C > 0$ , independent of  $\varepsilon$  but depending on  $\rho$  and  $T$ , such that

$$\frac{d}{dt} \left( \int_{\mathbb{R}^3} |x|^4 |u_\varepsilon|^2 \right) \leq C \int_{\mathbb{R}^3} |\partial_t u_\varepsilon|^2 + C \int_{\mathbb{R}^3} (1 + |x|^2)^2 |u_\varepsilon|^2$$

and since  $\frac{d}{dt} \left( \int_{\mathbb{R}^3} |u_\varepsilon|^2 \right) = 0$ , we obtain  $\frac{d}{dt} \left( \int_{\mathbb{R}^3} (1 + |x|^4) |u_\varepsilon|^2 \right) \leq C E_\varepsilon(t)$ .

We finally integrate on  $(0, t)$  and we get

$$\int_{\mathbb{R}^3} (1 + |x|^4) |u_\varepsilon|^2 \leq \int_{\mathbb{R}^3} (1 + |x|^4) |u_0|^2 + C \int_0^t E_\varepsilon(s) ds$$

which gives

$$\|u_\varepsilon(t)\|_{H_2}^2 \leq C \|u_0\|_{H_2}^2 + C \int_0^t E_\varepsilon(s) ds$$

we have completed the proof of (18).  $\square$

## 4.2 Second Step: $L^2$ -estimate of the time derivative

Here we obtain appropriate estimates on  $\partial_t u_\varepsilon$ :

**Lemma 8.** *Let  $E_\varepsilon(t)$  be defined as being  $E_\varepsilon(t) = \|u_\varepsilon(t)\|_{H_2}^2 + \|\partial_t u_\varepsilon(t)\|_{L^2}^2$ . There exists a constant  $C > 0$  depending only on  $T$ ,  $\alpha$  and  $\rho$  and a function  $\gamma \in L^1(0, T)$  such that for all  $t \in [0, T]$  we have:*

$$\|\partial_t u_\varepsilon(t)\|_{L^2}^2 \leq C \|u_0\|_{H^2 \cap H_2}^2 + \int_0^t \gamma(s) E_\varepsilon(s) ds. \quad (24)$$

**Proof.** We make the change of variables  $y = x - a(t)$  and we set

$$u_\varepsilon(x, t) = v_\varepsilon(y, t).$$

Then, we have

$$\partial_t v_\varepsilon(y, t) = \partial_t u_\varepsilon(x, t) + \frac{da}{dt}(t) \cdot \nabla u_\varepsilon(x, t) \quad (25)$$

and for all  $j = 1, 2$  or  $3$ ,

$$\frac{\partial v_\varepsilon}{\partial y_j}(y, t) = \frac{\partial u_\varepsilon}{\partial x_j}(x, t).$$

Therefore, the equation solved by  $v_\varepsilon$  can be written in the following way :

$$\begin{cases} i\partial_t v_\varepsilon + \Delta v_\varepsilon + \frac{v_\varepsilon}{|y|} + V_1(y + a(t), t)v_\varepsilon = i \frac{da}{dt}(t) \cdot \nabla v_\varepsilon, & (y, t) \in \mathbb{R}^3 \times (0, T) \\ v_\varepsilon(y, 0) = u_0(y + a(0)), & y \in \mathbb{R}^3. \end{cases}$$

Now, we set  $w_\varepsilon(y, t) = \partial_t v_\varepsilon(y, t)$  and since

$$\partial_t[V_1(y + a(t), t)] = \partial_t V_1(y + a(t), t) + \frac{da}{dt}(t) \cdot \nabla V_1(y + a(t), t),$$

then  $w$  satisfies the equation:

$$\begin{cases} i\partial_t w_\varepsilon + \Delta w_\varepsilon + \frac{w_\varepsilon}{|y|} + V_1(y + a(t), t)w_\varepsilon = i \frac{d^2 a}{dt^2}(t) \cdot \nabla v_\varepsilon + i \frac{da}{dt}(t) \cdot \nabla w_\varepsilon \\ \quad - \partial_t V_1(y + a(t), t)v_\varepsilon - \frac{da}{dt}(t) \cdot \nabla V_1(y + a(t), t)v_\varepsilon, & (26) \\ w_\varepsilon(y, 0) = \left( i\Delta + \frac{i}{|y|} + iV_1(y + a(0), 0) + \frac{da}{dt}(0) \cdot \nabla \right) u_0(y + a(0)). \end{cases}$$

If we multiply equation (26) by  $\bar{w}_\varepsilon$ , integrate on  $\mathbb{R}^3$  and take the imaginary part we have :

$$\begin{aligned} & \frac{1}{2} \frac{d}{dt} \int_{\mathbb{R}^3} |w_\varepsilon(y, t)|^2 dy \\ &= \operatorname{Im} \int_{\mathbb{R}^3} i \left( \frac{d^2 a}{dt^2}(t) \cdot \nabla v_\varepsilon(y, t) + \frac{da}{dt}(t) \cdot \nabla w_\varepsilon(y, t) \right) \bar{w}_\varepsilon(y, t) dy \\ &- \operatorname{Im} \int_{\mathbb{R}^3} \left( \partial_t V_1(y + a(t), t) + \frac{da}{dt}(t) \cdot \nabla V_1(y + a(t), t) \right) v_\varepsilon(y, t) \bar{w}_\varepsilon(y, t) dy \end{aligned}$$

and since

$$\operatorname{Im} \int_{\mathbb{R}^3} i \frac{da}{dt} \cdot \nabla w_\varepsilon \bar{w}_\varepsilon dy = \int_{\mathbb{R}^3} \frac{da}{dt} \cdot \operatorname{Re}(\bar{w}_\varepsilon \nabla w_\varepsilon) dy = \frac{1}{2} \int_{\mathbb{R}^3} \frac{da}{dt} \cdot \nabla(|w_\varepsilon|^2) dy = 0$$

we obtain

$$\begin{aligned} & \frac{1}{2} \frac{d}{dt} \int_{\mathbb{R}^3} |w_\varepsilon(y, t)|^2 dy \leq \left| \frac{d^2 a}{dt^2}(t) \right| \int_{\mathbb{R}^3} |\nabla v_\varepsilon(y, t)| |w_\varepsilon(y, t)| dy \\ &+ \left\| \frac{\partial_t V_1(t)}{1 + |x|^2} \right\|_{L^\infty} \int_{\mathbb{R}^3} (1 + |y + a(t)|^2) |v_\varepsilon(y, t)| |w_\varepsilon(y, t)| dy \\ &+ \left\| \frac{da}{dt} \right\|_{L^\infty(0, T)} \left\| \frac{\nabla V_1(t)}{1 + |x|^2} \right\|_{L^\infty} \int_{\mathbb{R}^3} (1 + |y + a(t)|^2) |v_\varepsilon(y, t)| |w_\varepsilon(y, t)| dy. \end{aligned}$$

Moreover one can notice that

$$\int_{\mathbb{R}^3} (1 + |y + a(t)|^2)^2 |v_\varepsilon(y, t)|^2 dy = \int_{\mathbb{R}^3} (1 + |x|^2)^2 |u_\varepsilon(x, t)|^2 dx = \|u_\varepsilon(t)\|_{H_2}^2$$

and after using Cauchy-Schwarz inequality and integrating in time variable on  $(0, t)$  we obtain

$$\begin{aligned} & \|w_\varepsilon(t)\|_{L^2}^2 \leq C \|u_0\|_{H^2 \cap H_2}^2 + 2 \int_0^t \left| \frac{d^2 a}{dt^2}(s) \right| \|\nabla v_\varepsilon(s)\|_{L^2} \|w_\varepsilon(s)\|_{L^2} ds \\ &+ 2 \int_0^t \left( \left\| \frac{\partial_t V_1(s)}{1 + |x|^2} \right\|_{L^\infty} + \left\| \frac{da}{dt} \right\|_{L^\infty(0, T)} \left\| \frac{\nabla V_1(s)}{1 + |x|^2} \right\|_{L^\infty} \right) \|u_\varepsilon(s)\|_{H_2} \|w_\varepsilon(s)\|_{L^2} ds \end{aligned}$$

where  $C > 0$  is a constant independent of  $\varepsilon$ . Furthermore, using (25) and reminding Theorem 5 and the definition of  $\rho_0$  and  $\alpha$ , we have

$$\begin{aligned} \|\partial_t u_\varepsilon(t)\|_{L^2}^2 &\leq 2 \|\partial_t v_\varepsilon(t)\|_{L^2}^2 + 2 \left\| \frac{da}{dt} \right\|_{L^\infty(0, T)}^2 \|\nabla u_\varepsilon(t)\|_{L^2}^2 \\ &\leq 2 \|\partial_t v_\varepsilon(t)\|_{L^2}^2 + C_{T, \alpha, \rho_0} \|u_0\|_{H^1 \cap H_1}^2. \end{aligned}$$



Since  $\partial_t v_\varepsilon = w_\varepsilon$  and since for all  $t \in (0, T)$ ,  $\|\nabla v_\varepsilon(t)\|_{L^2} = \|\nabla u_\varepsilon(t)\|_{L^2}$ , we get

$$\begin{aligned}
\|\partial_t u_\varepsilon(t)\|_{L^2}^2 &\leq C_{T,\alpha,\rho_0} \|u_0\|_{H^2 \cap H_2}^2 + 4 \int_0^t \left| \frac{d^2 a}{dt^2}(s) \right| \|\nabla u_\varepsilon(s)\|_{L^2} \|\partial_t v_\varepsilon(s)\|_{L^2} ds \\
&\quad + 4 \int_0^t \left( \left\| \frac{\partial_t V_1(s)}{1+|x|^2} \right\|_{L^\infty} + \alpha \left\| \frac{\nabla V_1(s)}{1+|x|^2} \right\|_{L^\infty} \right) \|u_\varepsilon(s)\|_{H_2} \|\partial_t v_\varepsilon(s)\|_{L^2} ds \\
&\leq C_{T,\alpha,\rho_0} \|u_0\|_{H^2 \cap H_2}^2 + 2 \int_0^t \left| \frac{d^2 a}{dt^2}(s) \right| (\|\nabla u_\varepsilon(s)\|_{L^2}^2 + \|\partial_t v_\varepsilon(s)\|_{L^2}^2) ds \\
&\quad + 2 \int_0^t \left( \left\| \frac{\partial_t V_1(s)}{1+|x|^2} \right\|_{L^\infty} + \alpha \left\| \frac{\nabla V_1(s)}{1+|x|^2} \right\|_{L^\infty} \right) (\|u_\varepsilon(s)\|_{H_2}^2 + \|\partial_t v_\varepsilon(s)\|_{L^2}^2) ds \\
&\leq C_{T,\alpha,\rho_0} \|u_0\|_{H^2 \cap H_2}^2 + 2 \int_0^t \gamma(s) (\|u_\varepsilon(s)\|_{H_2}^2 + \|\partial_t v_\varepsilon(s)\|_{L^2}^2) ds.
\end{aligned}$$

with

$$\gamma = \left| \frac{d^2 a}{dt^2} \right| + \left\| \frac{\partial_t V_1}{1+|x|^2} \right\|_{L^\infty} + \alpha \left\| \frac{\nabla V_1}{1+|x|^2} \right\|_{L^\infty} \in L^1(0, T).$$

Eventually, using (25) we also have

$$\|\partial_t v_\varepsilon(t)\|_{L^2}^2 \leq 2 \|\partial_t u_\varepsilon(t)\|_{L^2}^2 + 2 \left\| \frac{da}{dt} \right\|_{L^\infty(0,T)}^2 \|\nabla u_\varepsilon(t)\|_{L^2}^2$$

and for the same kind of reasons, we obtain

$$\|\partial_t u_\varepsilon(t)\|_{L^2}^2 \leq C_{T,\alpha,\rho} \|u_0\|_{H^2 \cap H_2}^2 + C \int_0^t \gamma(s) (\|u_\varepsilon(s)\|_{H_2}^2 + \|\partial_t u_\varepsilon(s)\|_{L^2}^2) ds.$$

where  $C$ ,  $C_{T,\alpha,\rho}$  and  $\gamma$  are independent of  $\varepsilon$ . This is precisely the claim of Lemma 8.  $\square$

**Remark.** One can notice that as we use this change of variables to prove the regularity result, we cannot generalize to the situation where more than one single nucleus is considered.

### 4.3 Third Step: Convergence and conclusion

Combining the estimates of Lemmas 7 and 8, we see that there exists a positive constant  $C$  and a function  $\gamma \in L^1(0, T)$ , depending on  $T$ ,  $\rho$  and  $\alpha$  but both independent of  $\varepsilon$ , such that for  $t \in [0, T]$ ,

$$\begin{aligned}
E_\varepsilon(t) &= \|u_\varepsilon(t)\|_{H_2}^2 + \|\partial_t u_\varepsilon(t)\|_{L^2}^2 \\
&\leq C \|u_0\|_{H^2 \cap H_2}^2 + \int_0^t \gamma(s) E_\varepsilon(s) ds.
\end{aligned}$$

We apply the Gronwall lemma and obtain that for all  $t$  in  $[0, T]$ ,

$$E_\varepsilon(t) \leq C e^{\|\gamma\|_{L^1(0,T)}} \|u_0\|_{H^2 \cap H_2}^2.$$

This shows that there exists  $C_{T,\alpha,\rho} > 0$  independent of  $\varepsilon$  such that

$$\|u_\varepsilon(t)\|_{H_2}^2 + \|\partial_t u_\varepsilon(t)\|_{L^2}^2 \leq C_{T,\alpha,\rho} \|u_0\|_{H^2 \cap H_2}^2, \quad \forall t \in [0, T].$$

Then, from Lemma 6, we derive that for all  $t \in [0, T]$ ,

$$\|u_\varepsilon(t)\|_{H^2 \cap H_2}^2 + \|\partial_t u_\varepsilon(t)\|_{L^2}^2 \leq C_{T,\alpha,\rho} \|u_0\|_{H^2 \cap H_2}^2 \quad (27)$$

and for all  $\varepsilon > 0$ , as we already know, the unique solution  $u_\varepsilon$  satisfies

$$u_\varepsilon \in C([0, T], H^2 \cap H_2) \cap C^1([0, T], L^2).$$

Then we let  $\varepsilon$  tend to 0 and pass to the limit in the distributions sense in equation (6). Indeed, estimate (27), implies the convergence of a subsequence  $(u_{\varepsilon'})$  in the following way:

$$\begin{aligned} u_{\varepsilon'} &\rightharpoonup u && \text{in } L^\infty(0, T; H^2 \cap H_2) \text{ w } \star \\ \partial_t u_{\varepsilon'} &\rightharpoonup \partial_t u && \text{in } L^\infty(0, T; L^2) \text{ w } \star. \end{aligned}$$

We also have these other convergences:

$$\begin{aligned} V_0^\varepsilon &\rightarrow \frac{1}{|x - a(t)|} && \text{in } L^\infty(0, T; L^p + L^\infty), p \in [2, 3[ \\ V_1^\varepsilon &\rightarrow V_1 && \text{in } L^\infty(0, T; L_{\text{loc}}^r), r > 1. \end{aligned}$$

Thus,  $u$  is the solution of equation (1) in the sense of distributions and satisfies  $u \in L^\infty(0, T; H^2 \cap H_2)$  and  $\partial_t u \in L^\infty(0, T; L^2(\mathbb{R}^3))$  and moreover

$$\|u(t)\|_{H^2 \cap H_2}^2 + \|\partial_t u(t)\|_{L^2}^2 \leq C_{T,\alpha,\rho} \|u_0\|_{H^2 \cap H_2}^2, \quad \forall t \in [0, T].$$

Since the uniqueness can easily be seen in  $L^\infty(0, T; H^2 \cap H_2)$ , the proof of Theorem 1 is complete.  $\square$

#### 4.4 Continuity results

We first point out that actually, under the hypothesis of Theorem 1, we also have  $u \in C_w([0, T]; H^2 \cap H_2)$ . Indeed, we have proved that the solution  $u$  belongs to  $L^\infty(0, T; H^2 \cap H_2)$  and since  $u \in W^{1,\infty}(0, T; L^2)$  we also have  $u \in C([0, T]; L^2)$ . Hence the weak continuity result.

Another way to formulate the result of Theorem 1 is the following.

**Corollary 9.** *Let  $a$  and  $V_1$  satisfy assumption (2) and  $u_0 \in H^2 \cap H_2$ . We define the family of Hamiltonians  $\{H(t), t \in [0, T]\}$  by  $H(t) = -\Delta - \frac{1}{|x-a|} - V_1$ . Then, there exists a unique family of evolution operators  $\{U(t, s), s, t \in [0, T]\}$*

(also called the propagator, or the Cauchy operator, associated with  $H(t)$ ) on  $H^2 \cap H_2$  such that for  $u_0 \in H^2 \cap H_2$ :

- (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  $[0, T]^2$  into  $H^2 \cap H_2$ ;
- (iv) the 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  $L^2$ .

We end this section by the proof of Theorem 2: our aim is to prove that  $u(s) \rightarrow u(t)$  strongly in  $H^1 \cap H_1$ , as  $s \rightarrow t$ .

To this end, note that on the one hand, for any  $R > 0$ , we have:

$$\begin{aligned} \|u(s) - u(t)\|_{H^1}^2 &\leq \int_{\mathbb{R}^3} (1 + |x|^2)|u(s) - u(t)|^2 dx \\ &\leq \int_{|x| < R} (1 + |x|^2)|u(s) - u(t)|^2 dx \\ &\quad + \int_{|x| > R} (1 + |x|^2)|u(s) - u(t)|^2 dx \\ &\leq (1 + R^2)\|u(s) - u(t)\|_{L^2}^2 \\ &\quad + \frac{2}{1 + R^2} \int_{\mathbb{R}^3} (1 + |x|^4)|u(s) - u(t)|^2 dx. \end{aligned}$$

On the other hand, recall that as in the proof of Lemma 6, for all  $\eta > 0$ , there exists a constant  $C_\eta > 0$  such that

$$\|u(s) - u(t)\|_{H^1}^2 \leq \eta \|u(s) - u(t)\|_{H^2}^2 + C_\eta \|u(s) - u(t)\|_{L^2}^2.$$

Therefore, for a fixed  $\eta > 0$  we may choose  $R > 0$  so that  $2(1 + R^2)^{-1} < \eta$ , and so

$$\begin{aligned} \|u(s) - u(t)\|_{H^1 \cap H_1}^2 &\leq \eta \|u(s) - u(t)\|_{H^2 \cap H_2}^2 + C_\eta \|u(s) - u(t)\|_{L^2}^2 \\ &\leq 2\eta \|u\|_{L^\infty(0, T; H^2 \cap H_2)}^2 + C_\eta \|u(s) - u(t)\|_{L^2}^2. \end{aligned} \quad (28)$$

Since we have already proved that  $u \in C([0, T]; L^2)$ , we know that  $\|u(s) - u(t)\|_{L^2}^2 \rightarrow 0$  as  $s \rightarrow t$ : thus we deduce from (28) that

$$\limsup_{s \rightarrow t} \|u(s) - u(t)\|_{H^1 \cap H_1}^2 \leq 2\eta \|u\|_{L^\infty(0, T; H^2 \cap H_2)}^2$$

for all  $\eta > 0$ , that is  $u \in C([0, T]; H^1 \cap H_1)$ , and thus the proof of Theorem 2 is complete.  $\square$

**Remark.** Actually, since for any  $\sigma < 2$ , and for all  $\eta > 0$  there exists  $C_\eta > 0$  such that

$$\|u\|_{H^\sigma} \leq \eta \|u\|_{H^2} + C_\eta \|u\|_{L^2},$$

one sees that if  $u_0 \in H^2 \cap H_2$ , the solution  $u$  of equation (1) belongs to the space  $C([0, T]; H^\sigma \cap H_\sigma)$  for all  $\sigma < 2$ .  $\square$

## 5 Application to the bilinear optimal control

We still consider equation (1)

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

where  $a \in W^{2,1}(0, T; \mathbb{R}^3)$  and  $V_1$  now satisfies the assumption:

$$\begin{aligned} (1 + |x|^2)^{-\frac{1}{2}} V_1 &\in L^\infty((0, T) \times \mathbb{R}^3), \\ (1 + |x|^2)^{-\frac{1}{2}} \partial_t V_1 &\in L^1(0, T; L^\infty) \text{ and} \\ (1 + |x|^2)^{-\frac{1}{2}} \nabla V_1 &\in L^1(0, T; L^\infty). \end{aligned} \quad (29)$$

On the one hand, we are concerned with the problem of proving the existence of a bilinear optimal control governed by equation (1). The electric potential  $V_1$  is the control, and if  $u_1 \in L^2$  is a given target, the problem reads:

$$\begin{aligned} &\text{Find a minimizer } V_1 \in H \text{ for} \\ &\inf \{J(V), V \in H\} \end{aligned}$$

where

$$H := \left\{ V, (1 + |x|^2)^{-\frac{1}{2}} V \in H^1(0, T; W) \right\} \quad (30)$$

with  $W$  an Hilbert space such that  $W \hookrightarrow W^{1,\infty}$ ,

$$J(V) = \frac{1}{2} \int_{\mathbb{R}^3} |u(T) - u_1|^2 dx + \frac{r}{2} \|V\|_H^2 \text{ with } r > 0,$$

and where  $u$  is the solution of

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

with  $u_0 \in H^2 \cap H_2$ .

On the other hand, we want to give an optimality condition for this bilinear optimal control problem. It means that if the optimal control problem described above is solved, then there exist  $V_1 \in H$  such that  $J(V_1) = \inf\{J(V), V \in H\}$

and we will prove that  $V_1$  satisfies a first order optimality condition.

**Remark.** Since we have to prove the differentiability of the cost functional  $J$ , we chose the Hilbert space  $H$  that makes it possible to differentiate the norm  $\|\cdot\|_H$  that appears in  $J$  and of course,  $V_1 \in H$  satisfies (29).

Let us now formulate the expected theorem.

**Theorem 10.** *There exists an optimal control  $V_1^*$  satisfying (29) such that*

$$J(V_1) = \inf_{V_1 \in H} J(V_1)$$

where  $H$  is defined by (30) and the cost functional  $J$  is given by

$$J(V) = \frac{1}{2} \int_{\mathbb{R}^3} |u(T) - u_1|^2 dx + \frac{r}{2} \|V_1\|_H^2$$

and it satisfies the optimality condition:

$$\forall \delta V \in H, \quad r \langle V_1^*, \delta V \rangle_H = \text{Im} \int_0^T \int_{\mathbb{R}^3} \delta V(x, t) u(x, t) \bar{p}(x, t) dx dt$$

with  $u$  solution of the state equation (1) and  $p$  solution of the adjoint problem

$$\begin{cases} i \partial_t p + \Delta p + \frac{p}{|x - a|} + V_1^* p = 0 & \text{in } \mathbb{R}^3 \times (0, T) \\ p(T) = u(T) - u_1 & \text{in } \mathbb{R}^3. \end{cases} \quad (31)$$

**Remark.** We would like to underline the fact that the regularity result described in Theorem 1 about the solution of equation (1) is strongly needed in the proof of this theorem.  $\square$

From a physical point of view, the problem linked with this situation is the laser control of chemical reactions. We are considering a single atom; as we already said, the coulombian potential  $V_0$  corresponds to the attraction of the nucleus placed in  $a(t)$  at instant  $t$ ,  $u$  is the wave function of the electron and  $V_1$  is the electric potential induced by a laser beam. Actually, the atom is subjected to an external electric field, where the corresponding potential may be unbounded at infinity, and is such that  $E(t, x) = \nabla V_1(x, t)$  where  $E$  is the field created by the laser beam.

Of course, this is a very simplified model and the lack here may be the absence of the more realistic Hartree nonlinearity

$$F(u) = (|u|^2 \star \frac{1}{|x|})u.$$

Nevertheless, the proof of the analogous theorem for the nonlinear Schrödinger equation is similar to this one and can be found in reference [2] (see also [1]). As a matter of fact, these results are a first step in order to study this kind of

optimal control problem on a coupled system of equations: namely, in such a situation, the function  $a(t)$  (that is the position of the nucleus) is unknown but satisfies a classical nuclear dynamics, coupled with the nonlinear Schrödinger equation where  $V_0 = |x - a(t)|^{-1}$  and  $u$  satisfies the equation ( $F(u)$  being given by the above relation)

$$i\partial_t u + \Delta u + \frac{u}{|x - a(t)|} + V_1 u = F(u).$$

An existence result for a bilinear optimal control, governed by a Schrödinger equation with Hartree non-linearity  $F(u)$ , has been given in [5], but with the special case in which the electric potential  $V_1$  is given by  $V_1 = -I(t) \cdot x$ , whose field is homogeneous in space, while we take into account here more general electric potentials.

The next subsections are devoted to the proof of Theorem 10 and one will find in the last subsection, for a particular case, an interpretation of the optimality condition in terms of partial differential equations.

## 5.1 Existence of a Bilinear Optimal Control

We consider an initial data  $u_0 \in H^2 \cap H_2$ , the potential  $V_0 = |x - a(t)|^{-1}$  with  $a \in W^{2,1}(0, T)$  and  $V_1$  satisfying assumption (29). Since this assumption is more restrictive and implies (2) (notice the power  $-\frac{1}{2}$  in assumption (29)), we know that for any given  $V_1$  in this class there exists a unique solution  $u$  to equation (1) such that

$$u \in C_w([0, T]; H^2 \cap H_2), \quad \partial_t u \in L^\infty(0, T; L^2), \quad u \in C([0, T]; H_1 \cap H^1).$$

In this subsection we will prove the first part of Theorem 10, that is the existence of an optimal control  $V_1^* \in H$  such that

$$J(V_1^*) = \inf\{J(V_1) ; V_1 \in H\}.$$

We begin with the following compactness result.

**Lemma 11.** *The imbeddings  $H^1 \cap H_1 \subset L^2$  and  $H^2 \cap H_2 \subset H^1 \cap H_1$  are compact.*

**Proof.** Consider for instance a sequence  $(\varphi_n)_n$  in  $H^2 \cap H_2$  converging weakly to zero in  $H^2 \cap H_2$  and such that

$$\|\varphi_n\|_{H^2 \cap H_2} \leq 1.$$

Then, for any  $R > 0$ , using Rellich-Kondrachov theorem on the compactness of the imbedding  $H^2(B(0, R)) \subset H^1(B(0, R))$ , we have that  $\|\varphi_n\|_{H^1(B(0, R))} \rightarrow 0$

as  $n \rightarrow \infty$ . And since

$$\begin{aligned}\|\varphi_n\|_{L^2}^2 &= \|\varphi_n\|_{L^2(B(0,R))}^2 + \int_{|x| \geq R} |\varphi_n|^2 dx \\ &\leq \|\varphi_n\|_{L^2(B(0,R))}^2 + \frac{1}{(1+R^2)^2} \|\varphi_n\|_{H_2}^2,\end{aligned}$$

one may see that  $\|\varphi_n\|_{L^2} \rightarrow 0$  as  $n \rightarrow +\infty$ . On the other hand since

$$\|\varphi_n\|_{H^1}^2 \leq C \|\varphi_n\|_{L^2} \|\varphi_n\|_{H^2} \leq C \|\varphi_n\|_{L^2},$$

we infer that  $\|\varphi_n\|_{H^1} \rightarrow 0$ . Finally, noting that

$$\begin{aligned}\|\varphi_n\|_{H^1}^2 &\leq (1+R^2) \|\varphi_n\|_{L^2(B(0,R))}^2 + \frac{1}{1+R^2} \int_{|x| \geq R} (1+|x|^2) |\varphi_n|^2 dx \\ &\leq (1+R^2) \|\varphi_n\|_{L^2(B(0,R))}^2 + \frac{1}{1+R^2},\end{aligned}$$

we see that  $\|\varphi_n\|_{H^1} \rightarrow 0$  as  $n \rightarrow +\infty$ . Summing up, we see that  $\|\varphi_n\|_{H^1 \cap H_1} \rightarrow 0$  for any sequence  $(\varphi_n)_n$  in  $H^2 \cap H_2$  which converges weakly to zero: this shows that the imbedding  $H^2 \cap H_2 \subset H^1 \cap H_1$  is compact. The proof of the compactness of  $H^1 \cap H_1 \subset L^2$  is analogous and can be omitted.  $\square$

In order to prove the existence of an optimal control, consider a minimizing sequence  $(V_1^n)_{n \geq 0}$  in  $H$  for the functional  $J$ . This means that

$$\inf_{V_1 \in H} J(V_1) = \lim_{n \rightarrow \infty} J(V_1^n)$$

and thus  $(V_1^n)_{n \geq +\infty}$  is bounded in  $H$ . Up to a subsequence, denoted again by  $(V_1^n)_n$ , we may find  $V_1^* \in H$  such that  $V_1^n \rightharpoonup V_1^*$  weakly in  $H$  and so

$$\|V_1^*\|_H \leq \liminf_{n \rightarrow \infty} \|V_1^n\|_H.$$

Denoting by  $u_n$  the unique solution of equation

$$\begin{cases} i\partial_t u_n + \Delta u_n + \frac{u_n}{|x-a|} + V_1^n u_n = 0, & \text{in } \mathbb{R}^3 \times (0, T) \\ u_n(0) = u_0, & \text{in } \mathbb{R}^3 \end{cases}, \quad (32)$$

and by  $u$  the solution to this equation corresponding to the potential  $V_1^*$ , we have to prove that

$$\|u(T) - u_1\|_{L^2}^2 \leq \underline{\lim} \|u_n(T) - u_1\|_{L^2}^2. \quad (33)$$

Indeed if this is done, then we have

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

that is the minimum is achieved.

Although a weak convergence would be enough, we will prove that  $u_n(T) \rightarrow u(T)$  in  $L^2$  (and even in  $H^1 \cap H_1$ ). From Theorem 1, we have:

$$\|u_n\|_{L^\infty(H^2 \cap H_2)} + \|\partial_t u_n\|_{L^\infty(L^2)} \leq C \|u_0\|_{H^2 \cap H_2}$$

where  $C$  is independent of  $n$  since  $(V_1^n)_{n \geq 0}$  is bounded in  $H$ . Then  $(u_n)_{n \geq 0}$  is bounded in  $L^\infty(0, T; H^2 \cap H_2) \cap W^{1, \infty}(0, T; L^2)$  and using the following compactness lemma (see for instance J. Simon, Theorem 5 in [9]), up to a subsequence we also have the strong convergence  $u_n \rightarrow u$  in  $C([0, T]; H_{\text{loc}}^1)$ .

**Lemma 12.** *Let  $X$ ,  $B$  and  $Y$  be Banach spaces such that the imbeddings  $X \subset B \subset Y$  are continuous and the embedding  $X \subset B$  is compact. Assume that a sequence  $(f_n)_{n \geq 1}$  is bounded in  $L^\infty(0, T; X)$  and is such that  $(\partial_t f_n)_{n \geq 1}$  is bounded in  $L^\infty(0, T; Y)$ . Then  $(f_n)_{n \geq 1}$  is relatively compact in  $C([0, T]; B)$ .*

Using this result with (see Lemma 11)

$$X = H^2 \cap H_2, \quad B = H^1 \cap H_1, \quad Y = L^2,$$

we conclude that the sequence  $(u_n)_n$  is relatively compact in  $C([0, T], H^1 \cap H_1)$ , and assuming that (up to a subsequence)  $u_n \rightarrow u_*$  in  $C([0, T], H^1 \cap H_1)$ , one checks that  $u_*$  satisfies equation (32), where  $V_1^n$  is replaced with  $V_1^*$ , in the sense of distributions: this means that one has actually  $u_* = u$ , where  $u$  is the solution of equation (32) where  $V_1^n$  is replaced with  $V_1^*$ . Thus in particular  $\|u_n(T) - u(T)\| \rightarrow 0$  and so

$$\|u(T) - u_1\|^2 = \lim_{n \rightarrow \infty} \|u_n(T) - u_1\|^2,$$

and the existence of an optimal control is proved.  $\square$

**Remark.** One can notice that we have actually prove the existence of an optimal control in the space  $\left\{V, (1 + |x|^2)^{-1} V \in W^{1, 1+\varepsilon}(0, T; W^{1, \infty})\right\}$ ,  $\varepsilon > 0$ . Indeed, the only important points are to ensure the existence of a solution to equation (1) and to take  $V_1$  in a reflexive space.

## 5.2 Optimality condition

In the definition of the space  $H$ , we can consider for instance

$$W = H^3 \oplus \text{Span}\{\psi_1, \psi_2, \dots, \psi_m\}$$

for some  $m \geq 1$ , and for  $1 \leq j \leq m$ ,  $\psi_j \in W^{1, \infty} \setminus H^3$  (indeed the case  $W = H^3$  can be treated in the same manner). This example enables us to deal both with the particular case of [4] where  $V_1(x, t) = I(t) \cdot x$ ,  $I \in H^1(0, T)$  and with general electric potentials  $(1 + |x|^2)^{-\frac{1}{2}} V_1(t) \in H^3$  which are non-homogeneous in space.



Let  $V_1 \in H$  be the bilinear optimal control obtained in previously. The usual way to obtain an optimality condition in this kind of situation is to prove that  $J$  is differentiable and to write the necessary condition

$$DJ(V_1)[\delta V_1] = 0, \quad \forall \delta V_1 \in H \quad (34)$$

in terms of the adjoint state. We postpone the proof of the following lemma and we recall that

$$V_0(x, t) = \frac{1}{|x - a(t)|}.$$

**Lemma 13.** *If  $u$  is the solution of equation (1), the functional*

$$\begin{aligned} \varphi : H &\rightarrow L^2(\mathbb{R}^3) \\ V_1 &\mapsto u(T) \end{aligned}$$

*is differentiable. Then, if  $z$  is the solution of*

$$\begin{cases} i\partial_t z + \Delta z + V_0 z + V_1 z = -\delta V_1 u, & \text{in } \mathbb{R}^3 \times (0, T) \\ z(0) = 0, & \text{in } \mathbb{R}^3 \end{cases} \quad (35)$$

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

Therefore,  $J$  is differentiable in  $V_1$  and since  $H$  is a Hilbert space, condition (34) now reads

$$\operatorname{Re} \int_{\mathbb{R}^3} (u(T) - u_1) \cdot \bar{z}(T) dx + r \langle V_1, \delta V_1 \rangle_H = 0. \quad (36)$$

**Remark.** Note that we prove the differentiability of the mapping  $V_1 \mapsto u(T)$  with values in  $L^2$ , but we do not know whether this remains true if we consider the same mapping with values in  $H^1$  for example. It is not clear whether the differentiability of  $J$  is still true. Therefore, in the functional  $J$ , the first term cannot be replaced by a stronger norm of  $u(T) - u_1$ .

Consider the adjoint state equation (31) which has a unique solution  $p \in C([0, T]; L^2)$  since  $u(T) - u_1 \in L^2$ . We multiply equation (35) by  $\bar{p}$  (the complex conjugate of  $p$ ), integrate on  $\mathbb{R}^3 \times [0, T]$  and take the imaginary part. We obtain:

$$\operatorname{Im} \int_0^T \int_{\mathbb{R}^3} (i\partial_t z + \Delta z + V_0 z + V_1 z) \bar{p} = \operatorname{Im} \int_0^T \int_{\mathbb{R}^3} -\delta V_1 u \bar{p}.$$

After an integration by parts and since  $z(0) = 0$ , we get

$$\begin{aligned} \operatorname{Im} \int_0^T \int_{\mathbb{R}^3} z \overline{i\partial_t p} - \operatorname{Im} \int_{\mathbb{R}^3} z(T) \overline{ip(T)} + \operatorname{Im} \int_0^T \int_{\mathbb{R}^3} z \overline{\Delta p} \\ + \operatorname{Im} \int_0^T \int_{\mathbb{R}^3} z \overline{(V_0 + V_1)p} = -\operatorname{Im} \int_0^T \int_{\mathbb{R}^3} \delta V_1 u \bar{p}. \end{aligned}$$

Since  $p$  satisfies equation (31), we then obtain

$$\operatorname{Re} \int_{\mathbb{R}^3} z(T) \overline{(u(T) - u_1)} = -\operatorname{Im} \int_0^T \int_{\mathbb{R}^3} \delta V_1 u \bar{p}.$$

We also have (36) and we finally obtain that for all  $\delta V_1$  in  $H$ ,

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

and the proof of the optimality condition of Theorem 10 is complete.  $\square$

We now give the proof of Lemma 13. Actually, we have to prove that  $z(T)$  is well defined in  $L^2$  when  $z$  is solution of (35) and that if  $w$  satisfies

$$\begin{cases} i\partial_t w + \Delta w + V_0 w + (V_1 + \delta V_1)w = -\delta V_1 z & \text{in } \mathbb{R}^3 \times (0, T) \\ w(0) = 0 & \text{in } \mathbb{R}^3 \end{cases} \quad (37)$$

then

$$\|w(T)\|_{L^2} = o(\|\delta V_1\|_H). \quad (38)$$

One can notice that  $w$  is actually the difference between  $z$  and  $\delta u$  where  $\delta u + u$  is the solution of equation (1) with electric potential  $\delta V_1 + V_1$ .

From Theorem 1, we know that  $u \in L^\infty([0, T]; H^2 \cap H_2)$  and since we also have  $(1 + |x|^2)^{-\frac{1}{2}} \delta V_1 \in H^1(0, T; W)$  and  $H^1(0, T; W) \hookrightarrow C(0, T; W^{1, \infty})$ , we obtain  $\delta V_1 u \in L^\infty(0, T; L^2)$ . It is then easy to prove, using Corollary 9 to formulate the integral equation equivalent to equation (35), and using a Picard fixed point theorem, that there exists a unique solution  $z \in C([0, T]; L^2)$  to equation (35). We can also specify that

$$\|z(t)\|_{L^2} \leq C \|\delta V_1\|_H \|u\|_{L^\infty(H^2 \cap H_2)}, \quad \forall t \in [0, T].$$

There and until the end of this proof,  $C$  denotes a generic constant depending on  $T$ .

Now we work on the equation solved by  $w$ . We multiply equation (37) by  $\bar{w}$ , integrate in space variable and take the imaginary part, and we obtain:

$$\begin{aligned} \frac{d}{dt} \|w(t)\|_{L^2}^2 &\leq 2 \|\delta V_1\|_H \int_{\mathbb{R}^3} (1 + |x|^2)^{\frac{1}{2}} |z(t)| |w(t)| dx \\ &\leq 2 \|\delta V_1\|_H \|z(t)\|_{H_1} \|w(t)\|_{L^2}. \end{aligned}$$

Applying Gronwall lemma, since  $w(0) = 0$  we get,  $\forall t \in [0, T]$ :

$$\|w(t)\|_{L^2} \leq C \|\delta V_1\|_H \max_{t \in [0, T]} \|z(t)\|_{H_1}. \quad (39)$$

At this point we need to consider more closely the solution  $z$  of equation (35) in order to obtain an estimate of  $\|z(t)\|_{H_1}$  for all  $t \in [0, T]$ . Actually, the

formulation of equation (35) as an integral equation allows to prove that  $z \in C([0, T]; H^1 \cap H_1)$  and the same kind of fixed point arguments then leads to prove that there exists a unique solution  $w \in C([0, T]; L^2)$  to equation (37). Usual calculations bring the following estimates :

$$\frac{d}{dt}(\|z(t)\|_{L^2}^2) \leq C\|\delta V_1\|_H\|u(t)\|_{H_1}\|z(t)\|_{L^2} \quad (40)$$

$$\begin{aligned} \frac{d}{dt}(\|x|z(t)\|_{L^2}^2) &\leq C\|\nabla z(t)\|_{L^2}\|x|z(t)\|_{L^2} \quad (41) \\ &+ C\|\delta V_1\|_H\|u(t)\|_{H_2}\|x|z(t)\|_{L^2} \end{aligned}$$

Let us now calculate  $\operatorname{Re} \int_{\mathbb{R}^3} (35) \cdot \partial_t \bar{z}(x) dx$ . We obtain, after some integrations by parts,

$$\begin{aligned} \frac{d}{dt} \left( \int_{\mathbb{R}^3} V_0 |z|^2 + \int_{\mathbb{R}^3} V_1 |z|^2 - \int_{\mathbb{R}^3} |\nabla z|^2 \right) &= \int_{\mathbb{R}^3} \partial_t V_0 |z|^2 + \int_{\mathbb{R}^3} \partial_t V_1 |z|^2 \\ &- 2 \frac{d}{dt} \left( \operatorname{Re} \int_{\mathbb{R}^3} \delta V_1 u \bar{z} \right) + 2 \operatorname{Re} \int_{\mathbb{R}^3} \partial_t (\delta V_1) u \bar{z} + 2 \operatorname{Re} \int_{\mathbb{R}^3} \delta V_1 \partial_t u \bar{z} \end{aligned}$$

We recall here that we have  $|\partial_t V_0(x, t)| = \frac{|\partial_t a(t)|}{|x - a(t)|^2}$  and we also remind the reader of Hardy's inequality:

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

Therefore, we obtain

$$\begin{aligned} \frac{d}{dt} \left( \int_{\mathbb{R}^3} |\nabla z|^2 - \int_{\mathbb{R}^3} (V_0 + V_1) |z|^2 \right) &\leq C \int_{\mathbb{R}^3} |\nabla z|^2 + 2 \frac{d}{dt} \left( \operatorname{Re} \int_{\mathbb{R}^3} \delta V_1 u \bar{z} \right) \\ &+ C\|V_1\|_H\|z(t)\|_{H_1}^2 \\ &+ C\|\delta V_1\|_H\|u(t)\|_{H_1}\|z(t)\|_{L^2} \\ &+ C\|\delta V_1\|_H\|\partial_t u(t)\|_{L^2}\|z(t)\|_{H_1} \end{aligned}$$

We integrate this between 0 and  $t \in [0, T]$  and since  $z(0) = 0$ , we get

$$\begin{aligned} \int_{\mathbb{R}^3} |\nabla z(t)|^2 &\leq \int_{\mathbb{R}^3} (V_0(t) + V_1(t)) |z(t)|^2 + \int_{\mathbb{R}^3} |\delta V_1(t)| |u(t)| |z(t)| \quad (42) \\ &+ C \int_0^t g(s) \|z(s)\|_{H_1} ds + C \int_0^t f(s) (\|z(s)\|_{H_1}^2 + \|\nabla z(s)\|_{L^2}^2) ds \end{aligned}$$

where we have set

$$g(s) = \|\delta V_1\|_H (\|u(s)\|_{H_2} + \|\partial_t u(s)\|_{L^2}) \quad \text{and} \quad f(s) = 1 + \|V_1\|_H.$$

Obviously we have  $f \in L^1(0, T)$ ,  $g \in L^1(0, T)$  and  $g \rightarrow 0$  uniformly in  $s$  when  $\delta V_1 \rightarrow 0$  in  $H$ .

We set

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

Moreover, we recall that from (40) we have

$$\|z(t)\|_{L^2}^2 \leq C \int_0^t g(s) \|z(s)\|_{L^2} ds, \quad (43)$$

which implies, with the above mentioned properties of  $g$ , that  $\|z(t)\|_{L^2} \rightarrow 0$  uniformly with respect to  $t \in [0, T]$ , when  $\|\delta V_1\|_H \rightarrow 0$ , and from (41),

$$\| |x|z(t) \|_{L^2}^2 \leq C \int_0^t \|z(s)\|_{H^1 \cap H_1}^2 ds + C \int_0^t g(s) \| |x|z(s) \|_{L^2} ds. \quad (44)$$

Thereafter, using (42), (43) and (44) we can write that for all  $t$  in  $[0, T]$ ,

$$\begin{aligned} E(t) &\leq C \int_0^t g(s) \sqrt{E(s)} ds + C \int_0^t f(s) E(s) ds \\ &\quad + \int_{\mathbb{R}^3} (V_0(t) + V_1(t)) |z(t)|^2 + C \|\delta V_1\|_H \|z(t)\|_{L^2}. \end{aligned}$$

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

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

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

$$\begin{aligned} \int_{\mathbb{R}^3} V_0(t) |z(t)|^2 &\leq \int_{\mathbb{R}^3} \frac{|z(t)|^2}{|x - a(t)|} \leq C \|z(t)\|_{H^1} \|z(t)\|_{L^2} \\ \int_{\mathbb{R}^3} V_1(t) |z(t)|^2 &\leq \|V_1\|_H \int_{\mathbb{R}^3} (1 + |x|^2)^{\frac{1}{2}} |z(t)|^2 \leq \|V_1\|_H \|z(t)\|_{L^2} \|z(t)\|_{H_1} \end{aligned}$$

and we obtain the expected result from Young's inequality.

Consequently, if we set  $h(t) = \|\delta V_1\|_H \|z(t)\|_{L^2} + \|z(t)\|_{L^2}^2$  and if we choose  $\eta$  small enough, we obtain

$$E(t) \leq C \int_0^t g(s) \sqrt{E(s)} ds + C \int_0^t f(s) E(s) ds + Ch(t) \quad (45)$$

where  $g \rightarrow 0$  in  $L^1(0, T)$  and  $h \rightarrow 0$  in  $L^\infty(0, T)$  when  $\delta V_1 \rightarrow 0$  in  $H$ .

We set  $F(t) = \left( \int_0^t g(s) \sqrt{E(s)} ds + \int_0^t f(s) E(s) ds + \|h\|_{L^\infty} \right)^{\frac{1}{2}}$  and we have  $E(t) \leq C F(t)^2$ . We use a Gronwall inequality on  $F$ .

$$\frac{dF(t)}{dt} = \frac{f(t)E(t) + g(t)\sqrt{E(t)}}{2F(t)} \leq C_1 f(t)F(t) + C_2 g(t).$$

Then, setting  $G(t) = \int_0^t C_1 f(s) ds$ , we have  $G$  bounded in  $L^\infty(0, T)$  and

$$\frac{d}{dt} \left( e^{-G(t)} F(t) \right) \leq C_2 g(t) e^{-G(t)}.$$

We obtain  $F(t) \leq C \|h\|_{L^\infty(0, T)}^{\frac{1}{2}} + C \int_0^t g(s) ds$  and we finally can write that

$$E(t) \leq C \left( \|h\|_{L^\infty} + \left| \int_0^t g(s) ds \right|^2 \right)$$

and when  $\|\delta V_1\|_H \rightarrow 0$ , we have (uniformly with respect to  $t \in [0, T]$ )

$$\|h\|_{L^\infty} + \left| \int_0^t g(s) ds \right|^2 \rightarrow 0.$$

Actually, what we have proved is the following uniform convergence:

$$\|z(t)\|_{H_1} + \|\nabla z(t)\|_{L^2} \xrightarrow{\|\delta V_1\|_H \rightarrow 0} 0.$$

Moreover, we have (39) and therefore, we obtain (38) and the proof of Lemma 13 is complete.  $\square$

### 5.3 Interpretation

We can finally give an interpretation of the optimality condition in terms of partial differential equation's in the particular case when  $W = H^3(\mathbb{R}^3)$ :

$$\tilde{H} = \left\{ V, (1 + |x|^2)^{-\frac{1}{2}} V \in H^1(0, T; H^3) \right\}.$$

Indeed, by now, we have the following optimality condition:

$$\forall \delta V \in \tilde{H}, \quad r \langle V_1, \delta V \rangle_{\tilde{H}} = \text{Im} \int_0^T \int_{\mathbb{R}^3} \delta V u \bar{p} dx dt$$

with  $u$  solution of the state equation (1),  $p$  solution of the adjoint state equation (31) and  $V_1 \in \tilde{H}$  the optimal control such that

$$J(V_1) = \inf \{ J(V), V \in \tilde{H} \}.$$

In this particular case, if  $V \in \tilde{H}$ , there exists  $X \in H^1(0, T; H^3)$  such that  $V = (1 + |x|^2)^{\frac{1}{2}} X$ . Moreover,  $X = (I - \Delta)^{-1} Y$  with  $Y \in H^1(0, T; H^1)$ . Therefore,

$$\langle V_1, \delta V \rangle_H = \langle X_1, \delta X \rangle_{H^1(0, T; H^2)} = \langle Y_1, \delta Y \rangle_{H^1(0, T; H^1)}$$

and on the one hand,

$$\langle Y_1, \delta Y \rangle_{H^1(0,T;L^2)} = \int_0^T \int_{\mathbb{R}^3} (I - \partial_t^2) Y_1 \delta Y + \int_{\mathbb{R}^3} (\partial_t Y_1(T) \delta Y(T) - \partial_t Y_1(0) \delta Y(0)).$$

while on the other hand,

$$\begin{aligned} \langle \nabla Y_1, \nabla \delta Y \rangle_{H^1(0,T;L^2)} &= \int_0^T \int_{\mathbb{R}^3} -(I - \partial_t^2) \Delta Y_1 \delta Y \\ &\quad + \int_{\mathbb{R}^3} (\partial_t \Delta Y_1(0) \delta Y(0) - \partial_t \Delta Y_1(T) \delta Y(T)). \end{aligned}$$

We obtain

$$\begin{aligned} \langle Y_1, \delta Y \rangle_{H^1(0,T;H^1)} &= \int_0^T \int_{\mathbb{R}^3} (I - \partial_t^2) (I - \Delta) Y_1 \delta Y \\ &\quad + \int_{\mathbb{R}^3} (\partial_t (Y_1 - \Delta Y_1)(T) \delta Y(T) - \partial_t (Y_1 - \Delta Y_1)(0) \delta Y(0)). \end{aligned}$$

The optimality condition becomes:

$$\begin{aligned} \forall \delta Y \in H^1(0,T;L^2), \\ r \int_0^T \int_{\mathbb{R}^3} (I - \partial_t^2) (I - \Delta) Y_1 \delta Y \, dx dt + r \int_{\mathbb{R}^3} \partial_t (Y_1 - \Delta Y_1)(T) \delta Y(T) \, dx \\ - r \int_{\mathbb{R}^3} \partial_t (Y_1 - \Delta Y_1)(0) \delta Y(0) \, dx \\ = \operatorname{Im} \int_0^T \int_{\mathbb{R}^3} u \bar{p} \sqrt{1 + |x|^2} (I - \Delta)^{-1} \delta Y \, dx dt \end{aligned}$$

and after an integration by parts, we obtain for all  $\delta Y$  in  $H^1(0,T;L^2)$ ,

$$\begin{aligned} r \int_0^T \int_{\mathbb{R}^3} (I - \partial_t^2) (I - \Delta) Y_1 \delta Y \, dx dt \\ + r \int_{\mathbb{R}^3} (\partial_t (Y_1 - \Delta Y_1)(T) \delta Y(T) - \partial_t (Y_1 - \Delta Y_1)(0) \delta Y(0)) \, dx \\ = \operatorname{Im} \int_0^T \int_{\mathbb{R}^3} \delta Y (I - \Delta)^{-1} \left( u \bar{p} \sqrt{1 + |x|^2} \right) \, dx dt. \end{aligned}$$

It can be noticed that if the target  $u_1$  is in  $L^2$  then  $p \in L^\infty(0,T;L^2)$  and since  $u \in L^\infty(0,T;H^2 \cap H_2)$ , we have  $u \bar{p} \sqrt{1 + |x|^2} \in L^\infty(0,T;L^1)$ . Then, as we have  $L^1(\mathbb{R}^3) \hookrightarrow H^{-2}(\mathbb{R}^3)$ , we get  $(I - \Delta)^{-1} \left( u \bar{p} \sqrt{1 + |x|^2} \right) \in L^\infty(0,T;L^2)$  and finally, the right hand side has a meaning.

Thus, the optimality condition corresponds to the system:

$$\begin{cases} r(I - \partial_t^2)(I - \Delta)Y_1 = (I - \Delta)^{-1} \left( \operatorname{Im}(u \bar{p}) \sqrt{1 + |x|^2} \right) & \text{in } \mathbb{R}^3 \times (0, T) \\ \partial_t(Y_1 - \Delta Y_1)(T) = \partial_t(Y_1 - \Delta Y_1)(0) = 0 & \text{in } \mathbb{R}^3. \end{cases}$$

where

$$V_1 = (1 + |x|^2)^{\frac{1}{2}} (I - \Delta)^{-1} Y_1.$$

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