Existence and Regularity of the Solution of a Time Dependent Hartree-Fock Equation Coupled with a Classical Nuclear Dynamics

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ABSTRACT

We study an Helium atom (composed of one nucleus and two electrons) submitted to a general time dependent electric field, modeled by the Hartree-Fock equation, whose solution is the wave function of the electrons, coupled with the classical Newtonian dynamics, for the position of the nucleus. We prove a result of existence and regularity for the Cauchy problem, where the main ingredients are a preliminary study of the regularity in a nonlinear Schrödinger equation with semi-group techniques and a Schauder fixed point theorem.

Key words: Hartree-Fock equation, classical dynamics, regularity, existence.

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1. Introduction, notations and main results

We are interested in the mathematical study of a simplified chemical system, in fact an atom consisting in a nucleus and two electrons, submitted to an external electric field. We need very classical approximations used in quantum chemistry to describe the chemical system in terms of partial differential equations. We choose a non-adiabatic approximation of the general time dependent Schrödinger equation

$$i\partial_t \Psi(x,t) = H(t)\Psi(x,t) - V_1(x,t)\Psi(x,t),$$

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where H is the Hamiltonian of the molecular system, Ψ its wave function, and V_1 the external electric potential, which allows, even under the effect of an electric field (see [5]), to neglect the quantum nature of the nucleus since it is much heavier than the electrons. On the one hand, we consider the nucleus 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 density (nucleus-electron attraction of Hellman-Feynman type). On the other hand, we obtain under the Restricted Hartree-Fock formalism, a time dependent Hartree-Fock equation whose solution is the wave function of the electrons.

Indeed, we consider the following coupled system:

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

where V_1 is the external electric potential which takes it values in $\mathbb{R}$ and satisfy the following assumptions:

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

Here, the time dependent Hartree-Fock equation is a Schrödinger equation (in the mathematical meaning) with a Coulombian potential due to the nucleus, singular at finite distance, an electric potential corresponding to the external electric field, singular at infinity, and a nonlinearity of Hartree type in the right hand side. Next, the classical nuclear dynamics is the second order in time ordinary differential equation solved by the position $a(t)$ of the nucleus (of mass m and charge equal to 1) responsible of the Coulombian potential.

This kind of situation has already 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 [7]). From then on, they have to deal with the nonlinear Schrödinger equation with only a time dependent Coulombian potential. Of course, we cannot use this technique here because of the generality of the potential V_1 we are considering.

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

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

- Re and Im are the real and the imaginary parts of a complex number,
- $W^{2,1}(0,T) = W^{2,1}(0,T;\mathbb{R}^3)$, for $p \geq 1$, $L^p = L^p(\mathbb{R}^3)$ and
- the usual Sobolev spaces are $H^1 = H^1(\mathbb{R}^3)$ and $H^2 = H^2(\mathbb{R}^3)$.

We also define

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

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

The main purpose of this paper is to prove the following result.

Theorem 1.1. *Let T be a positive arbitrary time. Under the assumptions* (2)*, and if we also assume $u_0 \in H^2 \cap H_2$ and $a_0, v_0 \in \mathbb{R}$, system* (1) *admits a solution*

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

The reader may notice at first sight that we do not give any uniqueness result for this coupled system. Actually, there is a proof of existence and uniqueness of solutions for the analogous system without electric potential in [5] (and also with a uniform electric potential, via the gauge transformation). Of course, their way of proving uniqueness cannot be applied here because the Marcinkiewicz spaces they used do not suit the electric potential V_1 we have. Even if one can be convinced that the solution in this class is unique, we do not have any proof of uniqueness yet. Nevertheless, for any solution of system (1) in the class given in Theorem 1.1, the following estimate holds:

Proposition 1.2. *Let (u,a) be a solution of the coupled system* (1) *under the assumptions* (2) *in the class*

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

If $\rho > 0$ satisfies

$$\Big\| \frac{V_1}{1+|x|^2} \Big\|_{W^{1,1}(0,T,L^\infty)} + \Big\| \frac{\nabla V_1}{1+|x|^2} \Big\|_{L^1(0,T,L^\infty)} \leq \rho,$$

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

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

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

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

The proof of Theorem 1.1 will be given in a first step in the case when the time T is small enough (section 3). Proposition 1.2 will then be useful to reach any arbitrary time T and prove Theorem 1.1 (section 4).

Finally, we would like to point out that the result given in Theorem 1.1 is a necessary step towards the study of the optimal control linked with system (1), the control being performed by the external electric field. This mathematical point of view participates to the understanding of the optimal control of simple chemical reactions by means of a laser beam action. One can notice that Theorem 1.1 ensures the existence of solution to the coupled equations for a large class of control parameters since V_1 satisfies (2). The optimal control problem has been described and studied in references [2] (nonlinear Schrödinger equation and coupled problem) and [3] (linear Schrödinger equation). One can read the whole study in [1].

Before working on the situation described above, we will consider the position $a(t)$ of the nucleus as known at any time $t \in [0,T]$. Of course, this is too restrictive for the study of chemical reactions but the next section is only a first step which leads to the proof of Theorem 1.1. We can refer to [6] for the study of the well-posedness of the Cauchy problem for fixed nuclei, in the Hartree-Fock approximation for the electrons. This reference precisely describes the N-electrons situation where the position of the nucleus is known. We consider here the 2-electrons 1-nucleus system.

2. A nonlinear Schrödinger equation

In this section, we will consider the position a of the nucleus as known at any moment and we will prove existence, uniqueness and regularity for the solution of the nonlinear Schrödinger equation of Hartree type which we are led to study. Indeed, we consider the following equation:

$$\begin{cases} i\partial_t u + \Delta u + \frac{1}{|x-a|}u + V_1 u = \left(|u|^2 * \frac{1}{|x|}\right)u, & \text{in } \mathbb{R}^3\times(0,T)\\ u(0) = u_0, & \text{in } \mathbb{R}^3, \end{cases} \tag{3}$$

where a and V_1 are given and satisfy the following assumptions:

$$
\begin{aligned}
a &\in W^{2,1}(0,T),\\
(1+|x|^2)^{-1}V_1 &\in L^\infty((0,T)\times\mathbb{R}^3),\\
(1+|x|^2)^{-1}\partial_t V_1 &\in L^1(0,T;L^\infty),\\
(1+|x|^2)^{-1}\nabla V_1 &\in L^1(0,T;L^\infty).
\end{aligned}
\tag{4}
$$

The study of this equation is submitted to the results known for the corresponding linear equation. We will use the main result given in references [3, 4] about existence and regularity of the solution of the linear Schrödinger equation

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

We set $\rho > 0$ such that

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

Theorem 2.1. *Let u_0 belong to $H^2\cap H_2$, a and V_1 satisfy the assumptions* (4). *We define the family of Hamiltonians $\{H(t), t\in[0,T]\}$ by*

$$
H(t) = -\Delta - \frac{1}{|x-a(t)|} - V_1(t).
$$

Then, there exists a unique family of evolution operators $\{\, U(t,s) \mid s,t\in[0,T] \,\}$ (the so called propagator associated with $H(t)$) on $H^2\cap H_2$ such that for all $u_0\in H^2\cap H_2$:

(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 : $\|U(t,s)u_0\|_{L^2} = \|u_0\|_{L^2}$,*

(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, for all $\alpha>0$, there exists $M_{T,\alpha,\rho}>0$ such that for all $t,s\in[0,T]$, and $f\in H^2\cap H_2$,*

$$
\|a\|_{W^{2,1}(0,T)} \le \alpha \;\Rightarrow\; \|U(t,s)f\|_{H^2\cap H_2} \le M_{T,\alpha,\rho}\|f\|_{H^2\cap H_2},
$$

(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.*

One shall notice that of course, in (iii), the constant $M_{T,\alpha,\rho}$ depends on the norm of V_1 in the space where it is defined, via ρ.

We would like to underline that the main difficulty to prove this theorem is to deal at the same time with the two potentials which have very different properties. The main reference is a paper by K. Yajima [11] which treats the case where $V_1 = 0$, using strongly T. Kato's results in reference [8]. In our situation, we first regularize V_0 and V_1 by V_0^ε and V_1^ε and obtain accurate estimates, independent of ε. The key point is to find an L^2-estimate of the time derivative of the solution u^ε. We use a change of variable $y = x - a(t)$ and considering then the equation solved by the time derivative of $v^\varepsilon(t,y) = u^\varepsilon(t,x)$ we prove an estimate of $\|\partial_t u^\varepsilon(t)\|_{L^2}$. Making ε tend to 0 ends the proof of Theorem 2.1.

We finally give the existence result on the nonlinear Schrödinger equation (3):

Theorem 2.2. *Let T be a positive arbitrary time. Under the assumptions* (4)*, and if we also assume $u_0 \in H^2 \cap H_2$, then equation* (3) *has a unique solution $u \in L^\infty(0,T; H^2 \cap H_2)$ which satisfies $\partial_t u \in L^\infty(0,T;L^2)$ and there exists a constant $C_{T,\alpha,\rho} > 0$ depending on T, α, and ρ where*

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

such that

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

An analogous 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 (3), one has $V_1 = -I(t)\cdot x$ as in reference [5] (but for a time T small enough) and in reference [7] (for the linear case). They both use a gauge transformation to remove the electric potential from the two equations such that they only have to deal with the usual difficulty corresponding to a time dependent Coulombian potential. The generality of potentials V_1 we are considering does not allow us to use this technique.

2.1. Local existence

We will begin with a local-in-time existence result for equation (3). We first need the following lemma to deal with the Hartree nonlinearity.

Lemma 2.3. *For $u \in H^1$, we define $F(u) = (|u|^2 * \frac{1}{|x|})u$ and one has the following estimates:*

(i) *There exists $C > 0$ such that for all $u, v \in H^1$,*

$$\|F(u) - F(v)\|_{L^2} \leq C(\|u\|_{H^1}^2 + \|v\|_{H^1}^2)\|u - v\|_{L^2} \tag{5}$$

(ii) *There exists $C_F > 0$ such that for all $u, v \in H^2 \cap H_2$,*

$$\|F(u) - F(v)\|_{H^2\cap H_2} \leq C_F(\|u\|_{H^1}^2 + \|v\|_{H^2\cap H_2}^2)\|u - v\|_{H^2\cap H_2} \tag{6}$$

$$\|F(u)\|_{H^2\cap H_2} \leq C_F\|u\|_{H^1}^2\|u\|_{H^2\cap H_2} \tag{7}$$

We notice that everywhere in this paper, C denotes a real non-negative generic constant. We may put in index a precise dependence of the constant (like C_F or $C_{T,\alpha,\rho}$).

Proof. From Cauchy-Schwarz and Hardy inequalities, we have

$$\begin{aligned}
\|F(u) - F(v)\|_{L^2} &\leq \left\| \left(|u|^2 * \frac{1}{|x|}\right)u - \left(|v|^2 * \frac{1}{|x|}\right)v \right\|_{L^2} \\
&\leq \left\| \left(|u|^2 * \frac{1}{|x|}\right)(u - v) \right\|_{L^2} + \left\| \left((|u|^2 - |v|^2) * \frac{1}{|x|}\right)v \right\|_{L^2} \\
&\leq 2\|u\|_{L^2}\|\nabla u\|_{L^2}\|u - v\|_{L^2} \\
&\quad + 2\|v\|_{L^2}\left(\|\nabla u\|_{L^2} + \|\nabla v\|_{L^2}\right)\|u - v\|_{L^2} \\
&\leq C(\|u\|_{H^1}^2 + \|v\|_{H^1}^2)\|u - v\|_{L^2}
\end{aligned}$$

which proves (5). Now, we have to establish (6) and (7). First of all we have

$$\begin{aligned}
\|F(u) - F(v)\|_{H^2\cap H_2}^2 = \|F(u) - F(v)\|_{L^2}^2 + \||x|^2F(u) - |x|^2F(v)\|_{L^2}^2 \\
+ \|\Delta F(u) - \Delta F(v)\|_{L^2}^2.
\end{aligned} \tag{8}$$

The first term of the right hand side is conveniently bounded in (5). We also use the same proof as for (5) to bound the second term:

$$\begin{aligned}
&\left\| |x|^2\left(|u|^2 * \frac{1}{|x|}\right)u - |x|^2\left(|v|^2 * \frac{1}{|x|}\right)v \right\|_{L^2} \\
&\quad\leq \left\| \left(|u|^2 * \frac{1}{|x|}\right)|x|^2(u - v) \right\|_{L^2} + \left\| \left((|u|^2 - |v|^2) * \frac{1}{|x|}\right)|x|^2v \right\|_{L^2} \\
&\quad\leq C\|u\|_{L^2}\|\nabla u\|_{L^2}\|u - v\|_{H_2} + C\|v\|_{H_2}\big(\|\nabla u\|_{L^2} + \|\nabla v\|_{L^2}\big)\|u - v\|_{L^2} \\
&\quad\leq C\big(\|u\|_{H^1}^2 + \|v\|_{H^1\cap H_2}^2\big)\|u - v\|_{H_2}.
\end{aligned} \tag{9}$$

Moreover

$$\begin{aligned}
&\|\Delta F(u) - \Delta F(v)\|_{L^2} \\
&\quad\leq \left\| \Delta\left[\left(|u|^2 * \frac{1}{|x|}\right)(u - v)\right] \right\|_{L^2} + \left\| \Delta\left[\left((|u|^2 - |v|^2) * \frac{1}{|x|}\right)v\right] \right\|_{L^2} \\
&\quad\leq \left\| \Delta\left[\left(|u|^2 * \frac{1}{|x|}\right)(u - v)\right] \right\|_{L^2} + \left\| \Delta\left[\left((|u| + |v|)||u| - |v|| * \frac{1}{|x|}\right)v\right] \right\|_{L^2}.
\end{aligned}$$

However, for any arbitrary function a, b, and $c \in H^2$, we have

$$\Delta\left[\left(ab * \frac{1}{|x|}\right)c\right] = 4\pi abc + 2\left(b\nabla a * \frac{1}{|x|}\right)\nabla c + 2\left(a\nabla b * \frac{1}{|x|}\right)\nabla c + \left(ab * \frac{1}{|x|}\right)\Delta c$$

and we thus obtain

$$\left\|\Delta\left[\left(ab * \frac{1}{|x|}\right)c\right]\right\|_{L^2} \leq C\|a\|_{H^1}\|b\|_{H^1}\|c\|_{H^2}.$$

Using that result, it is easy to conclude that

$$\|\Delta F(u) - \Delta F(v)\|_{L^2} \leq C_F\big(\|u\|^2_{H^1} + \|v\|^2_{H^2}\big)\|u - v\|_{H^2}. \tag{10}$$

Then, using (8), (9), and (10), we finally prove (6) and F is locally Lipschitz in $H^2 \cap H_2$. Therefore, taking $v = 0$, we also get (7). □

The proof of a local-in-time result is based on a Picard fixed point theorem and Theorem 2.1 and Lemma 2.3 are the main ingredients. We begin by fixing an arbitrary time $T > 0$ and considering $\tau \in]0, T]$. We also consider the functional

$$\varphi : u \longmapsto U(\cdot, 0)u_0 - i\int_0^{\cdot} U(\cdot, s)F(u(s))\,ds,$$

where U is the propagator given in Theorem 2.1, and the set

$$B = \{v \in L^\infty(0, \tau; H^2 \cap H_2), \|v\|_{L^\infty(0,\tau;H^2\cap H_2)} \leq 2M_{T,\alpha,\rho}\|u_0\|_{H^2\cap H_2}\}.$$

If $\tau > 0$ is small enough, the functional φ maps B into itself and is a strict contraction in the Banach space $L^\infty(0, \tau; H^2 \cap H_2)$. Indeed, on the one hand, from estimate (7) of Lemma 2.3, if $u \in B$, we have for all $t \in [0, \tau]$,

$$\begin{aligned}
\|\varphi(u)(t)\|_{H^2\cap H_2} &\leq \left\|U(t, 0)u_0 - i\int_0^t U(t, s)F(u(s))\,ds\right\|_{H^2\cap H_2} \\
&\leq M_{T,\alpha,\rho}\|u_0\|_{H^2\cap H_2} + \tau M_{T,\alpha,\rho}\|F(u)\|_{L^\infty(0,\tau;H^2\cap H_2)} \\
&\leq M_{T,\alpha,\rho}\|u_0\|_{H^2\cap H_2} + \tau C_F M_{T,\alpha,\rho}\|u\|^2_{L^\infty(0,\tau;H^1)}\|u\|_{L^\infty(0,\tau;H^2\cap H_2)} \\
&\leq M_{T,\alpha,\rho}\|u_0\|_{H^2\cap H_2} + 8\tau C_F M^4_{T,\alpha,\rho}\|u_0\|^3_{H^2\cap H_2}.
\end{aligned}$$

Then, if we choose $\tau > 0$ such that $8\tau C_F M^3_{T,\alpha,\rho}\|u_0\|^2_{H^2\cap H_2} < 1$ we obtain $\|\varphi(u)\|_{L^\infty(0,\tau;H^2\cap H_2)} \leq 2M_{T,\alpha,\rho}\|u_0\|_{H^2\cap H_2}$ and $\varphi(u)$ belongs to B.

On the other hand, if $u \in B$ and $v \in B$, then for all t in $[0,\tau]$ we have

$$\begin{aligned}
\|\varphi(u)(t)-\varphi(v)(t)\|_{H^2\cap H_2} &= \left\| \int_0^t U(t,s)\left(F(u(s))-F(v(s))\right) ds \right\|_{H^2\cap H_2} \\
&\le M_{T,\alpha,\rho} \int_0^t \|F(u(s))-F(v(s))\|_{H^2\cap H_2}\, ds \\
&\le C_F M_{T,\alpha,\rho}\big(\|u\|^2_{L^\infty(0,\tau;H^1)} + \|v\|^2_{L^\infty(0,\tau;H^2\cap H_2)}\big) \int_0^t \|u(s)-v(s)\|_{H^2\cap H_2}\, ds \\
&\le 8\tau C_F M^3_{T,\alpha,\rho}\|u_0\|^2_{H^2\cap H_2}\ \|u-v\|_{L^\infty(0,\tau;H^2\cap H_2)},
\end{aligned}$$

with $8\tau C_F M^3_{T,\alpha,\rho}\|u_0\|^2_{H^2\cap H_2} < 1$.

Therefore, we can deduce existence and uniqueness of the solution to the equation

$$u(t) = U(t,0)u_0 - i\int_0^t U(t,s)F(u(s))\, ds \tag{11}$$

in B, then in $L^\infty(0,\tau;H^2\cap H_2)$ for $\tau > 0$ small enough. Moreover, $\partial_t u$ belongs to $L^\infty(0,\tau;L^2)$ since from equation (3), we can write

$$\partial_t u = i\Delta u + i\frac{u}{|x-a|} + iV_1 u - iF(u).$$

Indeed, $u \in L^\infty(0,\tau;H^2\cap H_2)$ brings $F(u) \in L^\infty(0,\tau;H^2\cap H_2)$ and $\Delta u \in L^\infty(0,\tau;L^2)$ and we can prove that $V_1 u \in L^\infty(0,\tau;L^2)$ and $\frac{u}{|x-a|} \in L^\infty(0,\tau;L^2)$ in the following way: it is clear that for all t in $[0,\tau]$,

$$\|V_1(t)u(t)\|_{L^2} \le \left\| \frac{V_1(t)}{1+|x|^2} \right\|_{L^\infty} \|u(t)\|_{H_2},$$

and from Hardy's inequality,

$$\left\| \frac{u(t)}{|x-a(t)|} \right\|_{L^2} \le 2\|u(t)\|_{H^1}.$$

It is finally easy to prove that there exists a constant $C > 0$ depending on α, ρ, F and T such that for all t in $[0,\tau]$,

$$\|\partial_t u(t)\|_{L^2} \le C\|u_0\|_{H^2\cap H_2}.$$

The last point to prove is the uniqueness of the solution u of (11) in the space $L^\infty(0,\tau;H^2\cap H_2)\cap W^{1,\infty}(0,\tau;L^2)$. Let u and v be two solutions of (11) and w equal to $u-v$. Then $w(0)=0$ and

$$i\partial_t w + \Delta w + \frac{w}{|x-a|} + V_1 w = F(u) - F(v). \tag{12}$$

Calculating $\mathrm{Im} \int_{\mathbb{R}} (12) \cdot \bar{w}(x)\, dx$ and using Lemma 2.3 we obtain

$$\frac{d}{dt}(\|w\|_{L^2}^2) \leq C\|w\|_{L^2}^2$$

and uniqueness follows by Gronwall lemma.

Hence the proof of uniqueness, existence and regularity of the solution of equation (3) in $\mathbb{R}^3 \times [0, \tau]$ for any time τ such that $8\tau C_F M_{T,\alpha,\rho}^3 \|u_0\|_{H^2 \cap H_2}^2 < 1$.

2.2. A priori Energy estimate

We will prove here an a priori energy estimate of the solution of equation (3) for any arbitrary time T. We set $\alpha_0 > 0$ and $\rho_0 > 0$ such that

$$\left\|\frac{da}{dt}\right\|_{L^1(0,T)} \leq \alpha_0 \qquad \text{and} \qquad \left\|\frac{V_1}{1+|x|^2}\right\|_{W^{1,1}(0,T,L^\infty)} \leq \rho_0.$$

Proposition 2.4. *If u is a solution of equation* (3) *in the space $W^{1,\infty}(0,T;L^2) \cap L^\infty(0,T;H^2 \cap H_2)$, under assumption* (4) *for a and V_1, then there exists a non-negative constant C_{T,α_0,ρ_0}^0 depending on the time T, on ρ_0, α_0 and on $\|u_0\|_{H^2 \cap H_2}$ such that for all t in $[0,T]$,*

$$\|u(t)\|_{H^1 \cap H_1}^2 + \int_{\mathbb{R}^3} \left(|u(t,x)|^2 * \frac{1}{|x|}\right)|u(t,x)|^2 \leq C_{T,\alpha_0,\rho_0}^0.$$

Proof. On the one hand, we multiply equation (3) by $\partial_t \bar{u}$, integrate over $\mathbb{R}^3$ and take the real part. After an integration by parts we obtain

$$-\frac{1}{2}\frac{d}{dt}\int_{\mathbb{R}^3} |\nabla u|^2 + \mathrm{Re}\int_{\mathbb{R}^3} \frac{u\, \partial_t \bar{u}}{|x-a|} + \mathrm{Re}\int_{\mathbb{R}^3} V_1 u\, \partial_t \bar{u} = +\mathrm{Re}\int_{\mathbb{R}^3}\left(|u|^2 * \frac{1}{|x|}\right) u\, \partial_t \bar{u}$$

which is equivalent to

$$-\frac{d}{dt}\int_{\mathbb{R}^3} |\nabla u|^2 + \int_{\mathbb{R}^3}\left(\frac{1}{|x-a|} + V_1\right)\partial_t(|u|^2) = \frac{1}{2}\frac{d}{dt}\int_{\mathbb{R}^3}\left(|u|^2 * \frac{1}{|x|}\right)|u|^2.$$

Then,

$$\begin{aligned}\frac{d}{dt}\left(\int_{\mathbb{R}^3} |\nabla u|^2 + \frac{1}{2}\int_{\mathbb{R}^3}\left(|u|^2 * \frac{1}{|x|}\right)|u|^2 - \int_{\mathbb{R}^3}\left(\frac{1}{|x-a|} + V_1\right)|u|^2\right)& \\ = -\int_{\mathbb{R}^3}\left(\partial_t \frac{1}{|x-a|} + \partial_t V_1\right)|u|^2.& \quad (13)\end{aligned}$$

On the other hand, since V_1 satisfies assumption (4), we have

$$-\int_{\mathbb{R}^3} \partial_t V_1 |u|^2 \leq \left\|\frac{\partial_t V_1(t)}{1+|x|^2}\right\|_{L^\infty} \|u(t)\|_{H_1}^2$$

and from Hardy's inequality,

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

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

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

We define E at time t of $[0,T]$ by

$$E(t)=\int_{\mathbb{R}^3}|\nabla u(t,x)|^2\,dx+\lambda\int_{\mathbb{R}^3}(1+|x|^2)|u(t,x)|^2\,dx \\ +\frac{1}{2}\int_{\mathbb{R}^3}\left(|u(t,x)|^2*\frac{1}{|x|}\right)|u(t,x)|^2$$

where λ is a non-negative constant to be precised later. From now on, C denotes various positive constants, independent of anything but λ. We obviously have

$$\frac{dE(t)}{dt}\leq\frac{d}{dt}\left(\int_{\mathbb{R}^3}\left(\frac{1}{|x-a(t)|}+V_1(t)\right)|u(t)|^2\right) \\ +C\left(1+\left|\frac{da}{dt}(t)\right|+\left\|\frac{\partial_t V_1(t)}{1+|x|^2}\right\|_{L^\infty}\right)E(t)$$

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

$$E(t)\leq\int_{\mathbb{R}^3}\left(\frac{1}{|x-a(0)|}+|V_1(0)|\right)|u_0|^2+\int_{\mathbb{R}^3}\left(\frac{1}{|x-a(t)|}+V_1(t)\right)|u(t)|^2 \\ +C\int_0^t\left(1+\left|\frac{da}{dt}(s)\right|+\left\|\frac{\partial_t V_1(s)}{1+|x|^2}\right\|_{L^\infty}\right)E(s)\,ds+E(0)$$

Using Cauchy-Schwarz, Hardy and Young's inequalities, we prove that for all $\eta>0$,

$$\int_{\mathbb{R}^3}\frac{|u(t)|^2}{|x-a(t)|}\leq 2\left(\int_{\mathbb{R}^3}|\nabla u(t)|^2\right)^{\frac{1}{2}}\left(\int_{\mathbb{R}^3}|u(t)|^2\right)^{\frac{1}{2}} \\ \leq\eta\|\nabla u(t)\|_{L^2}^2+\frac{1}{4\eta}\|u_0\|_{L^2}^2$$

since it is easy to prove the conservation of the L^2-norm of u, and we also have

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

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 $(1+|x|^2)^{-1}V_1(0) \in L^\infty$ and we have for the same reasons as above,

$$\int_{\mathbb{R}^3}\Big(\frac{1}{|x-a(0)|}+|V_1(0)|\Big)|u_0|^2 \leq C_\rho \|u_0\|^2_{H^1\cap H_1}.$$

We also notice that

$$E(0) \leq C\|u_0\|^2_{H^1\cap H_1} + C\|u_0\|_{H^1}\|u_0\|^3_{L^2}.$$

Then, if we set $\eta = \frac{1}{2}$ and $\lambda = \frac{1}{2} + \big\|\frac{V_1}{1+|x|^2}\big\|_{L^\infty((0,T)\times\mathbb{R}^3)}$ we get

$$\begin{aligned} E(t) \leq C_\rho\|u_0\|^2_{H^1\cap H_1} &+ C\|u_0\|_{H^1}\|u_0\|^3_{L^2} + \frac{1}{2}\|u(t)\|^2_{H^1} \\ &+ \Big(\lambda - \frac{1}{2}\Big)\|u(t)\|^2_{H_1} + C\int_0^t \left(1 + \left|\frac{da}{dt}(s)\right| + \left\|\frac{\partial_t V_1(s)}{1+|x|^2}\right\|_{L^\infty}\right) E(s)\,ds. \end{aligned}$$

We define F at time t of $[0,T]$ by

$$\begin{aligned} F(t) = \int_{\mathbb{R}^3} |\nabla u(t,x)|^2\,dx &+ \int_{\mathbb{R}^3}(1+|x|^2)|u(t,x)|^2\,dx \\ &+ \int_{\mathbb{R}^3}\Big(|u(t,x)|^2 * \frac{1}{|x|}\Big)|u(t,x)|^2 \end{aligned}$$

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

$$\begin{aligned} F(t) \leq C(\|u_0\|^2_{H^1\cap H_1} &+ \|u_0\|_{H^1}\|u_0\|^3_{L^2}) \\ &+ C\int_0^t \left(1 + \left|\frac{da}{dt}(s)\right| + \left\|\frac{\partial_t V_1(s)}{1+|x|^2}\right\|_{L^\infty}\right) F(s)\,ds. \end{aligned}$$

We obtain from Gronwall's lemma

$$F(t) \leq C_T \exp\Big(\int_0^t \beta(s)ds\Big)\big(\|u_0\|^2_{H^1\cap H_1} + \|u_0\|_{H^1}\|u_0\|^3_{L^2}\big).$$

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

Therefore, there exists a non-negative constant C^0_{T,α_0,ρ_0} depending on the time T, on the initial data $\|u_0\|_{H^1\cap H_1}$ and on α_0, $\rho_0 > 0$, such that for all t in $[0,T]$,

$$\|u(t)\|^2_{H^1\cap H_1} + \int_{\mathbb{R}^3}\Big(|u(t)|^2 * \frac{1}{|x|}\Big)|u(t)|^2 \leq C^0_{T,\alpha_0,\rho_0}.$$

Hence the proof of Proposition 2.4. □

2.3. Global existence

Now, we can use Proposition 2.4 and equation (3) to obtain an a priori estimate of the solution in $W^{1,\infty}(0,T;L^2)\cap L^\infty(0,T;H^2\cap H_2)$ for any arbitrary time T. Indeed, since equation (3) is equivalent to the integral equation

$$u(t) = U(t,0)u_0 - i\int_0^t U(t,s)F(u(s))\,ds,$$

we have, from Theorem 2.1 and Lemma 2.3,

$$\begin{aligned}
\|u(t)\|_{H^2\cap H_2} &\leq M_{T,\alpha,\rho}\|u_0\|_{H^2\cap H_2} + M_{T,\alpha,\rho}\int_0^t \|F(u(s))\|_{H^2\cap H_2}\,ds \\
&\leq M_{T,\alpha,\rho}\|u_0\|_{H^2\cap H_2} + M_{T,\alpha,\rho}\int_0^t \|u(s)\|_{H^1}^2\|u(s)\|_{H^2\cap H_2}\,ds \\
&\leq C^0_{T,\alpha,\rho}\left(1+\int_0^t \|u(s)\|_{H^2\cap H_2}\,ds\right),
\end{aligned}$$

where $C^0_{T,\alpha,\rho} > 0$ is a generic constant depending on the time T, on ρ, α and on $\|u_0\|_{H^2\cap H_2}$. We obtain from Gronwall lemma and from equation (3), that

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

Now, in view of Segal's theorem [9], the local solution we obtained previously exists globally because we have a uniform bound on the norm

$$\|u(t)\|_{H^2\cap H_2} + \|\partial_t u(t)\|_{L^2}.$$

Hence the proof of Theorem 2.2. □

3. Proof of Theorem 1 for a small time τ

The position of the nucleus is now unknown but solution of classical dynamics. We recall the system we are concerned with, for $\tau\in(0,T)$,

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

We are going to choose τ small enough in this section in order to prove first existence of solutions for this system. In the sequel we make assumption (2):

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

3.1. Structure of the proof of local existence

Let $\alpha>0$ and $\rho>0$ be such that

$$\alpha=\max(|v_0|,1)$$

and

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

We define the following subsets

$$\mathcal{B}_{\mathsf{e}}=\{\,u\in L^\infty(0,\tau;H^2\cap H_2)\cap W^{1,\infty}(0,\tau;L^2)\mid \\ \|u\|_{L^\infty(0,\tau;H^2\cap H_2)}\le 2M_{T,\alpha,\rho}\|u_0\|_{H^2\cap H_2}\,\}$$

and

$$\mathcal{B}_{\mathsf{n}}=\left\{\,a\in W^{2,1}(0,\tau)\,\middle|\,\left\|\frac{d^2a}{dt^2}\right\|_{L^1(0,\tau)}\le\alpha\right\}.$$

The indexes e and n stand for "electrons" and "nucleus", while $u(x,t)$ correspond to the wave function of the electrons and $a(t)$ to the position of the nucleus.

We will prove here a local-in-time existence result for system (1), using a Schauder fixed point theorem. One can find a similar result in reference [5], where in a first time, $V_1=0$. We shall need the following lemmas, whose proofs are postponed until the next subsections.

On the one hand, we consider the wave function of the electrons as known and the second order differential equation which modelize the movement of the nucleus is to be solved:

Lemma 3.1. *Let $u_0\in H^2\cap H_2$, a_0, $v_0\in\mathbb{R}$, and let $\tau>0$ be small enough. We set $u\in\mathcal{B}_{\mathsf{e}}$ and we consider the equation*

$$m\frac{d^2z}{dt^2}=\int_{\mathbb{R}^3}|u(x)|^2\frac{x-z}{|x-z|^3}\,dx-\nabla V_1(z)\quad\text{in }(0,\tau)\tag{14}$$

with initial data $z(0)=a_0$ and $\frac{dz}{dt}(0)=v_0$. Then equation (14) has a unique solution $z\in C([0,\tau])$ such that $z\in\mathcal{B}_{\mathsf{n}}$.

On the other hand, we know the position of the nucleus at any moment and we use the previous section to prove

Lemma 3.2. *Let a_0, $v_0 \in \mathbb{R}$ and $u_0 \in H^2 \cap H_2$, and let $\tau > 0$ be small enough. We set $y \in \mathcal{B}_{\mathsf{n}}$ and we consider the equation*

$$i\partial_t u + \Delta u + \frac{u}{|x-y|} + V_1 u = \left(|u|^2 * \frac{1}{|x|}\right)u \quad \text{in } \mathbb{R}^3 \times (0,\tau) \tag{15}$$

with initial data $u(0) = u_0$. Then equation (15) *has a unique solution $u \in L^\infty(0,\tau; H^2 \cap H_2) \cap W^{1,\infty}(0,\tau; L^2)$ such that u belongs to $\mathcal{B}_{\mathsf{e}}$.*

From Lemma 3.1 and 3.2, the following mappings are well defined:

$$\begin{aligned} \phi : \mathcal{B}_{\mathsf{e}} &\longrightarrow \mathcal{B}_{\mathsf{n}} & \qquad \psi : \mathcal{B}_{\mathsf{n}} &\longrightarrow \mathcal{B}_{\mathsf{e}} \\ u &\longmapsto z, & y &\longmapsto u, \end{aligned}$$

and we finally consider the application $\mathcal{G} = \phi \circ \psi$ which maps $\mathcal{B}_{\mathsf{n}}$ into itself, where $\mathcal{B}_{\mathsf{n}}$ is convex and bounded. We will also prove the following lemma later on.

Lemma 3.3. *The application $\mathcal{G} : \mathcal{B}_{\mathsf{n}} \to \mathcal{B}_{\mathsf{n}}$ is continuous and $\mathcal{G}(\mathcal{B}_{\mathsf{n}})$ is compact in $\mathcal{B}_{\mathsf{n}}$.*

Therefore, we will be allowed to apply the Schauder fixed point theorem and if $y \in \mathcal{B}_{\mathsf{n}}$ then, with $u = \psi(y)$ and $z = \mathcal{G}(y)$, it satisfies

$$\begin{cases} i\partial_t u + \Delta u + \frac{1}{|x-y|}u + V_1 u = \big(|u|^2 * \frac{1}{|x|}\big)u, & \text{in } \mathbb{R}^3 \times (0,\tau), \\ u(0) = u_0, & \text{in } \mathbb{R}^3, \\ m\frac{d^2z}{dt^2} = \int_{\mathbb{R}^3} -|u(x)|^2 \nabla \frac{1}{|x-z|}\,dx - \nabla V_1(z), & \text{in } (0,\tau), \\ z(0) = a_0, \qquad \frac{dz}{dt}(0) = v_0. \end{cases}$$

Then, there exists $a \in \mathcal{B}_{\mathsf{n}}$ such that $a = \mathcal{G}(a)$. Therefore $(\psi(a), a)$ is solution of (1) with $\psi(a) \in \mathcal{B}_{\mathsf{e}}$ and $a \in \mathcal{B}_{\mathsf{n}}$. The proof of Theorem 1.1 for a small time τ will then be completed with the proofs of Lemma 3.1, Lemma 3.2, and Lemma 3.3. □

3.2. Second order differential equation, proof of Lemma 3.1

We are considering an ordinary differential equation of type

$$\frac{d^2z}{dt^2} = G(t,z)$$

with two initial conditions. In order to construct the proof of Lemma 3.1, we need to prove a general lemma about existence and regularity of solution for this type of equation and to study the right hand side

$$G(t,z) = \int_{\mathbb{R}^3} -|u(t,x)|^2 \nabla\Big(\frac{1}{|x-z|}\Big)\,dx - \nabla V_1(t,z)$$

to make sure we can apply this general lemma to our situation. Although it is a rather classical result, we give a short proof of the following result:

Lemma 3.4. *Let $\tau > 0$. We consider the differential equation*

$$\begin{cases} \frac{d^2\varphi}{dt^2} = G(t,\varphi) & \text{in } (0,\tau) \\ \varphi(0) = \varphi_0, \quad \frac{d\varphi}{dt}(0) = \psi_0. \end{cases} \tag{16}$$

If τ is small enough and if $G \in L^1(0,\tau; W^{1,\infty}_{loc}(\mathbb{R}^3))$ then there exists a unique solution $\varphi \in C([0,\tau])$ to equation (16)*.*

Proof. We consider the application Φ on $C([0,\tau])$ defined by

$$\Phi(\varphi)(t) = \varphi_0 + \psi_0 t + \int_0^t (t-s) G(s,\varphi(s))\, ds, \qquad \forall t \in [0,\tau]. \tag{17}$$

We will use a Picard fixed point theorem in the space $C([0,\tau])$ in order to prove existence and uniqueness of a solution to equation (17).

Let $R > 4$ be such that $|\varphi_0| \le \frac{R}{2}$. We also assume that $\tau > 0$ is small enough such that we have

$$\tau \max(|\psi_0|, 1) < 1, \qquad \tau \|G\|_{L^1(0,\tau;W^{1,\infty}(B_R))} < 1 \tag{18}$$

where $B_R = \{x \in \mathbb{R}^3, |x| \le R\}$.

Let $\varphi \in C([0,\tau])$ be such that $\|\varphi\|_{C([0,\tau])} = \sup_{t\in[0,\tau]} |\varphi(t)| \le R$. Then, for all t in $[0,\tau]$ we can write

$$\begin{aligned} |\Phi(\varphi)(t)| &\le |\varphi_0| + |\psi_0 t| + \int_0^t (t-s) |G(s,\varphi(s))|\, ds \\ &\le \frac{R}{2} + \tau|\psi_0| + \tau \int_0^\tau \|G(s)\|_{W^{1,\infty}(B_R)}\, ds \\ &\le \frac{R}{2} + \tau|\psi_0| + \tau \|G\|_{L^1(0,\tau;W^{1,\infty}(B_R))} \\ &\le \frac{R}{2} + 1 + 1 \le R \end{aligned}$$

and we obtain $\|\Phi(\varphi)\|_{C([0,\tau])} \le R$.

We ensure here that Φ is a strict contraction in $C([0,\tau])$. Let $\varphi_1, \varphi_2 \in C([0,\tau])$ be such that $\|\varphi_1\|_{C([0,\tau])} \le R$ and $\|\varphi_2\|_{C([0,\tau])} \le R$. We have, for all t in $[0,\tau]$,

$$\begin{aligned} |(\Phi(\varphi_1) - \Phi(\varphi_2))(t)| &\le \int_0^t (t-s) |G(s,\varphi_1(s)) - G(s,\varphi_2(s))|\, ds \\ &\le \tau \int_0^\tau \|G(s)\|_{W^{1,\infty}(B_R)} |\varphi_1(s) - \varphi_2(s)|\, ds \\ &\le \tau \|G\|_{L^1(0,\tau;W^{1,\infty}(B_R))} \|\varphi_1 - \varphi_2\|_{C([0,\tau])}, \end{aligned}$$

and since from (18), $\tau > 0$ is small enough such that $\tau \|G\|_{L^1(0,\tau;W^{1,\infty}(B_R))} < 1$, then Φ is a strict contraction.

We apply the Picard fixed point theorem to application Φ. Thus, if $\tau > 0$ satisfies (18), there exists a unique $\varphi \in C([0,\tau])$ such that $\Phi(\varphi) = \varphi$. Moreover, equation (17) is an integral equation equivalent to (16), hence the end of the proof of Lemma 3.4. □

Proof of Lemma 3.1. From Lemma 3.4, it is easy to deduce that if the mapping

$$(t,z) \mapsto \int_{\mathbb{R}^3} |u(t,x)|^2 \frac{x-z}{|x-z|^3}\, dx - \nabla V_1(t,z)$$

belongs to $L^1(0,\tau;W^{1,\infty}_{\text{loc}})$ then equation (14) of Lemma 3.1 has a unique solution in $C([0,\tau])$. Since we assume from the very beginning that $\nabla V_1 \in L^2(0,T;W^{1,\infty}_{\text{loc}})$, we only have to work on $f(t,z) = \int_{\mathbb{R}^3} |u(t,x)|^2 \frac{x-z}{|x-z|^3}\, dx$.

Lemma 3.5. *We set $u_1, u_2 \in H^2$ and $g(z) = \int_{\mathbb{R}^3} \frac{u_1(x)\bar{u}_2(x)}{|x-z|^3}(x-z)\, dx$. Then $g \in W^{1,\infty}(\mathbb{R}^3)$ and there exists a real constant $C > 4$ such that*

$$\|g\|_{L^\infty} \le C \|\nabla u_1\|_{L^2} \|\nabla u_2\|_{L^2}$$
$$\|Dg\|_{L^\infty} \le C \|u_1\|_{H^2} \|u_2\|_{H^2}$$

Proof. From Cauchy-Schwarz and Hardy's inequality, for all $z \in \mathbb{R}^3$ we have

$$\begin{aligned} |g(z)| &\le \int_{\mathbb{R}^3} \frac{|u_1(x)||u_2(x)|}{|x-z|^2}\, dx \\ &\le \left(\int_{\mathbb{R}^3} \frac{|u_1(x)|^2}{|x-z|^2}\, dx \right)^{\frac{1}{2}} \left(\int_{\mathbb{R}^3} \frac{|u_2(x)|^2}{|x-z|^2}\, dx \right)^{\frac{1}{2}} \\ &\le 4 \|\nabla u_1\|_{L^2} \|\nabla u_2\|_{L^2} \end{aligned}$$

Therefore, $\|g\|_{L^\infty} \le C \|\nabla u_1\|_{L^2} \|\nabla u_2\|_{L^2}$. Then we set, for all z in $\mathbb{R}^3$,

$$h(z) = \int_{\mathbb{R}^3} \frac{u_1(x)\ \bar{u}_2(x)}{|x-z|}\, dx.$$

The function h is well defined since $|h(z)| \le C \|u_1\|_{L^2} \|\nabla u_2\|_{L^2}$ and one can notice that $g = \nabla h$ and $h = (u_1 \bar{u}_2) * \frac{1}{|x|}$. Then, we only have to prove that h belongs to $W^{2,\infty}(\mathbb{R}^3)$ with $\|D^2 h\|_{L^\infty} \le C \|u_1\|_{H^2} \|u_2\|_{H^2}$. We set $\partial_i = \frac{\partial}{\partial x_i}$ and from Cauchy-Schwarz and Hardy's inequalities, for all $i, j = 1, 2, 3$ we get

$$\begin{aligned} \|\partial_i h\|_{L^\infty} &\le \left\| \partial_i (u_1 \bar{u}_2) * \frac{1}{|x|} \right\|_{L^\infty} \\ &\le \left\| \int_{\mathbb{R}^3} \frac{\partial_i u_1(y) \bar{u}_2(y)}{|x-y|}\, dy \right\|_{L^\infty} + \left\| \int_{\mathbb{R}^3} \frac{u_1(y) \partial_i \bar{u}_2(y)}{|x-y|}\, dy \right\|_{L^\infty} \\ &\le 4 \|\nabla u_1\|_{L^2} \|\nabla u_2\|_{L^2} \end{aligned}$$

and in the same way,

$$\begin{aligned}\|\partial_i\partial_j h\|_{L^\infty} &\le \left\|\partial_i\partial_j(u_1\bar{u}_2) * \frac{1}{|x|}\right\|_{L^\infty}\\ &\le \left\|\int_{\mathbb{R}^3}\frac{\partial_i\partial_j u_1(y)\bar{u}_2(y)}{|x-y|}\,dy\right\|_{L^\infty} + \left\|\int_{\mathbb{R}^3}\frac{u_1(y)\partial_i\partial_j\bar{u}_2(y)}{|x-y|}\,dy\right\|_{L^\infty}\\ &\quad + \left\|\int_{\mathbb{R}^3}\frac{\partial_i u_1(y)\partial_j\bar{u}_2(y)}{|x-y|}\,dy\right\|_{L^\infty} + \left\|\int_{\mathbb{R}^3}\frac{\partial_j u_1(y)\partial_i\bar{u}_2(y)}{|x-y|}\,dy\right\|_{L^\infty}\\ &\le 2\|u_1\|_{H^2}\|\nabla u_2\|_{L^2} + 2\|\nabla u_1\|_{L^2}\|u_2\|_{H^2} + 8\|\nabla u_1\|_{H^1}\|\nabla u_2\|_{H^1}\\ &\le 12\|u_1\|_{H^2}\|u_2\|_{H^2}.\end{aligned}$$

Therefore, $h \in W^{2,\infty}(\mathbb{R}^3)$ and $g \in W^{1,\infty}(\mathbb{R}^3)$ with

$$\|Dg\|_{L^\infty} \le C\|u_1\|_{H^2}\|u_2\|_{H^2},$$

hence the proof of Lemma 3.5. □

Thereafter, setting $u(t) = u_1 = u_2$, we get $f(t,z) = g(z)$ and we proved that $f(t) \in W^{1,\infty}(\mathbb{R}^3)$ with $\|f(t)\|_{W^{1,\infty}} \le C\|u(t)\|^2_{H^2}$. Then,

$$\|f\|_{L^\infty(0,T;W^{1,\infty})} \le C\|u\|^2_{L^\infty(0,T;H^2)} \le 4CM^2_{T,\alpha,\rho}\|u_0\|^2_{H^2\cap H_2}$$

and $f \in L^\infty(0,T;W^{1,\infty})$. Thus, if $\tau > 0$ is small enough, we have proved the existence of a unique solution $z \in C([0,\tau])$ for equation (14). More precisely, in this particular situation of equation (16) where the initial conditions are $\varphi(0) = a_0$ and $\frac{d\varphi}{dt}(0) = v_0$ and the right hand side is

$$G : (t,\varphi) \mapsto \frac{1}{m}(f(t,\varphi) - \nabla V_1(t,\varphi)),$$

we obtain that actually, if $\tau > 0$ is small enough such that we have

$$\begin{gathered}\tau\alpha < 1,\\ \frac{4C}{m}\tau M^2_{T,\alpha,\rho}\|u_0\|^2_{H^2\cap H_2} + \frac{\sqrt{\tau}}{m}\|\nabla V_1\|_{L^2(0,T;W^{1,\infty}(B_R))} < \alpha,\end{gathered} \tag{19}$$

where we recall that $\alpha = \max(|v_0|, 1)$, $R \ge \max(2|a_0|, 4)$ and $C > 4$, then assumption (18) is satisfied.

Eventually, in order to end the proof of Lemma 3.1, we only have to check that $z = \phi(u)$ belongs to $\mathcal{B}_\mathsf{n}$. We take $u \in \mathcal{B}_\mathsf{e}$ and we will prove here that

$$z = \phi(u) \in W^{2,1}(0,\tau) \qquad \text{with} \qquad \left\|\frac{d^2z}{dt^2}\right\|_{L^1(0,\tau)} \le \alpha.$$

We already have $z \in C([0,\tau])$ and R is such that $\|z\|_{C([0,\tau])} \leq R$. We recall equation (14):

$$m\frac{d^2z}{dt^2} = \int_{\mathbb{R}^3} |u(x)|^2 \frac{x-z}{|x-z|^3}\,dx - \nabla V_1(z) = f(z) - \nabla V_1(z)$$

and since $f \in L^\infty(0,T;W^{1,\infty})$ and $\nabla V_1 \in L^2(0,T;W^{1,\infty}_{\mathrm{loc}})$, we obtain $\frac{d^2z}{dt^2} \in L^2(0,\tau)$, thus $z \in W^{2,2}(0,\tau) \subset W^{2,1}(0,\tau)$. Moreover,

$$\begin{aligned}\left|\frac{d^2z}{dt^2}(t)\right| &\leq \frac{1}{m}\int_{\mathbb{R}^3} \frac{|u(x,t)|^2}{|x-z(t)|^2}\,dx + \frac{1}{m}|\nabla V_1(t,z(t))| \\ &\leq \frac{4}{m}\|\nabla u\|^2_{L^\infty(0,\tau;L^2)} + \frac{1}{m}\|\nabla V_1(t)\|_{W^{1,\infty}(B_R)}.\end{aligned}$$

Using Cauchy-Schwarz inequality and the fact that $u \in \mathcal{B}_{\mathsf{e}}$, we get

$$\begin{aligned}\left\|\frac{d^2z}{dt^2}\right\|_{L^1(0,\tau)} &\leq \frac{4}{m}\tau\|\nabla u\|^2_{L^\infty(0,\tau;L^2)} + \frac{1}{m}\int_0^\tau \|\nabla V_1(s)\|_{W^{1,\infty}(B_R)}\,ds \\ &\leq \frac{4}{m}\tau\|\nabla u\|^2_{L^\infty(0,\tau;L^2)} + \frac{\sqrt{\tau}}{m}\|\nabla V_1\|_{L^2(0,T;W^{1,\infty}(B_R))} \\ &\leq \frac{16}{m}\tau M^2_{T,\alpha,\rho}\|u_0\|^2_{H^2\cap H_2} + \frac{\sqrt{\tau}}{m}\|\nabla V_1\|_{L^2(0,T;W^{1,\infty}(B_R))}\end{aligned}$$

and if we choose $\tau > 0$ small enough to have (19), we obtain $\left\|\frac{d^2z}{dt^2}\right\|_{L^1(0,\tau)} \leq \alpha$ which means $z \in \mathcal{B}_{\mathsf{n}}$ and the proof of Lemma 3.1 is complete. □

3.3. Nonlinear Schrödinger equation, proof of Lemma 3.2

We already proved in section 2 that under assumption (4) for V_1 and if a belongs to $W^{2,1}(0,T)$, then equation (3):

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

has a unique solution

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

such that $u(0) = u_0 \in H^2 \cap H_2$ for any arbitrary time $T > 0$. The proof is based upon an existence and regularity result for the linear equation and on a fixed point argument. Fortunately, if $y \in \mathcal{B}_{\mathsf{n}}$ then $y \in W^{2,1}(0,\tau)$ and we obtain that equation (15) with initial condition $u(0) = u_0 \in H^2 \cap H_2$

$$i\partial_t u + \Delta u + \frac{u}{|x-y(t)|} + V_1 u = \left(|u|^2 * \frac{1}{x}\right)u \qquad \text{in } \mathbb{R}^3 \times (0,\tau)$$

has a unique solution $u \in L^\infty(0,\tau;H^2 \cap H_2) \cap W^{1,\infty}(0,\tau;L^2)$.

Following the proof of the local existence of a solution to equation (3) in paragraph 2.1, since $y \in \mathcal{B}_{\mathsf{n}}$ implies

$$\left\| \frac{dy}{dt} \right\|_{L^\infty(0,\tau)} \leq \alpha,$$

then, as soon as $8\tau C_F M^3_{T,\alpha,\rho} \|u_0\|^2_{H^2\cap H_2} \leq 1$, we get

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

This means $u \in \mathcal{B}_{\mathsf{e}}$ if τ is small enough. Hence the proof of Lemma 3.2. □

3.4. Continuity and compactness, proof of Lemma 3.3

First step. Continuity of $\mathcal{G}$. We consider $y \in \mathcal{B}_{\mathsf{n}}$ and a sequence $(y_n)_{n\in\mathbb{N}}$ of elements of $\mathcal{B}_{\mathsf{n}}$ such that

$$y_n \overset{n\to+\infty}{\longrightarrow} y \quad \text{in} \quad W^{2,1}(0,\tau).$$

We aim at proving that

$$\mathcal{G}(y_n) \overset{n\to+\infty}{\longrightarrow} \mathcal{G}(y) \quad \text{in} \quad W^{2,1}(0,\tau).$$

We recall that $\mathcal{G} = \phi \circ \psi$ where

$$\begin{aligned} \phi : \mathcal{B}_{\mathsf{e}} &\longrightarrow \mathcal{B}_{\mathsf{n}} & \qquad \psi : \mathcal{B}_{\mathsf{n}} &\longrightarrow \mathcal{B}_{\mathsf{e}} \\ u &\longmapsto z, & y &\longmapsto u \end{aligned}$$

and we set

$$\begin{aligned} u &= \psi(y), \\ z &= \mathcal{G}(y) = \phi(u), \\ u_n &= \psi(y_n), \qquad\qquad \forall n \in \mathbb{N}, \\ z_n &= \mathcal{G}(y_n) = \phi(u_n), \ \forall n \in \mathbb{N}. \end{aligned}$$

Then, z and z_n satisfy on $(0,\tau)$ the equations

$$\begin{aligned} m\frac{d^2z}{dt^2} &= \int_{\mathbb{R}^3} -|u(x)|^2 \nabla\Big(\frac{1}{|x-z|}\Big)\,dx - \nabla V_1(z), \\ m\frac{d^2z_n}{dt^2} &= \int_{\mathbb{R}^3} -|u_n(x)|^2 \nabla\Big(\frac{1}{|x-z_n|}\Big)\,dx - \nabla V_1(z_n), \end{aligned}$$

and we will prove that $z_n \overset{n\to+\infty}{\longrightarrow} z$ in $W^{2,1}(0,\tau)$.

Since y and y_n belong to $\mathcal{B}_{\mathsf{n}}$ for all $n \in \mathbb{N}$, then u and u_n belong to $\mathcal{B}_{\mathsf{e}}$ for all $n \in \mathbb{N}$. It implies that $(u_n)_{n\in\mathbb{N}}$ is bounded in $L^\infty(0,\tau;H^2 \cap H_2) \cap W^{1,\infty}(0,\tau;L^2)$ and thus, up to a subsequence, we get the strong convergence

$$u_n \overset{n\to+\infty}{\longrightarrow} u \;\text{ in } L^\infty(0,\tau;H^1_{\text{loc}}). \tag{20}$$

We use here the following result of J. Simon [10, Theorem 5]:

Lemma 3.6. *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 $p=\infty$).*

In the same way, we have z and z_n belonging to $\mathcal{B}_{\mathsf{n}}$ for all $n \in \mathbb{N}$ (since $\phi(\mathcal{B}_{\mathsf{e}}) = \mathcal{B}_{\mathsf{n}}$) and $(z_n)_{n\in\mathbb{N}}$ bounded in $W^{2,1}(0,\tau)$ implies, up to a subsequence, that

$$z_n \overset{n\to+\infty}{\longrightarrow} z \quad \text{in } W^{1,1}(0,\tau). \tag{21}$$

We notice that $z_n - z$ satisfies

$$\begin{aligned}\frac{d^2(z_n-z)}{dt^2} = \frac{1}{m}\int_{\mathbb{R}^3}\left(|u(x)|^2\nabla\frac{1}{|x-z|} - |u_n(x)|^2\nabla\frac{1}{|x-z_n|}\right)dx&\\ + \frac{1}{m}\,\left(\nabla V_1(z) - \nabla V_1(z_n)\right).&\end{aligned}$$

We first remark that since $\nabla V_1 \in L^2(0,T;W^{1,\infty}_{\text{loc}})$, then for almost every t in $[0,\tau]$, $\nabla V_1(t)$ is locally Lipschitz. And since there exists $R>0$ such that we have $\|z\|_{C([0,\tau])} \le R$ and for all $n \in \mathbb{N}$, $\|z_n\|_{C([0,\tau])} \le R$ (as z and z_n belong to $\mathcal{B}_{\mathsf{n}}$), we obtain

$$|\nabla V_1(z) - \nabla V_1(z_n)| \le \|\nabla V_1(t)\|_{W^{1,\infty}(B_R)}|z_n(t) - z(t)|.$$

We also have

$$\begin{aligned}\int_{\mathbb{R}^3} u\bar{u}\,\nabla\frac{1}{|x-z|}\,dx - \int_{\mathbb{R}^3} u_n\bar{u}_n\,\nabla\frac{1}{|x-z_n|}\,dx&\\ = \int_{\mathbb{R}^3}(u-u_n)\bar{u}_n\,\nabla\frac{1}{|x-z_n|}\,dx - \int_{\mathbb{R}^3} u\bar{u}_n\,\nabla\frac{1}{|x-z_n|}\,dx&\\ + \int_{\mathbb{R}^3}\overline{(u-u_n)}u\,\nabla\frac{1}{|x-z|}\,dx + \int_{\mathbb{R}^3}\bar{u}_n u\,\nabla\frac{1}{|x-z|}\,dx&\\ = \int_{\mathbb{R}^3}(u-u_n)\bar{u}_n\,\nabla\frac{1}{|x-z_n|}\,dx + \int_{\mathbb{R}^3}\overline{(u-u_n)}u\,\nabla\frac{1}{|x-z|}\,dx&\\ + \int_{\mathbb{R}^3} u\bar{u}_n\left(\nabla\frac{1}{|x-z|} - \nabla\frac{1}{|x-z_n|}\right)dx.&\end{aligned}$$

On the one hand, we can prove that there exists a constant $C > 0$ such that

$$\left|\int_{\mathbb{R}^3} u(x,t)\bar{u}_n(x,t)\left(\nabla\frac{1}{|x-z(t)|} - \nabla\frac{1}{|x-z_n(t)|}\right)dx\right| \leq C|z_n(t) - z(t)|.$$

Indeed, using Lemma 3.5, since g is Lipschitz (here, $u_1 = u(t)$ and $u_2 = u_n(t)$), we have for all t in $[0,\tau]$,

$$\left|\int_{\mathbb{R}^3} \frac{u(x,t)\bar{u}_n(x,t)}{|x-z_n(t)|^3}(x-z_n(t))\,dx - \int_{\mathbb{R}^3} \frac{\bar{u}_n(x,t)u(x,t)}{|x-z(t)|^3}(x-z(t))\,dx\right| \\ = |g(z_n(t)) - g(z(t))| \leq C\|u(t)\|_{H^2}\|u_n(t)\|_{H^2}|(z_n - z)(t)|,$$

and since u and u_n belong to $\mathcal{B}_{\mathsf{e}}$, $\|u(t)\|_{H^2}$ and $\|u_n(t)\|_{H^2}$ are bounded independently of n.

On the other hand, we can deal with both of the two other terms in the same way. For instance, we have in fact for any $R > 0$, from Hardy's inequality,

$$\begin{aligned}&\left|\int_{\mathbb{R}^3}(u-u_n)(x,t)\bar{u}_n(x,t)\nabla\frac{1}{|x-z_n(t)|}\,dx\right| \\ &\quad\leq \int_{B(0,R)}\frac{|(u-u_n)(x,t)||u_n(x,t)|}{|x-z_n(t)|^2}\,dx + \int_{B(0,R)^C}\frac{|(u-u_n)(x,t)||u_n(x,t)|}{|x-z_n(t)|^2}\,dx \\ &\quad\leq C\|(u-u_n)(t)\|_{H^1(B(0,R))}\|u_n(t)\|_{H^1} + \frac{C}{R^2}\|u_n(t)\|_{L^2}(\|u_n(t)\|_{L^2} + \|u(t)\|_{L^2})\end{aligned}$$

and since u and u_n belong to $\mathcal{B}_{\mathsf{e}}$ for all $n \in \mathbb{N}$, then

$$\left|\int_{\mathbb{R}^3}(u-u_n)\bar{u}_n\ \nabla\frac{1}{|x-z_n|}\,dx\right| \leq C\|u-u_n\|_{L^\infty(0,\tau;H^1(B(0,R)))} + \frac{C}{R^2}.$$

Thus, for all $\varepsilon > 0$, there exists $R > 0$ such that $\frac{C}{R^2} \leq \frac{\varepsilon}{2}$ and from (20) there exists $N_0 \in \mathbb{N}$ such that

$$C\|u-u_n\|_{L^\infty(0,\tau;H^1(B(0,R))} \leq \frac{\varepsilon}{2}, \quad \forall n \geq N_0.$$

We get

$$\forall\varepsilon > 0, \quad \exists N_0 \in \mathbb{N}, \quad \forall n \geq N_0, \qquad \left|\int_{\mathbb{R}^3}(u-u_n)\bar{u}_n\nabla\frac{1}{|x-z_n|}\,dx\right| \leq \varepsilon.$$

Eventually, we obtain that for all t in $(0,\tau)$ and for all $\varepsilon > 0$,

$$\left|\left(\frac{d^2z_n}{dt^2} - \frac{d^2z}{dt^2}\right)(t)\right| \leq C\big(1 + \|\nabla V_1(t)\|_{W^{1,\infty}(B_R)}\big)|z_n(t) - z(t)| + 2\varepsilon,$$

then

$$\left\| \frac{d^2 z_n}{dt^2} - \frac{d^2 z}{dt^2} \right\|_{L^1(0,\tau)} \le C_\tau \big(1+\|\nabla V_1\|_{L^2(0,T;W^{1,\infty}(B_R))}\big)\|z_n - z\|_{L^\infty(0,\tau)} + 2\varepsilon.$$

Therefore, since we have the strong convergence (21) and $W^{1,1}(0,\tau) \hookrightarrow L^\infty(0,\tau)$, we obtain

$$\frac{d^2 z_n}{dt^2} \overset{n\to+\infty}{\longrightarrow} \frac{d^2 z}{dt^2} \quad \text{in } L^1(0,\tau),$$

what means $\mathcal{G}(y_n) \overset{n\to+\infty}{\longrightarrow} \mathcal{G}(y)$ in $W^{2,1}(0,\tau)$ and $\mathcal{G}$ is continuous.

Second step. Compactness of $\mathcal{G}(\mathcal{B}_{\mathsf{n}})$ in $\mathcal{B}_{\mathsf{n}}$. We consider a sequence $(y_n)_{n\in\mathbb{N}}$ of elements of $\mathcal{B}_{\mathsf{n}}$ and we aim at proving that $z_n = \mathcal{G}(y_n)$ is precompact in $\mathcal{B}_{\mathsf{n}}$. If we set

$$f_n(t,z) = \int_{\mathbb{R}^3} |u_n(t,x)|^2 \frac{x - z(t)}{|x - z(t)|^3}\, dx,$$

then we have

$$\frac{d^2 z_n}{dt^2}(t) = f_n(t, z_n(t)) - \nabla V_1(t, z_n(t)).$$

We will first prove that $\tilde{f}_n : t \mapsto f_n(t, z_n(t)) = \tilde{f}_n(t)$ is bounded in $C^{0,\frac{1}{2}}([0,\tau])$ as soon as $z_n \in \mathcal{B}_{\mathsf{n}}$. Let t, h in $[0,\tau]$ be such that $t+h \in [0,\tau]$. Using again Lemma 3.5, we can write

$$\begin{aligned}
\left|\tilde{f}_n(t+h) - \tilde{f}_n(t)\right| &= |f(t+h, z_n(t+h)) - f(t, z_n(t))| \\
&\le \left| \int_{\mathbb{R}^3} (u_n(t+h) - u_n(t))\bar{u}_n(t+h)\ \nabla \frac{1}{|x - z_n(t+h)|}\, dx \right| \\
&\quad + \left| \int_{\mathbb{R}^3} (\bar{u}_n(t+h) - \bar{u}_n(t)) u_n(t)\ \nabla \frac{1}{|x - z_n(t)|}\, dx \right| \\
&\quad + \left| \int_{\mathbb{R}^3} u_n(t)\bar{u}_n(t+h) \left(\nabla \frac{1}{|x - z_n(t)|} - \nabla \frac{1}{|x - z_n(t+h)|} \right) dx \right| \\
&\le \int_{\mathbb{R}^3} \frac{|u_n(t+h) - u_n(t)||u_n(t+h)|}{|x - z_n(t+h)|^2}\, dx \\
&\quad + \int_{\mathbb{R}^3} \frac{|u_n(t+h) - u_n(t)||u_n(t)|}{|x - z_n(t)|^2}\, dx \\
&\quad + C\|u_n(t)\|_{H^2}\|u_n(t+h)\|_{H^2}|(z_n(t+h) - z_n(t)| \\
&\le C\|u_n\|_{L^\infty(0,\tau;H^1)}\|u_n(t+h) - u_n(t)\|_{H^1} \\
&\quad + C\|u_n\|^2_{L^\infty(0,\tau;H^2)}|(z_n(t+h) - z_n(t)|.
\end{aligned}$$

Moreover, on the one hand, since $(z_n)_{n\in\mathbb{N}}$ belongs $\mathcal{B}_{\mathsf{n}}$, we have

$$|(z_n(t+h) - z_n(t)| \leq h\left\|\frac{dz_n}{dt}\right\|_{L^\infty(0,\tau)} \leq C_{\tau,\alpha} h^{\frac{1}{2}}$$

and on the other hand, using the Fourier transform, we can prove that

$$\|u_n(t+h) - u_n(t)\|_{L^2} \leq h\|\partial_t u_n\|_{L^\infty(0,\tau;L^2)},$$
$$\|u_n(t+h) - u_n(t)\|_{H^2} \leq 2\|u_n\|_{L^\infty(0,\tau;H^2)}$$

imply

$$\|u_n(t+h) - u_n(t)\|_{L^2} \leq C^0_{\tau,\alpha,\rho} h^{\frac{1}{2}}$$

where $C^0_{\tau,\alpha,\rho} > 0$ only depends on τ, $\|u_0\|_{H^2\cap H_2}$, ρ, and α. Therefore,

$$\left|\tilde{f}_n(t+h) - \tilde{f}_n(t)\right| \leq C^0_{\tau,\alpha,\rho} h^{\frac{1}{2}} \qquad \text{and} \qquad \tilde{f}_n \in C^{0,\frac{1}{2}}([0,\tau])$$

and we obtain $(\tilde{f}_n)_{n\in\mathbb{N}}$ bounded in $C^{0,\frac{1}{2}}([0,\tau])$. In addition, since $(z_n)_{n\in\mathbb{N}}$ is bounded in $W^{2,1}(0,\tau)$ and since $(u_n)_{n\in\mathbb{N}}$ is bounded in $\mathcal{B}_{\mathsf{e}}$, we have, up to a subsequence,

$$z_n \overset{n\to+\infty}{\longrightarrow} z \quad \text{in } W^{1,1}(0,\tau) \cap C([0,T])$$

and

$$u_n \overset{n\to+\infty}{\longrightarrow} u \quad \text{in } L^\infty(0,\tau; H^1_{\text{loc}}).$$

Thereafter, the fact that we have the compact injection

$$C^{0,\frac{1}{2}}(0,\tau) \hookrightarrow C([0,\tau])$$

(from Ascoli's theorem), implies, up to a subsequence, the strong convergence

$$\tilde{f}_n \overset{n\to+\infty}{\longrightarrow} \tilde{f} \quad \text{in } C([0,\tau]) \quad \text{where } \tilde{f}(t) = \int_{\mathbb{R}^3} |u(t,x)|^2 \frac{x - z(t)}{|x-z(t)|^3}\, dx.$$

Finally, since $\nabla V_1 \in L^2(0,T; W^{1,\infty}_{\text{loc}})$ and $z_n \overset{n\to+\infty}{\longrightarrow} z$ in $L^\infty(0,\tau)$, we also obtain, from

$$\|\nabla V_1(z_n) - \nabla V_1(z)\|_{L^2(0,T)} \leq \|\nabla V_1(t)\|_{L^2(0,T;W^{1,\infty}(B(0,\alpha)))} \|z_n - z\|_{L^\infty(0,\tau)},$$

that

$$\nabla V_1(z_n) \overset{n\to+\infty}{\longrightarrow} \nabla V_1(z) \ \text{ in } \ L^2(0,\tau).$$

Eventually, $\left(\frac{d^2 z_n}{dt^2}\right)_{n\in\mathbb{N}}$ converges in $L^2(0,\tau)$ as the sum of $(\tilde{f}_n)_{n\in\mathbb{N}}$ and $(\nabla V_1(z_n))_{n\in\mathbb{N}}$. Then, $(z_n = \mathcal{G}(y_n))_{n\in\mathbb{N}}$ is precompact in $W^{2,2}(0,\tau)$ thus in $\mathcal{B}_{\mathsf{n}}$.

Hence the end of the proof of Lemma 3.3. □

4. Global existence of solutions

We recall the coupled system (1) for an arbitrary time T:

$$i\partial_t u + \Delta u + \frac{1}{|x-a|}u + V_1 u = \Big(|u|^2 * \frac{1}{|x|}\Big)u, \qquad \text{in } \mathbb{R}^3 \times (0,T), \tag{22}$$

$$u(0) = u_0, \qquad \text{on } \mathbb{R}^3,$$

$$m\frac{d^2a}{dt^2} = \int_{\mathbb{R}^3} -|u(x)|^2 \nabla \frac{1}{|x-a|}\,dx - \nabla V_1(a), \qquad \text{in } (0,T), \tag{23}$$

$$a(0) = a_0, \qquad \partial_t a(0) = v_0,$$

and we consider a solution (u,a) in $W^{1,\infty}(0,T;L^2)\cap L^\infty(0,T;H^2\cap H_2)\times W^{2,1}(0,T)$. We will prove here Proposition 1.2.

The global approach is the same as for the a priori estimate of the energy for the nonlinear Schrödinger equation with $a(t)$ known. Indeed, on the one hand, using equation (22) we have

$$\frac{d}{dt}\Big(\int_{\mathbb{R}^3}|\nabla u|^2 + \frac{1}{2}\int_{\mathbb{R}^3}\Big(|u|^2 * \frac{1}{|x|}\Big)|u|^2 - \int_{\mathbb{R}^3}\Big(\frac{1}{|x-a|} + V_1\Big)|u|^2\Big) = -\int_{\mathbb{R}^3}\Big(\partial_t \frac{1}{|x-a|} + \partial_t V_1\Big)|u|^2 \tag{24}$$

and on the other hand, since $\nabla\frac{1}{|x-a|} = \frac{a-x}{|x-a|^3}$, when we multiply (23) by $\frac{da}{dt}$ we get

$$\frac{m}{2}\frac{d}{dt}\Big(\Big|\frac{da}{dt}\Big|^2\Big) = \int_{\mathbb{R}^3}|u(x)|^2\frac{da}{dt}\cdot\frac{x-a}{|x-a|^3}\,dx - \nabla V_1(a)\cdot\frac{da}{dt}. \tag{25}$$

Now $\partial_t\big(\frac{1}{|x-a|}\big) = \frac{da}{dt}\cdot\frac{x-a}{|x-a|^3}$ and the sum of (24) and (25) gives

$$\begin{aligned}\frac{d}{dt}\Big(\int_{\mathbb{R}^3}|\nabla u|^2 + \frac{m}{2}\Big|\frac{da}{dt}\Big|^2 + \frac{1}{2}\int_{\mathbb{R}^3}\Big(|u|^2 * \frac{1}{|x|}\Big)|u|^2 - \int_{\mathbb{R}^3}\Big(\frac{1}{|x-a|} + V_1\Big)|u|^2\Big)& \\ = -\nabla V_1(a)\cdot\frac{da}{dt} - \int_{\mathbb{R}^3}\partial_t V_1|u|^2& \\ = -\frac{dV_1}{dt}(a) + \partial_t V_1(a) - \int_{\mathbb{R}^3}\partial_t V_1|u|^2.&\end{aligned}$$

Moreover, from assumption (2), V_1 satisfies $\frac{\partial_t V_1}{1+|x|^2} \in L^1(0,T;L^\infty(\mathbb{R}^3))$ and we have

$$\partial_t V_1(a) - \int_{\mathbb{R}^3}\partial_t V_1|u|^2 \le \Big\|\frac{\partial_t V_1(t)}{1+|x|^2}\Big\|_{L^\infty}(1 + |a(t)|^2 + \|u(t)\|_{H_1}^2)$$

and in order to get an H_1-estimate of u, we then calculate the imaginary part of the product of equation (22) by $(1+|x|^2)\bar{u}(x)$, integrated over $\mathbb{R}^3$. This gives

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

We define E at time t of $[0,T]$ by

$$E(t) = \int_{\mathbb{R}^3}|\nabla u(t,x)|^2\,dx + \lambda\int_{\mathbb{R}^3}(1+|x|^2)|u(t,x)|^2\,dx + \frac{m}{2}\left|\frac{da(t)}{dt}\right|^2 + \frac{1}{2}\int_{\mathbb{R}^3}\left(|u(t,x)|^2 * \frac{1}{|x|}\right)|u(t,x)|^2\,dx$$

where λ is a non-negative constant to be precised later. We obviously have a constant $C>0$ depending on λ such that

$$\frac{dE(t)}{dt} \leq \frac{d}{dt}\left(-V_1(t,a(t)) + \int_{\mathbb{R}^3}\left(\frac{1}{|x-a(t)|} + V_1(t)\right)|u(t)|^2\right) + C\left(1+\left\|\frac{\partial_t V_1(t)}{1+|x|^2}\right\|_{L^\infty}\right)E(t) + \left\|\frac{\partial_t V_1(t)}{1+|x|^2}\right\|_{L^\infty}(1+|a(t)|^2)$$

and if we set $\beta = \left\|\frac{\partial_t V_1}{1+|x|^2}\right\|_{L^\infty} \in L^1(0,T)$ and integrate over $(0,t)$, we obtain

$$\begin{aligned} E(t) \leq E(0) + V_1(0,a_0) &+ \int_{\mathbb{R}^3}\left(\frac{1}{|x-a_0|} + |V_1(0)|\right)|u_0|^2 \\ &+ |V_1(t,a(t))| + \int_{\mathbb{R}^3}\left(\frac{1}{|x-a(t)|} + V_1(t)\right)|u(t)|^2 \\ &+ C\int_0^t \left(1+\beta(s)\right)E(s) + \beta(s)(1+|a(s)|^2)\,ds \end{aligned}$$

Then, as shown in subsection 2.2, we have

$$\int_{\mathbb{R}^3}\frac{|u(t,x)|^2}{|x-a(t)|}\,dx \leq \eta\|\nabla u(t)\|_{L^2}^2 + \frac{1}{4\eta}\|u_0\|_{L^2}^2, \quad \forall \eta>0,$$

$$\int_{\mathbb{R}^3}V_1(t,x)|u(t,x)|^2\,dx \leq \left\|\frac{V_1}{1+|x|^2}\right\|_{L^\infty((0,T)\times\mathbb{R}^3)}\|u(t)\|_{H_1}^2,$$

and

$$\int_{\mathbb{R}^3}\left(\frac{1}{|x-a_0|} + |V_1(0,x)|\right)|u_0(x)|^2\,dx \leq \|u_0\|_{H^1\cap H_1}^2.$$

Moreover, for all t in $[0,T]$,

$$|V_1(t,a(t))| \leq \left\| \frac{V_1}{1+|x|^2} \right\|_{L^\infty(0,T;L^\infty)} (1+|a(t)|^2)$$

and we also notice that

$$E(0) \leq C\|u_0\|^2_{H^1\cap H_1} + \frac{m}{2}|v_0|^2 + C\|u_0\|_{H^1}\|u_0\|^3_{L^2}.$$

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

$$\begin{aligned} E(t) \leq{}& C\|u_0\|^2_{H^1\cap H_1} + \frac{m}{2}|v_0|^2 + C\|u_0\|_{H^1}\|u_0\|^3_{L^2} + C(1+|a_0|^2) \\ &+ \frac{1}{2}\|u(t)\|^2_{H^1} + \Big(\lambda - \frac{1}{2}\Big)\|u(t)\|^2_{H_1} + C(1+|a(t)|^2) \\ &+ C\int_0^t (1+\beta(s))E(s) + \beta(s)(1+|a(s)|^2)\,ds. \end{aligned} \tag{26}$$

We define F at time t of $[0,T]$ by

$$\begin{aligned} F(t) = \int_{\mathbb{R}^3} |\nabla u(t,x)|^2\,dx + \int_{\mathbb{R}^3}(1+|x|^2)|u(t,x)|^2\,dx + m\left|\frac{da}{dt}(t)\right|^2 \\ + \int_{\mathbb{R}^3}\left(|u(t,x)|^2 * \frac{1}{|x|}\right)|u(t,x)|^2 \end{aligned}$$

and it is easy to deduce from (26) that we have, for all t in $[0,T]$,

$$\begin{aligned} F(t) \leq C(1 + \|u_0\|^2_{H^1\cap H_1} + |a_0|^2 + |v_0|^2 + \|u_0\|_{H^1}\|u_0\|^3_{L^2}) \\ + C(1+|a(t)|^2) + C\int_0^t (1+\beta(s))F(s) + \beta(s)(1+|a(s)|^2)\,ds. \end{aligned}$$

Then, we set

$$\begin{aligned} \Psi(t) = (1+|a(t)|^2) + \int_0^t (1+\beta(s))F(s) + \beta(s)(1+|a(s)|^2)\,ds \\ + 1 + \|u_0\|^2_{H^1\cap H_1} + |a_0|^2 + |v_0|^2 + \|u_0\|_{H^1}\|u_0\|^3_{L^2} \end{aligned}$$

and we have $F(t) \leq C\Psi(t)$, $\Psi(0) = 1 + \|u_0\|^2_{H^1\cap H_1} + |a_0|^2 + |v_0|^2 + \|u_0\|_{H^1}\|u_0\|^3_{L^2}$ and since $C > 0$ denotes a generic constant,

$$\begin{aligned} \frac{d\Psi}{dt}(t) &= 2|a(t)|\left|\frac{da}{dt}(t)\right| + (1+\beta(t))F(t) + \beta(t)(1+|a(t)|^2) \\ &\leq C\sqrt{\Psi(t)}\sqrt{F(t)} + C(1+\beta(t))\Psi(t) + \beta(t)\Psi(t) \\ &\leq C(1+\beta(t))\Psi(t). \end{aligned}$$

From Gronwall's lemma, we then get

$$\Psi(t) \leq C_T \exp\left(\int_0^t \beta(s)ds\right)\Psi(0).$$

Therefore, there exists a non-negative constant K^0_{T,ρ_0} depending on the time T, on the initial data $\|u_0\|_{H^1\cap H_1}$, $|a_0|$ and $|v_0|$ and on $\rho_0 > 0$, where

$$\left\|\frac{V_1}{1+|x|^2}\right\|_{W^{1,1}(0,T,L^\infty)} \leq \rho_0,$$

such that for all t in $[0,T]$,

$$\|u(t)\|_{H^1\cap H_1} + m\left|\frac{da}{dt}(t)\right| + \left(\int_{\mathbb{R}^3}\left(|u(t)|^2 * \frac{1}{|x|}\right)|u(t)|^2\right)^{\frac{1}{2}} \leq K^0_{T,\rho_0}. \tag{27}$$

Notice that this estimate does not use any assumption on ∇V_1. Of course, we also obtain that a is bounded on $[0,T]$ which means that there exists $R>0$, depending on T, ρ_0, $\|u_0\|_{H^1\cap H_1}$, $|a_0|$, and $|v_0|$, such that for all t in $[0,T]$, $|a(t)| \leq R$.

Moreover, from equation (23) and since a is bounded, we have

$$\begin{aligned} m\left|\frac{d^2a}{dt^2}(t)\right| &\leq \int_{\mathbb{R}^3} \frac{|u(t,x)|^2}{|x-a(t)|^2}\,dx + |\nabla V_1(t,a(t))| \\ &\leq 4\,\|u(t)\|^2_{H^1} + \|\nabla V_1(t)\|_{W^{1,\infty}(B_R)} \end{aligned}$$

and if we define $\rho_1 > 0$ such that

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

we obtain from (27) that there exists a constant $K^0_{T,\rho_1} > 0$ depending on T, $\|u_0\|_{H^1\cap H_1}$, $|a_0|$, $|v_0|$, and ρ_1 such that

$$\begin{aligned} m\left\|\frac{d^2a}{dt^2}\right\|_{L^1(0,T)} &\leq 4T\|u\|^2_{L^\infty(0,T;H^1)} + \sqrt{T}\|\nabla V_1\|_{L^2(0,T;W^{1,\infty}(B_R))} \\ &\leq 4T(K^0_{T,\rho_0})^2 + \sqrt{T}\|\nabla V_1\|_{L^2(0,T;W^{1,\infty}(B_R))} \leq K^0_{T,\rho_1}. \end{aligned}$$

Now, we can use estimate (27) and equation (22) to obtain the estimate of Proposition 1.2. Indeed, since equations (22) is equivalent to the integral equation

$$u(t) = U(t,0)u_0 - i\int_0^t U(t,s)F(u(s))\,ds,$$

we have, from Theorem 2.1 and from Lemma 2.3,

$$\begin{aligned}\|u(t)\|_{H^2\cap H_2} &\leq M_{T,\alpha,\rho}\|u_0\|_{H^2\cap H_2} + M_{T,\alpha,\rho}\int_0^t \|F(u(s))\|_{H^2\cap H_2}\,ds\\ &\leq M_{T,\alpha,\rho}\|u_0\|_{H^2\cap H_2} + M_{T,\alpha,\rho}\int_0^t \|u(s)\|_{H^1}^2\|u(s)\|_{H^2\cap H_2}\,ds\end{aligned}$$

where $\alpha = \frac{K^0_{T,\rho_1}}{m}$. Therefore, we can deduce from estimate (27) that there exists a constant C^0_{T,ρ_1} such that

$$\|u(t)\|_{H^2\cap H_2} \leq C^0_{T,\rho_1}\|u_0\|_{H^2\cap H_2} + C^0_{T,\rho_1}\int_0^t \|u(s)\|_{H^2\cap H_2}\,ds.$$

Eventually, from Gronwall lemma, we get

$$\forall t\in[0,T],\quad \|u(t)\|_{H^2\cap H_2} \leq e^{C^0_{T,\rho_1}T}\|u_0\|_{H^2\cap H_2}.$$

It is then easy to estimate $\|\partial_t u(t)\|_{L^2}$ using equation (22). Hence the end of the proof of Proposition 1.2. $\square$

We will conclude here the proof of Theorem 1.1. We begin by setting an arbitrary time $T > 0$. We already obtained the local-in-time existence of solutions for the coupled problem. Indeed, by now, we have a solution (u,a) for the system (1) in the class

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

where $\|a\|_{C([0,\tau])} \leq R$ and τ satisfies

$$\begin{gathered}\tau\alpha < 1,\\ 8\tau C_F M^3_{T,\alpha}\|u_0\|^2_{H^2\cap H_2} < 1,\\ \frac{4C}{m}\tau M^2_{T,\alpha}\|u_0\|^2_{H^2\cap H_2} + \frac{\sqrt{\tau}}{m}\|\nabla V_1\|_{L^2(0,T;W^{1,\infty}(B_R))} < \alpha,\end{gathered}\tag{28}$$

where $\alpha = \max(|v_0|,1)$ and $C > 4$.

Let us consider the maximal time T_0 such that (1) has a maximal solution defined on $[0,T_0[$ in the class mentioned above. From Proposition 1.2, we have a local uniform estimate on the following norm of (u,a):

$$\|u(t)\|_{H^2\cap H_2} + \|\partial_t u(t)\|_{L^2} + \left\|\frac{d^2a}{dt^2}\right\|_{L^1(0,T)} + \left|\frac{da}{dt}(t)\right|$$

which means that this quantity remains bounded for t less or equal to T. Therefore, as one can read in [9], and in [5, 6], global existence follows. Indeed, if (u,a) is a maximal solution on $[0, T_0[$ with $T_0 < T$, then its norm in the ad hoc class has to blow up when t reaches the maximal time T_0. However, if we consider $s \in [0, T_0[$ close enough to T_0 and if we take T^* as the largest τ satisfying

$$\tau \max(|v_s|, 1) < 1$$
$$8\tau C_F M^3_{T,|v_s|} \|u_s\|^2_{H^2\cap H_2} < 1$$
$$\frac{4C}{m}\tau M^2_{T,|v_s|}\|u_s\|^2_{H^2\cap H_2} + \frac{\sqrt{\tau}}{m}\|\nabla V_1\|_{L^2(0,T;W^{1,\infty}(B_R))} < \max(|v_s|, 1),$$

where $\frac{da}{dt}(s) = v_s$ and $u(s) = u_s$, then we can bound the norm of (u, a) for all t in $[s, s + T^*]$ which brings a contradiction since $T_0 \in [s, s + T^*]$. The important point is that T^* only depends on the time T since $\|u_s\|_{H^2\cap H_2}$ and $|v_s|$ are bounded by the local uniform estimate of Proposition 1.2. Thus, for any arbitrary time T we have a solution (u, a) to the system (1) such that

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

and the proof of Theorem 1.1 in then complete. □

References

[1] L. Baudouin, *Contributions à l'étude de l'équation de Schrödinger : problème inverse en domaine borné et contrôle optimal bilinéaire d'une équation de Hartree-Fock*, Thése, 2004.

[2] ———, *A bilinear optimal control problem applied to a time dependent Hartree-Fock equation coupled with classical nuclear dynamics*, preprint.

[3] L. Baudouin, O. Kavian, and J.-P. Puel, *Regularity for a Schrödinger equation with a singular potentials and application to bilinear optimal control*, J. Differential Equations, to appear.

[4] ———, *Régularité dans une équation de Schrödinger avec potentiel singulier à distance finie et à l'infini*, C. R. Math. Acad. Sci. Paris **337** (2003), no. 11, 705–710.

[5] E. Cancès and C. Le Bris, *On the time-dependent Hartree-Fock equations coupled with a classical nuclear dynamics*, Math. Models Methods Appl. Sci. **9** (1999), no. 7, 963–990.

[6] J. M. Chadam and R. T. Glassey, *Global existence of solutions to the Cauchy problem for time-dependent Hartree equations*, J. Mathematical Phys. **16** (1975), 1122–1130.

[7] R. J. Iório Jr. and D. Marchesin, *On the Schrödinger equation with time-dependent electric fields*, Proc. Roy. Soc. Edinburgh Sect. A **96** (1984), no. 1-2, 117–134.

[8] T. Kato, *Linear evolution equations of "hyperbolic" type*, J. Fac. Sci. Univ. Tokyo Sect. I **17** (1970), 241–258.

[9] I. Segal, *Non-linear semi-groups*, Ann. of Math. (2) **78** (1963), 339–364.

[10] J. Simon, *Compact sets in the space $L^p(0, T; B)$*, Ann. Mat. Pura Appl. (4) **146** (1987), 65–96.

[11] K. Yajima, *Existence of solutions for Schrödinger evolution equations*, Comm. Math. Phys. **110** (1987), no. 3, 415–426.