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HIGHER ORDER SCHRÖDINGER AND HARTREE-FOCK EQUATIONS

RÉMI CARLES AND EMMANUEL MOULAY

ABSTRACT. In this article, we extend the domain of validity of the higher order Schrödinger equations to the use of a Coulomb potential. Then we develop the higher order Hartree-Fock equations with bounded and Coulomb potentials.

1. INTRODUCTION

The higher order Schrödinger equations have been developed in [5, 25]. They are Schrödinger type equations involving a higher order Schrödinger operator [10, 16, 21, 23] and dedicated to particles whose norm of their velocity vector is below $c/\sqrt{2}$. They are an interpolation between Schrödinger and relativistic equations, valid in the semi-relativistic domain between non-relativistic and ultra-relativistic extremes. The fundamental Schrödinger equation was published in 1926 by Erwin Schrödinger in [39]. The semi-relativistic equation is studied for instance in [19, 20]. The existence of a solution of the higher order Schrödinger equations is studied without potential for free particles in [5, 25]. The case of bounded potential (particles in finite potential wells) and of linear potentials (neutrons in free fall in the gravity field and electrons accelerated by an electric field) is treated in [5]. Moreover, the higher order Schrödinger operator with quasi-periodic potentials in dimension two is developed in [23].

The Hartree equation was developed by Douglas Rayner Hartree in the 20s [12]. It arises in the mean-field limit of large systems of identical bosons, as for instance the Gross-Pitaevskii equation in a Bose-Einstein condensate [18, 33], by taking into account the self interaction between bosons. A semi-relativistic version of the Hartree equation was developed in [11, 27] for modeling boson stars. The Hartree-Fock equation was also developed by Vladimir Aleksandrovich Fock [13]. It is dedicated to large systems of identical fermions with applications in electronic structure theory by taking into account the self interaction between charged fermions plus an exchange term which is a consequence of the Pauli principle. A semi-relativistic version of the Hartree-Fock equation was developed in [14] for modeling white dwarfs. The Hartree equation is also used for fermions as an approximation of the Hartree-Fock equation where spin effects are neglected. The Hartree and Hartree-Fock equations are used for several applications in many-particle physics [31, Section 2.2].

The first idea of this article is to extend the scope of the higher order Schrödinger equations to the Coulomb potential by using a perturbation theory. The Coulomb potential has been widely studied for the Schrödinger equation, see for instance [17, 26, 38, 35, 44]. It is possible to use the higher order Schrödinger equations

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with a Coulomb potential for the alpha particles which are fast charged semi-relativistic particles coming from the alpha decay and composed of two protons and two neutrons [30]. Maximum alpha particle velocities are on the order of one-tenth of the speed of light [40, 42]. The second idea of this article is to develop higher order Hartree-Fock equations with bounded and Coulomb potentials which are able to take into account some relativistic effects in many-particle physics, as for instance the electrons of heavy atoms in quantum chemistry [22, 34, 43], the semi-relativistic electron gas in a finite potential well [32, Section 4.2], the metal clusters [31, Section 2.2.1] or the modeling of white dwarfs [14].

The paper is organized as follows. After some notations and definitions given in Section 2, the case of the higher order Schrödinger equations with a Coulomb potential is studied in Section 3. The Section 4 is devoted to the Cauchy problem of the higher order Hartree-Fock equations with a bounded potential. The Cauchy problem of the higher order Hartree-Fock equations with a Coulomb potential is addressed in Section 5. Finally, a conclusion is given in Section 6.

2. NOTATIONS AND DEFINITIONS

The wave function of a particle is denoted by $\psi(t, x)$ where x is the position of the particle and t the time. Moreover, ψ stands for $\psi(t, x)$. $\Delta := \nabla^2$ denotes the Laplace operator.

For $x \in \mathbf{R}^3$, $|x|$ denotes the Euclidean norm of x . The notation $*$ stands for the convolution

$$(2.1) \quad (f * g)(x) = \int_{\mathbf{R}^3} f(x-y)g(y)dy.$$

By using the following approximation

$$(2.2) \quad E_J = mc^2 \left(1 + \sum_{j=1}^J (-1)^{j+1} \alpha(j) \frac{\mathbf{p}^{2j}}{m^{2j} c^{2j}} \right)$$

of the energy

$$(2.3) \quad E = \sqrt{\mathbf{p}^2 c^2 + m^2 c^4}$$

of a particle of mass m and of momentum \mathbf{p} , and the correspondence principle [3]

$$(2.4) \quad E \leftrightarrow i\hbar \frac{\partial}{\partial t} \quad \mathbf{p} \leftrightarrow -i\hbar \frac{\partial}{\partial x} = -i\hbar \nabla,$$

we obtain the *higher order Schrödinger equations*

$$(2.5) \quad i\hbar \frac{\partial \psi}{\partial t} = - \sum_{j=0}^J \frac{\alpha(j) \hbar^{2j}}{m^{2j-1} c^{2j-2}} \Delta^j \psi + V\psi,$$

where V is an external potential, $J \in \mathbb{N}^*$, $\hbar = \frac{h}{2\pi}$ is the reduced Planck constant and

$$(2.6) \quad \alpha(j) = \frac{(2j-2)!}{j!(j-1)!2^{2j-1}},$$

with $\alpha(0) = -1$. See [5] for more details.

Let us introduce the integro-differential Hartree and Hartree-Fock equations given for instance in [14, 31, 32]. The *Hartree equation* of N particles is defined by

$$(2.7) \quad i\hbar \frac{\partial}{\partial t} \psi_k = -\frac{\hbar^2}{2m} \Delta \psi_k + \sum_{\ell=1}^N \left(\frac{\kappa}{|x|} * |\psi_\ell|^2 \right) \psi_k + V \psi_k$$

with V an external bounded potential, κ a positive constant and $k = 1, \dots, N$. The Hartree term

$$H_k = \sum_{\ell=1}^N \left(\frac{\kappa}{|x|} * |\psi_\ell|^2 \right)$$

describes the self interaction between charged particles as a repulsive force. The *Hartree-Fock equation* of N particles is given by

$$(2.8) \quad i\hbar \frac{\partial}{\partial t} \psi_k = -\frac{\hbar^2}{2m} \Delta \psi_k + H_k \psi_k - \sum_{\ell=1}^N \left(\frac{\kappa}{|x|} * \overline{\psi_\ell} \psi_k \right) \psi_\ell + V \psi_k.$$

The Fock term

$$(2.9) \quad F(\psi_k) = \sum_{\substack{\ell=1 \\ \ell \neq k}}^N \left(\frac{\kappa}{|x|} * (\overline{\psi_\ell} \psi_k) \right) \psi_\ell$$

is an exchange term which is a consequence of the Pauli principle. It is non zero for fermions which have a non zero spin.

The *semi-relativistic Hartree equation* is given by

$$(2.10) \quad i\hbar \frac{\partial}{\partial t} \psi_k = \sqrt{-c^2 \hbar^2 \Delta + m^2 c^4} \psi_k + H_k \psi_k + V \psi_k,$$

and the *semi-relativistic Hartree-Fock equation* by

$$(2.11) \quad i\hbar \frac{\partial}{\partial t} \psi_k = \sqrt{-c^2 \hbar^2 \Delta + m^2 c^4} \psi_k + H_k \psi_k - F(\psi_k) + V \psi_k,$$

with $k = 1, \dots, N$. Both equations (2.10) and (2.11) are studied for instance in [1, 9, 14]. The main difficulty of these equations leads in the use of a non local pseudo-differential operator $\sqrt{-c^2 \hbar^2 \Delta + m^2 c^4}$, see for instance [28, Chapter 7]. Indeed, it causes problem for practical simulations on a bounded domain where an infinite number of boundary conditions are necessary.

For $J \in \mathbb{N}^*$, we have the following *higher order Hartree-Fock equations*

$$(2.12) \quad i\hbar \frac{\partial}{\partial t} \psi_k = - \sum_{j=0}^J \frac{\alpha(j) \hbar^{2j}}{m^{2j-1} c^{2j-2}} \Delta^j \psi_k + H_k \psi_k - F(\psi_k) + V \psi_k$$

with $k = 1, \dots, N$ and V an external potential.

3. HIGHER ORDER SCHRÖDINGER EQUATIONS WITH A COULOMB POTENTIAL

It is proved in [5] that equations (2.5) have a unique solution without external potential, and for a bounded or linear (in x) potential V . The main objective of this section is to prove that this is also true with a Coulomb potential.

For $J \in \mathbb{N}^*$, let us consider the higher order Schrödinger equations

$$(3.1) \quad i\hbar \frac{\partial \psi}{\partial t} = - \sum_{j=0}^J \frac{\alpha(j) \hbar^{2j}}{m^{2j-1} c^{2j-2}} \Delta^j \psi + V_\alpha \psi; \quad \psi(x, 0) = \psi_0(x),$$

where

$$(3.2) \quad V_\alpha(x) = \frac{\alpha}{|x|}$$

is the Coulomb potential with α a positive constant. We can prove the existence of a solution of Equation (3.1) by using perturbative arguments based on the Kato-Rellich theorem.

Theorem 3.1. *Let $\psi_0 \in L^2(\mathbf{R}^3)$. Equation (3.1) has a unique solution $\psi \in C(\mathbf{R}; L^2(\mathbf{R}^3))$, given by $\psi(x, t) = e^{i\frac{t}{\hbar}\mathcal{H}_J}\psi_0(x)$ where*

$$(3.3) \quad \mathcal{H}_J = - \sum_{j=0}^J \frac{\alpha(j)\hbar^{2j}}{m^{2j-1}c^{2j-2}} \Delta^j + V_\alpha.$$

In addition, the following conservation holds,

$$\frac{d}{dt} \|\psi(t)\|_{L^2(\mathbf{R}^3)}^2 = 0.$$

Proof. First, let us prove that we can apply the Kato-Rellich Theorem. By using $2J$ integration by parts, it is easy to prove that the Hamiltonian

$$(3.4) \quad \mathcal{H}_{0J} = - \sum_{j=0}^J \frac{\alpha(j)\hbar^{2j}}{m^{2j-1}c^{2j-2}} \Delta^j$$

is essentially self-adjoint. We will show that V_α is \mathcal{H}_{0J} -bounded

$$(3.5) \quad \|V_\alpha\psi\|_{L^2(\mathbf{R}^3)} \leq a\|\mathcal{H}_{0J}\psi\|_{L^2(\mathbf{R}^3)} + b\|\psi\|_{L^2(\mathbf{R}^3)}, \quad \forall \psi \in \mathcal{S}(\mathbf{R}^3),$$

with $a < 1$, and where \mathcal{S} denotes the Schwartz space. By using the Kato-Rellich Theorem (see e.g. [37, Theorem X.12]), we deduce that the Hamiltonian

$$\mathcal{H}_J = \mathcal{H}_{0J} + V_\alpha$$

is a self adjoint operator and $D(\mathcal{H}_J) = W^{2,2}(\mathbb{R}^3) = H^2(\mathbb{R}^3)$. Then, we apply the Stone Theorem (see e.g. [37]) to conclude that for $\psi_0 \in L^2(\mathbf{R}^3)$, the Schrödinger type equation

$$i\hbar \frac{\partial \psi}{\partial t} = \mathcal{H}_J \psi$$

has a unique solution given by $\psi(x, t) = e^{i\frac{t}{\hbar}\mathcal{H}_J}\psi_0(x)$, and $\|\psi(t)\|_{L^2} = \|\psi_0\|_{L^2}$ for all time t . We are left with the proof of (3.5). From Hardy inequality (see e.g. [2]), there exists $C > 0$ such that

$$\|V_\alpha\psi\|_{L^2(\mathbf{R}^3)} \leq C\|\nabla\psi\|_{L^2(\mathbf{R}^3)}.$$

An integration by parts and Cauchy-Schwarz inequality yield

$$\|V_\alpha\psi\|_{L^2(\mathbf{R}^3)} \leq C\|\psi\|_{L^2(\mathbf{R}^3)}^{1/2}\|\Delta\psi\|_{L^2(\mathbf{R}^3)}^{1/2} \leq \frac{C}{\varepsilon}\|\psi\|_{L^2(\mathbf{R}^3)} + C\varepsilon\|\Delta\psi\|_{L^2(\mathbf{R}^3)},$$

where we have used the Young inequality $2ab \leq a^2 + b^2$ for the last estimate, and $\varepsilon > 0$ is to be fixed later. By considering E_J as a polynomial in \mathbf{p} , and distinguishing the small values of \mathbf{p} from the large values of \mathbf{p} , we readily check that there exist $C_J > 0$ such that

$$\mathbf{p}^2 \leq C_J(1 + E_J^2).$$

Using Plancherel identity, we infer

$$\|\Delta\psi\|_{L^2(\mathbf{R}^3)} \leq C_J(\|\psi\|_{L^2(\mathbf{R}^3)} + \|\mathcal{H}_{0J}\psi\|_{L^2(\mathbf{R}^3)}), \quad \forall \psi \in \mathcal{S}(\mathbf{R}^3).$$

Gathering all the estimates together, we obtain

$$\|V_\alpha \psi\|_{L^2(\mathbf{R}^3)} \leq \left(\frac{C}{\varepsilon} + C_J C \varepsilon \right) \|\psi\|_{L^2(\mathbf{R}^3)} + C_J C \varepsilon \|\mathcal{H}_{0J} \psi\|_{L^2(\mathbf{R}^3)}, \quad \forall \psi \in \mathcal{S}(\mathbf{R}^3).$$

Choosing ε sufficiently small, we conclude that V_α is \mathcal{H}_{0J} -bounded, with a relative bound $a < 1$. \square

Example 3.2. The alpha decay is modeled by the equation

$$(3.6) \quad \frac{A+4}{Z+2} \mathbf{X} \rightarrow \frac{A}{Z} \mathbf{Y} + \alpha$$

where Z is the atomic number of the residual nucleus Y , A the mass number of the residual nucleus Y and α denotes the alpha particle composed of 2 protons and 2 neutrons. Let us suppose that the origin is taken at the center of the mother nucleus. For $|x| > R$ with R the radius of the residual nucleus, the potential of an alpha particle after its decay is given by

$$(3.7) \quad V_\alpha(x) = \frac{\tilde{\alpha}}{|x|},$$

where $\tilde{\alpha} = \frac{2Ze^2}{4\pi\epsilon_0}$ with e the elementary charge and ϵ_0 the vacuum permittivity [15, 36]. The alpha particle is a semi-relativistic particle whose maximum velocity is of the order of one-tenth of the speed of light [40, 42]. It can be described by the Schrödinger equation

$$(3.8) \quad i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m_\alpha} \Delta \psi + V_\alpha \psi,$$

where m_α is the mass of the alpha particle after its quantum tunnelling out of the mother nucleus X [41, Section 3.6]. By using a 2-order Schrödinger equation, we obtain the following equation

$$(3.9) \quad i\hbar \frac{\partial \psi}{\partial t} = (m_\alpha c^2 + V_\alpha) \psi - \frac{\hbar^2}{2m_\alpha} \Delta \psi - \frac{\hbar^4}{8m_\alpha^3 c^2} \Delta^2 \psi,$$

for an alpha particle after its quantum tunnelling out of the mother nucleus X . It has been shown in [5, Example 3.3] that the accuracy is improved with several orders of magnitudes by taking into account a 2-order Schrödinger equation rather than the Schrödinger equation.

4. HIGHER ORDER HARTREE-FOCK EQUATIONS WITH A BOUNDED EXTERNAL POTENTIAL

In this section, we study the Cauchy problem associated to (2.12), in the case where V is a bounded potential. We denote by

$$U_J(t) = e^{-it\mathcal{H}_{0J}}$$

the propagator corresponding to the case $H_k = F = V = 0$, where we recall that \mathcal{H}_{0J} is defined in (3.4). Given $\psi_{01}, \dots, \psi_{0N} \in L^2(\mathbf{R}^3)$, we rewrite the Cauchy problem (2.12) with $\psi_k|_{t=0} = \psi_{0k}$ in an integral form (Duhamel's principle): for $k = 1, \dots, N$,

$$(4.1) \quad \begin{aligned} \psi_k(t) &= U_J(t) \psi_{0k} - i \int_0^t U_J(t-s) (H_k \psi_k)(s) ds \\ &\quad + i \int_0^t U_J(t-s) (F(\psi_k))(s) ds - i \int_0^t U_J(t-s) (V \psi_k)(s) ds. \end{aligned}$$

In the case $J = 1$ (Hartree-Fock equation), the existence and uniqueness of a solution has been established in [8] (see also [4] for a proof using more recent tools). Therefore, we shall focus our presentation on the case $J \geq 2$. We emphasize a difference with previous results: when $J = 1$, the H^2 -regularity of the solution to (2.8) is proven by showing that ψ_k and $\partial_t \psi_k$ belong to $C([0, T]; L^2(\mathbf{R}^3))$, and using the equation (2.8) to infer that $\Delta \psi_k \in C([0, T]; L^2(\mathbf{R}^3))$, hence $\psi_k \in C([0, T]; H^2(\mathbf{R}^3))$. This is so even in the linear case, see the proof on Lemma 2.1 in [44] (a property which is used also in [4]). In the case of (2.12), this method can be adapted to pass from an L^2 -regularity to an H^{2J} -regularity: this may correspond to a rather large regularity, and we choose to present a different approach.

Theorem 4.1. *Let $J \geq 2$, $V \in L^\infty(\mathbf{R}^3)$, $\psi_{01}, \dots, \psi_{0N} \in L^2(\mathbf{R}^3)$. Then (4.1) has a unique, global, solution*

$$(\psi_1, \dots, \psi_N) \in \left(C(\mathbf{R}; L^2(\mathbf{R}^3)) \cap L_{\text{loc}}^{4J/3}(\mathbf{R}; L^\infty(\mathbf{R}^3)) \right)^N.$$

In addition, the following conservations hold, for all $\ell, k \in \{1, \dots, N\}$:

$$(4.2) \quad \frac{d}{dt} \int_{\mathbf{R}^3} \overline{\psi_\ell}(t, x) \psi_k(t, x) dx = 0.$$

Remark 4.2. The space $L_{\text{loc}}^{4J/3}(\mathbf{R}; L^\infty(\mathbf{R}^3))$ is mentioned in order to guarantee uniqueness. Other spaces based on the Strichartz type estimates presented below would do the job as well.

4.1. Dispersive estimates and consequences. From [25, Theorem 4.1], we have the following local in time dispersive estimate. There exists $C > 0$ such that

$$\|U_J(t)\|_{L^1(\mathbf{R}^3) \rightarrow L^\infty(\mathbf{R}^3)} \leq \frac{C}{|t|^{3/(2J)}}, \quad 0 < |t| \leq 1.$$

This estimate is the same as the one associated to the usual Schrödinger group $e^{it\Delta}$ ($J = 1$) on \mathbf{R}^n , with $n = 3/J$. This remark is purely algebraic, since n need not be an integer. Large time decay properties for $U_J(t)$ (with a different rate) are also established in [25, Theorem 4.1], but we shall not need them here. Invoking [24, Theorem 1.2], we infer the following lemma.

Lemma 4.3 (Local Strichartz estimates). *Let $J \geq 2$, and (q_1, r_1) , (q_2, r_2) be admissible pairs, in the sense that they satisfy*

$$(4.3) \quad \frac{2}{q} = n \left(\frac{1}{2} - \frac{1}{r} \right), \quad 2 \leq r \leq \infty, \quad n = \frac{3}{J}.$$

Let I be some finite time interval, of length at most one, $|I| \leq 1$.

1. *There exists $C = C(r_1)$ such that for all $\phi \in L^2(\mathbf{R}^3)$,*

$$(4.4) \quad \|U(\cdot)\phi\|_{L^{q_1}(I; L^{r_1}(\mathbf{R}^3))} \leq C \|\phi\|_{L^2(\mathbf{R}^3)}.$$

2. *If I contains the origin, $0 \in I$, denote*

$$D_I(f)(t, x) = \int_{I \cap \{s \leq t\}} U(t-s)f(s, x) ds.$$

There exists $C = C(r_1, r_2)$ such that for all $f \in L^{q_2'}(I; L^{r_2'}(\mathbf{R}^3))$,

$$(4.5) \quad \|D_I(f)\|_{L^{q_1}(I; L^{r_1}(\mathbf{R}^3))} \leq C \|f\|_{L^{q_2'}(I; L^{r_2'}(\mathbf{R}^3))},$$

where p' stands for the Hölder conjugate exponent of p , $\frac{1}{p} + \frac{1}{p'} = 1$.

Remark 4.4. The value $r = \infty$ is always allowed in the present context, because we morally consider a Schrödinger equation in space dimension $n < 2$.

4.2. The fixed point argument. In order to unify the treatment of the terms H_k and F in (4.1), consider the trilinear operator

$$\mathbf{T}(\phi_1, \phi_2, \phi_3) = \left(\frac{1}{|x|} * (\phi_1 \phi_2) \right) \phi_3.$$

Lemma 4.5. *There exists $C > 0$ such that for all $\phi_1, \phi_2, \phi_3 \in C_0^\infty(\mathbf{R}^3)$,*

$$\|\mathbf{T}(\phi_1, \phi_2, \phi_3)\|_{L^2(\mathbf{R}^3)} \leq C \|\phi_1\|_{L^{24/11}(\mathbf{R}^3)} \|\phi_2\|_{L^{24/11}(\mathbf{R}^3)} \|\phi_3\|_{L^4(\mathbf{R}^3)}.$$

Proof. Hölder inequality yields

$$\|\mathbf{T}(\phi_1, \phi_2, \phi_3)\|_{L^2(\mathbf{R}^3)} \leq \left\| \frac{1}{|x|} * (\phi_1 \phi_2) \right\|_{L^4(\mathbf{R}^3)} \|\phi_3\|_{L^4(\mathbf{R}^3)}.$$

Since $x \in \mathbf{R}^3$, Hardy-Littlewood-Sobolev inequality (see e.g. [2]) yields

$$\left\| \frac{1}{|x|} * (\phi_1 \phi_2) \right\|_{L^4(\mathbf{R}^3)} \leq C \|\phi_1 \phi_2\|_{L^{12/11}(\mathbf{R}^3)},$$

and the lemma follows from Hölder inequality. \square

Lemma 4.6. *Let $\psi_{01}, \dots, \psi_{0N} \in L^2(\mathbf{R}^3)$. There exists $T > 0$ depending on $\psi_{01}, \dots, \psi_{0N}$ only through $\|\psi_{01}\|_{L^2}, \dots, \|\psi_{0N}\|_{L^2}$ such that (4.1) has a unique solution*

$$(\psi_1, \dots, \psi_N) \in \left(C([0, T]; L^2(\mathbf{R}^3)) \cap L^{4J/3}([0, T]; L^\infty(\mathbf{R}^3)) \right)^N.$$

Proof. Denote by $\Phi_k(\psi_1, \dots, \psi_L)$ the right hand side of (4.1), and for $T > 0$, let

$$X_T = \{(\psi_1, \dots, \psi_N) \in L^\infty([0, T]; L^2(\mathbf{R}^3))^N; \|\psi_k\|_{L^\infty([0, T]; L^2(\mathbf{R}^3))} \leq 2\|\psi_{0k}\|_{L^2}, \\ \|\psi_k\|_{L^{4J/3}([0, T]; L^\infty(\mathbf{R}^3))} \leq 2C_\infty \|\psi_{0k}\|_{L^2}, \quad k = 1, \dots, N\},$$

where the constant C_∞ stems from (4.4) in the case $r_1 = \infty$. The lemma follows from a standard fixed point argument: for $T > 0$ sufficiently small (depending on $\|\psi_{01}\|_{L^2}, \dots, \|\psi_{0N}\|_{L^2}$), all the Φ_k 's leave X_T invariant, and are contractions on that space.

From Lemma 4.3, and denoting by $L_T^q L^r = L^q([0, T]; L^r(\mathbf{R}^3))$, we have

$$\|\Phi_k\|_{L_T^\infty L^2} \leq \|\psi_{0k}\|_{L^2} + C \|H_k \psi_k\|_{L_T^1 L^2} + C \|F(\psi_k)\|_{L_T^1 L^2} + \|V \psi_k\|_{L_T^1 L^2}.$$

Lemma 4.5 and the boundedness of V yield

$$\|\Phi_k\|_{L_T^\infty L^2} \leq \|\psi_{0k}\|_{L^2} + C \sum_{\ell=1}^N \left\| \|\psi_k(t)\|_{L^{24/11}} \|\psi_\ell(t)\|_{L^{24/11}} \|\psi_\ell(t)\|_{L^4} \right\|_{L_T^1} \\ + C \|\psi_k\|_{L_T^1 L^2}.$$

The last term is readily estimated by $CT \|\psi_k\|_{L_T^\infty L^2}$. Each term of the sum is controlled by

$$\left\| \|\psi_k(t)\|_{L^\infty}^{1/12} \|\psi_k(t)\|_{L^2}^{11/12} \|\psi_\ell(t)\|_{L^\infty}^{1/12} \|\psi_\ell(t)\|_{L^2}^{11/12} \|\psi_\ell(t)\|_{L^\infty}^{1/2} \|\psi_\ell(t)\|_{L^2}^{1/2} \right\|_{L_T^1}$$

Neglecting the indices k and ℓ , which are irrelevant at this step of the analysis, Hölder inequality in time yields

$$\left\| \|\psi(t)\|_{L^\infty}^{2/3} \|\psi(t)\|_{L^2}^{7/3} \right\|_{L_T^1} \leq \|\psi\|_{L_T^\infty L^2}^{7/3} \|\psi\|_{L_T^{4J/3} L^\infty}^{2/3} T^{3(2J-1)/4},$$

and we come up with an estimate of the form

$$\|\Phi_k\|_{L_T^\infty L^2} \leq \|\psi_{0k}\|_{L^2} + C(\|\psi_{01}\|_{L^2}, \dots, \|\psi_{0N}\|_{L^2}) \left(T + T^{3(2J-1)/4} \right).$$

Choosing $T > 0$ sufficiently small, the right hand side does not exceed $2\|\psi_{0k}\|_{L^2}$, uniformly in k . Similarly, Lemma 4.3 yields

$$\|\Phi_k\|_{L_T^{4J/3} L^\infty} \leq C_\infty \|\psi_{0k}\|_{L^2} + C \|H_k \psi_k\|_{L_T^1 L^2} + C \|F(\psi_k)\|_{L_T^1 L^2} + \|V \psi_k\|_{L_T^1 L^2},$$

and so, X_T is invariant under the action of Φ provided that $T > 0$ is sufficiently small.

Up to diminishing T , contraction follows readily, since \mathbf{T} is a trilinear operator. So there exists a unique (in X_T) fixed point for Φ , that is, a solution to (4.1). Uniqueness in the larger space $(C([0, T]; L^2(\mathbf{R}^3)) \cap L^{4J/3}([0, T]; L^\infty(\mathbf{R}^3)))^N$ follows from the same estimates. \square

Since the L^2 norm of ψ_k , $k = 1, \dots, N$ is invariant under the flow of (2.12) (like in the case $J = 1$), the above local existence result can be iterated indefinitely in order to cover any arbitrary time interval, and Theorem 4.1 follows.

4.3. Higher order regularity. We infer the propagation of higher order Sobolev regularity, which essentially reflects the fact that (2.12) is L^2 -subcritical, and the nonlinearity is smooth. Roughly speaking, the point is to differentiate (4.1) with respect to the space variable (such derivatives commute with U_J), and use the fact that the nonlinearity is a trilinear operator, along with Sobolev embedding.

Corollary 4.7. *Let $s \in \mathbf{N}$. Suppose that $V \in W^{s, \infty}(\mathbf{R}^3)$, and that $\psi_{0k} \in H^s(\mathbf{R}^3)$, $k = 1, \dots, N$. Then the solution to (2.12) provided by Theorem 4.1 satisfies*

$$\psi_k \in C(\mathbf{R}; H^s(\mathbf{R}^3)), \quad k = 1, \dots, N.$$

If $s \geq J$, then we have in addition:

$$\psi_k \in L^\infty(\mathbf{R}; H^J(\mathbf{R}^3)), \quad k = 1, \dots, N.$$

Proof. We refer to the proof of [6, Theorem 8.1] for precise details concerning the proof of the first statement. In the case $s \geq J$, we take advantage of the Hamiltonian structure of (2.12). The quantity

$$\begin{aligned} \mathcal{E} &= \sum_{k=1}^N \langle \psi_k, \mathcal{H}_{0J} \psi_k \rangle + \int_{\mathbf{R}^3} V(x) \rho_\Psi(x) dx \\ &\quad + \frac{\kappa}{2} \iint_{\mathbf{R}^3 \times \mathbf{R}^3} \frac{\rho_\Psi(x) \rho_\Psi(y) - |\rho_\Psi(x, y)|^2}{|x - y|} dx dy, \end{aligned}$$

is formally independent of time, where

$$(4.6) \quad \rho_\Psi(x, y) = \sum_{k=1}^N \psi_k(x) \overline{\psi_k}(y), \quad \text{and } \rho_\Psi(x) = \rho_\Psi(x, x),$$

and we recall that we have denoted

$$\mathcal{H}_{0J} = - \sum_{j=0}^J \frac{\alpha(j)\hbar^{2j}}{m^{2j-1}c^{2j-2}} \Delta^j = - \sum_{j=0}^J (-1)^j \frac{\alpha(j)\hbar^{2j}}{m^{2j-1}c^{2j-2}} (-\Delta)^j,$$

where the last equality is here to stress the fact that $-\Delta$ is a positive operator. In view of Cauchy-Schwarz inequality, the integral on $\mathbf{R}^3 \times \mathbf{R}^3$ in \mathcal{E} is non-negative. At leading order (in terms of regularity),

$$\langle \psi_k, \mathcal{H}_{0J} \psi_k \rangle = (-1)^{J+1} \frac{\alpha(J)\hbar^{2J}}{m^{2J-1}c^{2J-2}} \|(-\Delta)^{J/2} \psi_k\|_{L^2}^2 + \text{l.o.t.}$$

In view of the conservation of the L^2 norm, we infer that if $(-1)^{J+1}$ and κ have the same sign, then the conservation of \mathcal{E} yields an a priori bound of the form

$$(4.7) \quad \psi_k \in L^\infty(\mathbf{R}; H^J(\mathbf{R}^3)), \quad k = 1, \dots, N.$$

In passing, we have used the following interpolation estimates, for $0 \leq s \leq J$:

$$\|(-\Delta)^{s/2} \psi\|_{L^2} \leq C \|\psi\|_{L^2}^{1-\theta} \|(-\Delta)^{J/2} \psi\|_{L^2}^\theta, \quad \theta = 1 - \frac{s}{J}.$$

If $(-1)^{J+1}$ and κ have different signs, we recall from [29] the estimate

$$\begin{aligned} \iint_{\mathbf{R}^3 \times \mathbf{R}^3} \frac{\rho_\Psi(x)\rho_\Psi(y)}{|x-y|} dx dy &\leq C \left(\int_{\mathbf{R}^3} \rho_\Psi(x) dx \right)^{2/3} \left(\int_{\mathbf{R}^3} \rho_\Psi^{4/3}(x) dx \right) \\ &\leq C \sum_{k=1}^N \|\psi_k\|_{L^{8/3}(\mathbf{R}^3)}^{8/3} \leq C \sum_{k=1}^N \|\psi_k\|_{H^{3/8}(\mathbf{R}^3)}^{8/3}, \end{aligned}$$

where we have used the conservation of the L^2 -norm and Sobolev embedding, successively. Therefore, the leading order in the “kinetic” part always dominates the potential part ($J > 3/8$), and (4.7) is always true. Finally, the conservation of \mathcal{E} can be rigorously established by following classical arguments (see e.g. [7]). \square

5. HIGHER ORDER HARTREE-FOCK EQUATIONS WITH A COULOMB POTENTIAL

In the case where the external potential V in (2.12) is a Coulomb potential (3.2), we prove:

Theorem 5.1. *Let $J \geq 2$, V given by (3.2), $\psi_{01}, \dots, \psi_{0N} \in L^2(\mathbf{R}^3)$. Then (4.1) has a unique, global, solution*

$$(\psi_1, \dots, \psi_N) \in \left(C(\mathbf{R}; L^2(\mathbf{R}^3)) \cap L_{\text{loc}}^{4J/3}(\mathbf{R}; L^\infty(\mathbf{R}^3)) \right)^N.$$

In addition, the following conservations hold, for all $\ell, k \in \{1, \dots, N\}$:

$$(5.1) \quad \frac{d}{dt} \int_{\mathbf{R}^3} \overline{\psi_\ell}(t, x) \psi_k(t, x) dx = 0.$$

If moreover $\psi_{01}, \dots, \psi_{0N} \in H^{2J}(\mathbf{R}^3)$, then

$$\psi_k \in C(\mathbf{R}; H^{2J}(\mathbf{R}^3)) \cap L^\infty(\mathbf{R}; H^J(\mathbf{R}^3)), \quad k = 1, \dots, N,$$

and the energy

$$\begin{aligned} \mathcal{E} &= \sum_{k=1}^N \langle \psi_k, \mathcal{H}_{0J} \psi_k \rangle + \int_{\mathbf{R}^3} V(x) \rho_{\Psi}(x) dx \\ &\quad + \frac{\kappa}{2} \iint_{\mathbf{R}^3 \times \mathbf{R}^3} \frac{\rho_{\Psi}(x) \rho_{\Psi}(y) - |\rho_{\Psi}(x, y)|^2}{|x - y|} dx dy \end{aligned}$$

is independent of time, where ρ_{Ψ} is defined in (4.6).

Sketch of the proof. The global existence at the L^2 level follows the same lines as in the previous section. The only difference is that the term $V\psi_k$ must be handled differently. Since the pair $(4J/3, \infty)$ is admissible, we may write

$$\begin{aligned} \|\Phi_k\|_{L_T^\infty L^2} &\leq \|\psi_{0k}\|_{L^2} + C \|H_k \psi_k\|_{L_T^1 L^2} + C \|F(\psi_k)\|_{L_T^1 L^2} \\ &\quad + \|V_1 \psi_k\|_{L_T^{4J/(4J-3)} L^1} + \|V_2 \psi_k\|_{L_T^1 L^2}, \end{aligned}$$

where we have decomposed the Coulomb potential as the sum of a singular potential with compact support and a bounded potential,

$$V_1(x) = \frac{\alpha}{|x|} \mathbf{1}_{|x| < 1}, \quad V_2(x) = \frac{\alpha}{|x|} \mathbf{1}_{|x| \geq 1}.$$

Since $V_2 \in L^\infty(\mathbf{R}^3)$, the last term is treated like in the previous case. We also have, in view of Cauchy-Schwarz inequality (in x),

$$\begin{aligned} \|V_1 \psi_k\|_{L_T^{4J/(4J-3)} L^1} &\leq \|V_1\|_{L^2(\mathbf{R}^3)} \|\psi_k\|_{L_T^{4J/(4J-3)} L^2} \\ &\leq T^{(4J-3)/(4J)} \|V_1\|_{L^2(\mathbf{R}^3)} \|\psi_k\|_{L_T^\infty L^2}, \end{aligned}$$

and we can conclude like in the proof of Lemma 4.6, and Theorem 4.1, successively, to obtain the first part of the theorem.

For the second part, we follow the same strategy as in [44] and [4]: the above fixed point argument can be repeated in

$$\begin{aligned} Y_T &= \{(\psi_1, \dots, \psi_N) \in L^\infty([0, T]; H^J(\mathbf{R}^3))^N; \|\psi_k\|_{L^\infty([0, T]; L^2(\mathbf{R}^3))} \leq 2\|\psi_{0k}\|_{L^2}, \\ &\quad \|\psi_k\|_{L^{4J/3}([0, T]; L^\infty(\mathbf{R}^3))} \leq 2C_\infty \|\psi_{0k}\|_{L^2}, \\ &\quad \|\partial_t \psi_k\|_{L^\infty([0, T]; L^2(\mathbf{R}^3))} \leq 2K_{0k}, \\ &\quad \|\partial_t \psi_k\|_{L^{4J/3}([0, T]; L^\infty(\mathbf{R}^3))} \leq 2C_\infty K_{0k}, \quad k = 1, \dots, N\}, \end{aligned}$$

where K_{0k} corresponds morally to $\|\partial_t \psi_k|_{t=0}\|_{L^2}$. Since the time variable is characteristic, this quantity is given by the equation, and we can take

$$\hbar K_{0k} = \sum_{j=0} \frac{|\alpha(j)| \hbar^{2j}}{m^{2j-1} c^{2j-2}} \|\psi_{0k}\|_{\dot{H}^{2j}} + \|H_k \psi_{0k}\|_{L^2} + \|F(\psi_{0k})\|_{L^2} + \|V \psi_{0k}\|_{L^2}.$$

The sum of the right hand side is finite by assumption, the nonlinear terms are finite by Sobolev embedding, and the last term is controlled by $\|\nabla \psi_{0k}\|_{L^2}$ thanks to Hardy inequality (see e.g. [2]).

The fixed point argument performed in X_T is readily adapted to the case of Y_T , hence

$$\psi_k \in C([0, T]; H^{2J}(\mathbf{R}^3)), \quad k = 1, \dots, N.$$

Since T depends on the L^2 norms of the initial data, and not of higher order norms, this local argument can be repeated in order to cover any given time interval, hence

$$\psi_k \in C(\mathbf{R}; H^{2J}(\mathbf{R}^3)), \quad k = 1, \dots, N.$$

The conservation of the energy \mathcal{E} follows from standard arguments, and the proof of Corollary 4.7 can be repeated to obtain the global boundedness of the H^J norm. \square

6. CONCLUSION

In this article, we have shown that the higher order Schrödinger equations are compatible with the Coulomb potential. These kind of equations can be used for instance for alpha particles. Moreover, we have expanded the scope to the higher order Hartree-Fock equations with bounded and Coulomb potentials which can be used in many-particle physics.

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