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HIGHER-ORDER SCHRÖDINGER AND HARTREE–FOCK EQUATIONS

RÉMI CARLES, WOLFGANG LUCHA, AND EMMANUEL MOULAY

ABSTRACT. The domain of validity of the higher-order Schrödinger equations is analyzed for harmonic-oscillator and Coulomb potentials as typical examples. Then the Cauchy theory for higher-order Hartree–Fock equations with bounded and Coulomb potentials is developed. Finally, the existence of associated ground states for the odd-order equations is proved. This renders these quantum equations relevant for physics.

1. INTRODUCTION

In this work, we discuss, in a rather general setting, various equations of motion enjoying considerable interest in numerous areas of physics and, by establishing the well-posedness of the corresponding problems, we try to put applications of these equations of motion on a solid basis: The higher-order Schrödinger equations have been developed in, e.g., [1, 2]. These are Schrödinger-type equations involving a higher-order Schrödinger operator [3, 4, 5, 6] and converging towards the semirelativistic bound-state equation called the spinless Salpeter equation. The original Schrödinger equation has been formulated by Schrödinger in 1926 [7]. The spinless Salpeter equation is studied, for instance, in [8, 9]. The Cauchy problem of the higher-order Schrödinger equations without potential, i.e., for free particles, is studied in [1, 2]. The case of bounded potentials (e.g., particles in finite potential wells) and of linear potentials (e.g., neutrons in free fall in the gravity field and electrons accelerated by an electric field) is treated in [1]. Moreover, the higher-order Schrödinger operator with quasi-periodic potentials in two dimensions is discussed in [6].

The extraordinarily high interest of the particle physics community in the spinless Salpeter equation derives primarily from the fact that this semirelativistic equation of motion constitutes a well-defined approximation to the Bethe–Salpeter formalism [10] designed for the Lorentz-covariant description of bound states within relativistic quantum field theory. Within this framework, it may be obtained along the course of a “three-dimensional reduction” effected by a sequence of reasonable and physically justified assumptions [11, 12]: In the limit of all bound-state constituents interacting instantaneously [13] as well as propagating freely, the homogeneous Bethe–Salpeter equation reduces to Salpeter’s equation [14], which, upon neglect of negative-energy contributions and spin degrees of freedom and restriction of the involved interaction kernels to convolution form, eventually simplifies to the spinless Salpeter equation. The latter may be regarded as the straightforward generalization of the Schrödinger equation towards inclusion of the relativistically correct free-particle kinetic energy.

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The semirelativistic bound-state equation emerging from the derivation sketched above is the eigenvalue equation of a nonlocal Hamiltonian composed of the sums of the relativistic kinetic energies of the bound-state constituents — represented by the famous square-root operators — and of the interactions of these particles — encoded in appropriately chosen potentials. The inconvenience induced by the nonlocality of such a spinless-Salpeter Hamiltonian, however, occasionally tempts practitioners to expand each square-root operator, regarded as a function of the involved momentum squared, in a (truncated) Taylor series not only up to the lowest nontrivial order — which gives the usual Schrödinger equation — but (at least) up to the next-to-lowest nontrivial order, without paying attention to obviously crucial questions such as the well-posedness of the problem or the existence of a ground state. Unfortunately, the Hamiltonian involving this expansion up to next-to-lowest nontrivial order proves to be unbounded from below. In this situation, a remedy *might* be, *if done properly*, to construct merely approximate solutions to such *pseudo* spinless Salpeter equation by taking into account all the worrisome terms in the Hamiltonian only perturbatively.

In order to settle this question once and forever, we analyze such semirelativistic equations of motion for expansions of the relativistic kinetic energy up to arbitrarily high order. The outcomes of such expansions are known as higher-order Schrödinger equations.

Logically, the next steps then are to consider the corresponding time-dependent equations, to allow for the general case of systems composed of more than one or two interacting particles, which yields the Hartree equation, and to take into account the fermionic nature of the involved particles, which leads to the Hartree–Fock equation.

The Hartree equation, found by Hartree in the 1920s [15], arises in the mean-field limit of large systems of identical bosons (as, e.g., the Gross–Pitaevskii equation for Bose-Einstein condensates [16, 17]) by taking into account the self-interactions of the bosons. A semirelativistic version of the Hartree equation was obtained in [18, 19] for modeling boson stars. The Hartree–Fock equation, also developed by Fock [20], describes large systems of identical fermions (finding application in, e.g., electronic structure theory) by taking into account the self-interactions of charged fermions as well as an exchange term resulting from Pauli’s principle. A semirelativistic version of the Hartree–Fock equation was developed in [21] for modeling white dwarfs. The Hartree equation is also used for fermions as an approximation of the Hartree–Fock equation neglecting the impact of their fermionic nature. Hartree and Hartree–Fock equations are used for several applications in many-particle physics [22, Section 2.2].

Our first issue is to extend the scope of the higher-order Schrödinger equations to the Coulomb potential by using perturbation theory. Coulomb potentials have been widely employed for the Schrödinger equation (see, for instance, [23, 24, 25, 26, 27]); among others, it is conceivable to apply the higher-order Schrödinger equations with a Coulomb potential to the α particles, semirelativistically moving charged bosons composed of two protons and two neutrons and produced in the nuclear α decay [28]. Generalizing a result obtained in [1], we also prove that the higher-order Schrödinger equations converge towards the spinless Salpeter equation. Our second issue is to develop higher-order Hartree–Fock equations for bounded and Coulomb potentials. This allows us to take into account some relativistic effects in many-particle physics, as, for instance, the electrons of heavy atoms in quantum chemistry [29, 30, 31], the semirelativistic electron gas in a finite potential well [32, Section 4.2], the metal

clusters [22, Section 2.2.1] or the modeling of white dwarfs [21]. Last but not least, in order to give a physical meaning to the higher-order Schrödinger and Hartree–Fock equations, the existence of a ground state is proved for the odd-order equations.

This paper is organized as follows. After recalling some notations and definitions in Section 2, the case of higher-order Schrödinger equations with harmonic-oscillator or Coulomb potentials is discussed in Section 3. Section 4 is devoted to the Cauchy problem of the higher-order Hartree–Fock equations. An important special case, the Cauchy problem of higher-order Hartree–Fock equations with a Coulomb potential, is addressed in Subsection 4.2. In Section 5, we prove the existence of a ground state for the odd-order Schrödinger and Hartree–Fock equations. Our conclusions may be found in Section 6. In the Appendix, an extension of the convergence of the higher-order Schrödinger equations towards the spinless Salpeter equation is provided.

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, defined, in the case of integrable functions, by the formula

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

Upon approximating the relativistically correct expressions for the kinetic energy

$$(2.2) \quad E = \sqrt{\mathbf{p}^2 c^2 + m^2 c^4}$$

of a free particle of mass m and momentum \mathbf{p} by its expansion in powers of \mathbf{p}^2/m^2 ,

$$(2.3) \quad E_J = mc^2 \left(1 + \sum_{j=1}^J (-1)^{j+1} \alpha(j) \frac{\mathbf{p}^{2j}}{m^{2j} c^{2j}} \right),$$

and applying the correspondence principle [33]

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

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, $J \in \mathbf{N}^*$, $\hbar = \frac{h}{2\pi}$ the reduced Planck constant, c the speed of light, and

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

with $\alpha(0) = -1$. Stirling's formula yields, in particular,

$$(2.7) \quad \alpha(j) = \mathcal{O}\left(\frac{1}{j^{3/2}}\right) \quad \text{as } j \rightarrow \infty.$$

See [1] for more details. We denote the higher-order kinetic-energy operator by

$$(2.8) \quad \mathcal{H}_{0J} = - \sum_{j=0}^J \frac{\alpha(j)\hbar^{2j}}{m^{2j-1}c^{2j-2}} \Delta^j.$$

Example 2.1. For $J = 1$, we get the regular Schrödinger operator

$$\mathcal{H}_{01} = mc^2 - \frac{\hbar^2}{2m} \Delta.$$

For $J = 2$, we get

$$\mathcal{H}_{02} = mc^2 - \frac{\hbar^2}{2m} \Delta - \frac{\hbar^4}{8m^3c^2} \Delta^2.$$

The semirelativistic *time-dependent spinless Salpeter equation* is given by

$$(2.9) \quad i\hbar \frac{\partial}{\partial t} \psi = \sqrt{-c^2\hbar^2\Delta + m^2c^4} \psi + V\psi.$$

Let us introduce the integro-differential Hartree and Hartree–Fock equations given, for instance, in [21, 22, 32]. The *Hartree equation* of N particles is defined by

$$(2.10) \quad i\hbar \frac{\partial}{\partial t} \psi_k = -\frac{\hbar^2}{2m} \Delta \psi_k + \sum_{\ell=1}^N \left(\frac{\kappa}{|x|} * |\psi_\ell|^2 \right) \psi_k + V\psi_k,$$

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

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

describes the self-interaction between charged particles as a repulsive force if $\kappa > 0$, attractive force if $\kappa < 0$. The *Hartree–Fock equation* of N particles is given by

$$(2.11) \quad i\hbar \frac{\partial}{\partial t} \psi_k = -\frac{\hbar^2}{2m} \Delta \psi_k + H\psi_k - \sum_{\ell=1}^N \left(\frac{\kappa}{|x|} * \overline{\psi_\ell} \psi_k \right) \psi_\ell + V\psi_k.$$

The Fock term

$$(2.12) \quad F_k(\psi_k) = \sum_{\substack{\ell=1 \\ \ell \neq k}}^N \left(\frac{\kappa}{|x|} * (\overline{\psi_\ell} \psi_k) \right) \psi_\ell$$

is an exchange term that is a consequence of the Pauli principle and thus applies to fermions.

The *semirelativistic Hartree equation* is given by

$$(2.13) \quad i\hbar \frac{\partial}{\partial t} \psi_k = \sqrt{-c^2\hbar^2\Delta + m^2c^4} \psi_k + H\psi_k + V\psi_k,$$

and the *semirelativistic Hartree–Fock equation* by

$$(2.14) \quad i\hbar \frac{\partial}{\partial t} \psi_k = \sqrt{-c^2\hbar^2\Delta + m^2c^4} \psi_k + H\psi_k - F_k(\psi_k) + V\psi_k,$$

with $k = 1, \dots, N$. Both equations (2.13) and (2.14) are studied, for instance, in [34, 35, 21]. The main difficulty of all these equations relies in the use of the nonlocal pseudo-differential operator $\sqrt{-c^2\hbar^2\Delta + m^2c^4}$ (see, e.g., [36, Chapter 7] or [37]).

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

$$(2.15) \quad i\hbar \frac{\partial}{\partial t} \psi_k = \mathcal{H}_{0J} \psi_k + H \psi_k - F_k(\psi_k) + V \psi_k,$$

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

3. HIGHER-ORDER SCHRÖDINGER EQUATIONS WITH AN EXTERNAL POTENTIAL

It is proved in [1] that equations (2.5) have a unique solution without external potential, and for a bounded or linear (in x) potential V . On the other hand, for a harmonic potential, the flow associated to (2.5) is not well-defined for $J = 2$.

The first main objective of this section is to prove that if one sticks to *odd* values of J , then the flow associated to (2.5) is well-defined with V a harmonic-oscillator potential. Then we consider the presence of a Coulomb potential.

3.1. Harmonic-oscillator potential.

Introduce the Schwartz space

$$\mathcal{S}(\mathbf{R}^d) = \left\{ f \in C^\infty(\mathbf{R}^d; \mathbf{C}) \mid \sup_{x \in \mathbf{R}^d} |x^\alpha \partial^\beta f(x)| < \infty, \quad \forall \alpha, \beta \in \mathbf{N}^d \right\}.$$

For $f \in \mathcal{S}(\mathbf{R}^d)$, the (semi-classical) Fourier transform of f , denoted by \widehat{f} or $\mathcal{F}(f)$, is defined by

$$\widehat{f}(p) = \frac{1}{(2\pi\hbar)^{d/2}} \int_{x \in \mathbf{R}^d} e^{-ix \cdot p/\hbar} f(x) dx,$$

where p is the Fourier variable. The Fourier Inversion Formula reads

$$(3.1) \quad f(x) = \frac{1}{(2\pi\hbar)^{d/2}} \int_{p \in \mathbf{R}^d} e^{+ix \cdot p/\hbar} \widehat{f}(p) dp.$$

The Fourier transform is uniquely continuously extended to the space of tempered distributions, $\mathcal{S}'(\mathbf{R}^d)$, and is unitary on $L^2(\mathbf{R}^d)$ (Plancherel formula):

$$(3.2) \quad \|u\|_{L^2(\mathbf{R}^d)} = \|\widehat{u}\|_{L^2(\mathbf{R}^d)}, \quad \forall u \in L^2(\mathbf{R}^d).$$

Among other features, the Fourier transform exchanges differentiation and multiplication by a polynomial, typically

$$\mathcal{F}(-\hbar^2 \Delta u)(p) = |p|^2 \widehat{u}(p),$$

and

$$\mathcal{F}(\mathcal{H}_{0J} u)(p) = - \sum_{j=0}^J \frac{\alpha(j)}{m^{2j-1} c^{2j-2}} (-1)^j |p|^{2j} \widehat{u}(p).$$

In the presence of a harmonic-oscillator potential, we get

$$\mathcal{F} \left(\left(\mathcal{H}_{0J} + \frac{|x|^2}{2} \right) u \right) (p) = \left(-\frac{\hbar^2}{2} \Delta_p - \sum_{j=0}^J \frac{\alpha(j)}{m^{2j-1} c^{2j-2}} (-1)^j |p|^{2j} \right) \widehat{u}(p).$$

If $J = 1$, we see that the Fourier transform maps the harmonic oscillator to another harmonic oscillator, in agreement with Example 2.1. For $J = 2$, we find, still in view of Example 2.1,

$$\mathcal{F} \left(\left(\mathcal{H}_{02} + \frac{|x|^2}{2} \right) u \right) (p) = \left(-\frac{\hbar^2}{2} \Delta_p + mc^2 + \frac{|p|^2}{2m} - \frac{|p|^4}{8m^3 c^2} \right) \widehat{u}(p).$$

Since the operator on the right-hand side is not essentially self-adjoint on $C_0^\infty(\mathbf{R}^d)$ (see, e.g., [38]), the flow associated to the operator $\mathcal{H}_{02} + \frac{|x|^2}{2}$ is not well-defined.

This is so essentially because trajectories associated to the Hamiltonian on the right-hand side may reach an infinite speed, due to the fact that the potential (in p) goes to $-\infty$ faster than quadratic. Such a feature is ruled out if J is restricted to odd values, $J = 2n + 1$, $n \in \mathbf{N}$, since then

$$\mathcal{F} \left(\left(\mathcal{H}_{0J} + \frac{|x|^2}{2} \right) u \right) (p) = \left(-\frac{\hbar^2}{2} \Delta_p - \sum_{j=0}^{2n+1} \frac{\alpha(j)}{m^{2j-1} c^{2j-2}} (-1)^j |p|^{2j} \right) \widehat{u}(p),$$

and the potential in p behaves for large p as

$$+\frac{\alpha(2n+1)}{m^{4n+1} c^{4n}} |p|^{4n+2}.$$

This potential is therefore uniformly bounded from below (going to $+\infty$ at infinity, hence it is confining), and the flow associated to the corresponding Hamiltonian is well-defined (see, e.g., [39]):

Proposition 3.1. *Let $\psi_0 \in L^2(\mathbf{R}^3)$ and J be an odd integer. Then \mathcal{H}_{0J} is essentially self-adjoint, and the Cauchy problem*

$$i\hbar \frac{\partial \psi}{\partial t} = \mathcal{H}_{0J} \psi + \frac{|x|^2}{2} \psi, \quad \psi(x, 0) = \psi_0(x),$$

has a unique solution $\psi \in C(\mathbf{R}; L^2(\mathbf{R}^3))$. In addition, the following conservation law holds:

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

Remark 3.2. As noticed in [1] and recalled above, the assumption that J is odd is sharp.

3.2. Coulomb potential. For $J \in \mathbf{N}^*$, let us consider the higher-order Schrödinger equations

$$(3.3) \quad i\hbar \frac{\partial \psi}{\partial t} = \mathcal{H}_{0J} \psi + V_\alpha \psi, \quad \psi(x, 0) = \psi_0(x),$$

where

$$(3.4) \quad V_\alpha(x) = \frac{\alpha}{|x|}$$

is the — attractive or repulsive — Coulomb potential with coupling constant $\alpha \in \mathbf{R}$. We can prove the existence of a solution of Equation (3.3) by adopting perturbative arguments based on the Kato–Rellich theorem.

Theorem 3.3. *Let $\psi_0 \in L^2(\mathbf{R}^3)$. Equation (3.3) 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*

$$(3.5) \quad \mathcal{H}_J = \mathcal{H}_{0J} + V_\alpha = - \sum_{j=0}^J \frac{\alpha(j) \hbar^{2j}}{m^{2j-1} c^{2j-2}} \Delta^j + V_\alpha.$$

In addition, the following conservation law holds:

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

Finally, the same conclusions hold if J is odd and \mathcal{H}_{0J} is replaced by

$$\mathcal{H}_{0J} + \frac{|x|^2}{2}.$$

Proof. The proof relies on the Kato–Rellich Theorem. By using $2J$ integrations by parts, it is easy to prove that the Hamiltonian \mathcal{H}_{0J} , defined in (2.8), is essentially self-adjoint. We will show that V_α is \mathcal{H}_{0J} -bounded:

$$(3.6) \quad \|V_\alpha \psi\|_{L^2(\mathbf{R}^3)} \leq a \|\mathcal{H}_{0J} \psi\|_{L^2(\mathbf{R}^3)} + b \|\psi\|_{L^2(\mathbf{R}^3)}, \quad \forall \psi \in \mathcal{S}(\mathbf{R}^3),$$

with $a < 1$, and where \mathcal{S} denotes the Schwartz space. By using the Kato–Rellich Theorem (see, e.g., [39, Theorem X.12]), we deduce that the Hamiltonian

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

is a self-adjoint operator and $D(\mathcal{H}_J) = W^{J,2}(\mathbf{R}^3) = H^J(\mathbf{R}^3)$. Then, we apply the Stone Theorem (see, e.g., [39]) 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 (3.6). From the Hardy inequality (see, e.g., [40]), 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 the 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

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

skipping here irrelevant parameters m and c . Using the Plancherel identity, we infer

$$(3.7) \quad \|\Delta \psi\|_{L^2(\mathbf{R}^3)} \leq C_J (\|\psi\|_{L^2(\mathbf{R}^3)} + \|\mathcal{H}_{0J} \psi\|_{L^2(\mathbf{R}^3)}), \quad \forall \psi \in \mathcal{S}(\mathbf{R}^3).$$

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 $a < 1$. The case of a harmonic-oscillator potential follows the same line. If J is odd, then, as noticed in Section 3.1, the symbol of the operator $\mathcal{H}_{0J} + \frac{|x|^2}{2}$ is bounded from below, and so an inequality analogous to (3.7) holds:

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

provided that J is odd. We can then conclude as above. \square

4. HIGHER-ORDER HARTREE–FOCK EQUATIONS

4.1. Bounded external potential. In this section, we study the Cauchy problem associated to (2.15), 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 $H = F_k = V = 0$, where we recall that \mathcal{H}_{0J} is defined in (2.8). Given $\psi_{01}, \dots, \psi_{0N} \in L^2(\mathbf{R}^3)$, we rewrite the Cauchy problem (2.15) with $\psi_k|_{t=0} = \psi_{0k}$ in an integral form (Duhamel's principle): for $k = 1, \dots, N$,

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

We prove the global existence of a unique solution to (4.1) with initial data in $L^2(\mathbf{R}^3)$, thanks to dispersive estimates for U_J . The corresponding argument is presented in the case of a bounded potential, and we show in Section 4.2 how it can be adapted to the case of a Coulomb potential. At the end of Section 4.1, we show that if the initial data belong to $H^J(\mathbf{R}^3)$ (which, of course, as J increases, is a stronger and stronger requirement) and the external potential is sufficiently smooth, then global existence of a unique solution can be established with more basic tools than dispersive estimates (an approach which does not seem to be easily extended to the case of a Coulomb potential though). See Proposition 4.8.

In the case $J = 1$ (the Hartree–Fock equation), the existence and uniqueness of a solution has been established in [41] (see also [42] for a proof using more recent tools). Therefore, we shall focus our presentation on the case $J \geq 2$. We emphasize a difference with the previous results: for $J = 1$, the H^2 -regularity of the solution to (2.11) is proven by showing that ψ_k and $\partial_t \psi_k$ belong to $C([0, T]; L^2(\mathbf{R}^3))$ and using equation (2.11) 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 of Lemma 2.1 in [27] (a property which is used also in [42]). In the case of (2.15), this method can be adapted to pass from an L^2 -regularity to an H^{2J} -regularity: this approach will be followed to prove Theorem 4.9 below (case of a Coulomb potential).

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 conservation laws hold, for all $\ell, k \in \{1, \dots, N\}$:

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

This result will follow from Lemma 4.6 in Subsection 4.1.2 below.

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.

4.1.1. *Dispersive estimates and consequences.* From [2, Theorem 4.1], we have the following local-in-time dispersive estimate. There exists $C > 0$ such that

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

Formally, 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 [2, Theorem 4.1], but we shall not need them here. Invoking [43, 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 $\phi \in L^2(\mathbf{R}^3)$,

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

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

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

There exists $C = C(r_1, r_2)$ such that for all $f \in L^{q'_2}(I; L^{r'_2})$,

$$(4.5) \quad \|D_I(f)\|_{L^{q_1}(I; L^{r_1}(\mathbf{R}^3))} \leq C \|f\|_{L^{q'_2}(I; L^{r'_2}(\mathbf{R}^3))},$$

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 $n < 2$.

4.1.2. *The fixed-point argument.* In order to unify the treatment of the terms H 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. The 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 $x \in \mathbf{R}^3$, the Hardy–Littlewood–Sobolev inequality (see, e.g., [40]) 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 the 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

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

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

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

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, the Hölder inequality in time yields

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

and we come up with an estimate of the form

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

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

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

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 (2.15) (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.

4.1.3. *Higher-order regularity.* We infer the propagation of higher-order Sobolev regularity, which essentially reflects the fact that (2.15) 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 (2.15) 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 [44, 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 (2.15). The quantity

$$(4.6) \quad \begin{aligned} \mathcal{E}_{\text{HF}} &= \sum_{k=1}^N \langle \psi_k, \mathcal{H}_{0J} \psi_k \rangle + \int_{\mathbf{R}^3} V(x) \rho_\Psi(x) dx \\ &+ \frac{\kappa}{2} \iint_{\mathbf{R}^3 \times \mathbf{R}^3} \frac{\rho_\Psi(x) \rho_\Psi(y) - |\rho_\Psi(x, y)|^2}{|x - y|} dx dy, \end{aligned}$$

is formally independent of time, where

$$(4.7) \quad \rho_\Psi(x, y) = \sum_{k=1}^N \psi_k(x) \overline{\psi_k}(y), \quad \text{and } \rho_\Psi(x) = \rho_\Psi(x, x),$$

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 stresses the fact that $-\Delta$ is a positive operator. In view of the Cauchy–Schwarz inequality, the integral on $\mathbf{R}^3 \times \mathbf{R}^3$ in \mathcal{E}_{HF} is nonnegative. 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}_{HF} yields an a priori bound of the form

$$(4.8) \quad \psi_k \in L^\infty(\mathbf{R}; H^J(\mathbf{R}^3)), \quad k = 1, \dots, N.$$

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

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

If $(-1)^{J+1}$ and κ have different signs, we recall from [45] 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 (4.8) is always true. Finally, the conservation of \mathcal{E}_{HF} can be rigorously established by the following classical arguments (see, e.g., [46]). \square

To conclude this section, we sketch a more direct proof of the above result.

Proposition 4.8. *Let $s \in \mathbf{N}$, with $s \geq J \geq 2$. 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 (2.15) has a unique, global, solution*

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

with initial data ψ_{0k} .

Sketch of the proof. Since $s \geq J \geq 2$, $H^s(\mathbf{R}^3)$ is a Banach algebra, continuously embedded into $L^p(\mathbf{R}^3)$ for all $p \in [2, \infty]$. We have

$$\|V\psi\|_{H^s} \leq C\|V\|_{W^{s,\infty}}\|\psi\|_{H^s},$$

and the estimate of Lemma 4.5 can be replaced by

$$(4.9) \quad \|\mathbf{T}(\phi_1, \phi_2, \phi_3)\|_{H^s(\mathbf{R}^3)} \leq C\|\phi_1\|_{H^s(\mathbf{R}^3)}\|\phi_2\|_{H^s(\mathbf{R}^3)}\|\phi_3\|_{H^s(\mathbf{R}^3)}.$$

To see this, decompose $1/|x|$ as the sum of $K_1(x) = \mathbf{1}_{|x|<1}/|x| \in L^1(\mathbf{R}^3)$ and $K_2(x) = \mathbf{1}_{|x|\geq 1}/|x| \in L^\infty(\mathbf{R}^3)$. We have

$$\begin{aligned} \|\mathbf{T}(\phi_1, \phi_2, \phi_3)\|_{H^s} &\leq C\|K_1 * (\phi_1\phi_2)\|_{H^s}\|\phi_3\|_{H^s} \\ &\quad + C \sum_{|\beta_1|+|\beta_2|\leq s} \|K_2 * (\partial^{\beta_1}\phi_1\partial^{\beta_2}\phi_2)\|_{L^\infty}\|\phi_3\|_{H^s}. \end{aligned}$$

Then (4.9) follows from

$$\begin{aligned} \|K_1 * (\partial^{\beta_1}\phi_1\partial^{\beta_2}\phi_2)\|_{L^2} &\leq \|K_1\|_{L^1}\|\partial^{\beta_1}\phi_1\partial^{\beta_2}\phi_2\|_{L^2} \leq \|K_1\|_{L^1}\|\phi_1\phi_2\|_{H^s}, \\ \|K_2 * (\partial^{\beta_1}\phi_1\partial^{\beta_2}\phi_2)\|_{L^\infty} &\leq \|K_2\|_{L^\infty}\|\partial^{\beta_1}\phi_1\partial^{\beta_2}\phi_2\|_{L^1} \\ &\leq \|K_2\|_{L^\infty}\|\partial^{\beta_1}\phi_1\|_{L^2}\|\partial^{\beta_2}\phi_2\|_{L^2}, \end{aligned}$$

and the fact that H^s is an algebra. A classical fixed-point argument yields the local existence of a solution in H^s (see, e.g., [47]). Global existence when $s = J$ follows from the same arguments as in the proof of Corollary 4.7: we have an a priori estimate in $H^J(\mathbf{R}^3)$, hence in $L^\infty(\mathbf{R}^3)$, so the solution is global in time. Propagation of higher regularity (when $s > J$) follows easily, thanks to tame estimates (see [40]). \square

4.2. Coulomb potential. In the case where the external potential V in (2.15) is a Coulomb potential (3.4), we prove:

Theorem 4.9. *Let $J \geq 2$, V given by (3.4), $\psi_{01}, \dots, \psi_{0N} \in L^2(\mathbf{R}^3)$. 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 conservation laws hold, for all $\ell, k \in \{1, \dots, N\}$:

$$(4.10) \quad \frac{d}{dt} \int_{\mathbf{R}^3} \overline{\psi_\ell}(t, x) \psi_k(t, x) dx = 0.$$

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

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

is independent of time, where ρ_Ψ is defined in (4.7).

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

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

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 the 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 [27] and [42]: the above fixed-point argument can be repeated in

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

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

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

The sum on 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 the Hardy inequality (see, e.g., [40]).

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 on 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}_{HF} 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

5. GROUND STATE

The existence of a ground state for the semirelativistic Hartree equation goes back to [45]. See also [48] for the introduction of an external potential as well as for more references.

The problem of the existence of a ground state for the higher-order Schrödinger equations has been raised in [49] (see also [50]). In particular, the second-order Schrödinger equation ($J = 2$) has no ground state. We will see in this section that the odd-order Schrödinger and Hartree–Fock equations have a ground state and are relevant in quantum physics.

5.1. Higher-order Schrödinger equation. In the case of the higher-order Schrödinger equation with a potential, (2.5), the associated energy reads

$$(5.1) \quad \mathcal{E}_S = \langle \psi, \mathcal{H}_{0,J} \psi \rangle + \int_{\mathbf{R}^3} V(x) |\psi(x)|^2 dx.$$

Integrations by parts show that the energy also takes the form

$$(5.2) \quad \mathcal{E}_S = \sum_{j=0}^J \frac{\alpha(j) \hbar^{2j}}{m^{2j-1} c^{2j-2}} (-1)^{j+1} \int_{\mathbf{R}^3} |(-\Delta)^{j/2} \psi(x)|^2 dx + \int_{\mathbf{R}^3} V(x) |\psi(x)|^2 dx.$$

Let

$$(5.3) \quad \underline{m} = \inf \{ \mathcal{E}_S ; \langle \psi, \psi \rangle = 1 \}.$$

The main cases we are interested in are when V is a harmonic-oscillator potential or when V is a Coulomb potential. In the first case, we have $V \geq 0$: in view of (5.2), we readily see that \underline{m} is finite if and only if J is odd ($\underline{m} = -\infty$ if J is even). Recall that we have seen in [1] and in Section 3.1 that for J even, the dynamics associated to (2.5) is not well-defined when V is a harmonic-oscillator potential. Consequently, the case J odd seems to be the only reliable one. When V is a Coulomb potential (3.4), the dynamics associated to (3.3) is well-defined for all $J \in \mathbf{N}$, as stated in Theorem 3.3. In view of the Cauchy–Schwarz and Hardy inequalities,

$$\left| \int_{\mathbf{R}^3} V(x) |\psi(x)|^2 dx \right| \leq |\alpha| \left\| \frac{\psi}{|x|} \right\|_{L^2(\mathbf{R}^3)} \|\psi\|_{L^2(\mathbf{R}^3)} \leq C |\alpha| \|\nabla \psi\|_{L^2(\mathbf{R}^3)} \|\psi\|_{L^2(\mathbf{R}^3)}.$$

On the other hand, if J is even, and unlike what happens when V is a harmonic-oscillator potential, one can consider

$$M = \sup \{ \mathcal{E}_S ; \langle \psi, \psi \rangle = 1 \} = - \inf \{ -\mathcal{E}_S ; \langle \psi, \psi \rangle = 1 \},$$

which is finite, for the same reason by which \underline{m} is finite when J is odd. It is then classical to infer (see, e.g., [51, 52]):

Proposition 5.1. *Suppose that J is odd, and that V is the sum of a harmonic-oscillator potential and a Coulomb potential,*

$$V(x) = \frac{\alpha}{|x|} + \sum_{j=1}^3 \omega_j^2 x_j^2, \quad \alpha \in \mathbf{R}, \omega_j \geq 0.$$

Then there exists ψ such that $\langle \psi, \psi \rangle = 1$ and $\mathcal{E}_S = \underline{m}$, with \underline{m} defined in (5.3). If J is even and V is a Coulomb potential ($\omega_j = 0$ for all j), there exists ψ such that $\langle \psi, \psi \rangle = 1$ and $\mathcal{E}_S = M$.

5.2. Higher-order Hartree–Fock equation. In the case of the higher-order Hartree–Fock equation (2.15), the associated energy is given by (4.6). When $J = 1$ (classical Hartree–Fock equation), the existence of minimizers for \mathcal{E}_{HF} and their properties have been studied in, e.g., [51, 52, 53, 54]. As we have seen in Section 4, \mathcal{E}_{HF} controls the H^J -norm, so for $J \geq 2$, the Hartree nonlinearity plays a weaker role in the analysis compared to the standard case $J = 1$. If a harmonic confinement is present in all three spatial directions,

$$V(x) = \frac{\alpha}{|x|} + \sum_{j=1}^3 \omega_j^2 x_j^2, \quad \alpha \in \mathbf{R}, \omega_j > 0,$$

then any minimizing sequence is compact, since the embedding

$$H^J(\mathbf{R}^3) \cap \mathcal{F}(H^1) \hookrightarrow L^2(\mathbf{R}^3) \cap L^6(\mathbf{R}^3)$$

is compact (see, e.g., [39]).

Proposition 5.2. *Let $N \geq 1$, $\kappa = 1$. Suppose that $J \geq 3$ is odd, and that V is the sum of a harmonic-oscillator potential and a Coulomb potential,*

$$V(x) = \frac{\alpha}{|x|} + \sum_{j=1}^3 \omega_j^2 x_j^2, \quad \alpha \in \mathbf{R}, \omega_j \geq 0.$$

In either of the cases,

- *full confinement: $\omega_j > 0$, $\forall j = 1, \dots, 3$, or*
- *$\alpha > N - 1$,*

there exists $\psi \in H^J(\mathbf{R}^3)^N$ such that

$$\mathcal{E}_{\text{HF}}(\psi) = \min \left\{ \mathcal{E}_{\text{HF}}(\phi), \phi \in H^J(\mathbf{R}^3)^N ; \int_{\mathbf{R}^3} \phi_j \bar{\phi}_k = \delta_{jk} \right\}.$$

If $J \geq 2$ is even, V is a Coulomb potential ($\omega_j = 0$ for all j) and $\alpha > N - 1$, there exists $\psi \in H^J(\mathbf{R}^3)^N$ such that

$$\mathcal{E}_{\text{HF}}(\psi) = \max \left\{ \mathcal{E}_{\text{HF}}(\phi), \phi \in H^J(\mathbf{R}^3)^N ; \int_{\mathbf{R}^3} \phi_j \bar{\phi}_k = \delta_{jk} \right\}.$$

6. CONCLUSION

In this article, we have shown that the higher-order Schrödinger equations are compatible with both the harmonic-oscillator potential and the Coulomb potential. Moreover, we have expanded the scope to higher-order Hartree–Fock equations with bounded and Coulomb potentials, which may become a useful tool in many-particle physics. Finally, we have proved the existence of a ground state for the odd-order ones among both types of equations, which thus are the only ones to have a physical meaning.

APPENDIX A. CONVERGENCE OF THE HIGHER-ORDER SCHRÖDINGER EQUATION
WITHOUT POTENTIAL

Recall that for $s \in \mathbf{N}$, the (semi-classical) Sobolev space $H^s(\mathbf{R}^d)$ is the space of L^2 functions whose distributional derivatives of order at most s are in $L^2(\mathbf{R}^d)$. It is equipped with the norm

$$\|f\|_{H^s} = \sum_{|\alpha| \leq s} \hbar^{|\alpha|} \|\partial^\alpha f\|_{L^2(\mathbf{R}^d)}.$$

We denote by $H^\infty(\mathbf{R}^d)$ the intersection of all the spaces $H^s(\mathbf{R}^d)$, $s \in \mathbf{N}$. These spaces can also be characterized in terms of their Fourier transform, as defined in Section 3. For $s \in \mathbf{N}$, we have the equivalence of norms:

$$(A.1) \quad \|f\|_{H^s}^2 \approx \int_{p \in \mathbf{R}^d} (1 + |p|^2)^s |\widehat{f}(p)|^2 dp.$$

The *homogeneous* Sobolev space $\dot{H}^s(\mathbf{R}^d)$ is equipped with the norm

$$\|f\|_{\dot{H}^s} = \sum_{|\alpha|=s} \hbar^{|\alpha|} \|\partial^\alpha f\|_{L^2(\mathbf{R}^d)} \approx \left(\int_{p \in \mathbf{R}^d} |p|^{2s} |\widehat{f}(p)|^2 dp \right)^{1/2}.$$

Theorem A.1. *Let $\psi_0 \in H^\infty(\mathbf{R}^d)$, and consider the solutions ψ and ψ_J to (2.9) and (2.5), respectively, in the case $V = 0$. Suppose that $\psi|_{t=0} = \psi_J|_{t=0} = \psi_0$. Then for all $T > 0$,*

$$(A.2) \quad \sup_{t \in [0, T]} \|\psi(t, \cdot) - \psi_J(t, \cdot)\|_{L^2(\mathbf{R}^d)} \leq \frac{2T}{\hbar} \frac{\alpha(J+1)}{m^{2J+1} c^{2J}} \|\psi_0\|_{\dot{H}^{2J+2}(\mathbf{R}^d)}.$$

In particular, if there exists C_0 independent of $s \in \mathbf{N}$ such that

$$(A.3) \quad \|\psi_0\|_{\dot{H}^s(\mathbf{R}^d)} \leq C_0 (mc)^s,$$

then, by (2.7),

$$\sup_{t \in [0, T]} \|\psi(t) - \psi_J(t)\|_{L^2(\mathbf{R}^d)} = \mathcal{O}(T\alpha(J+1)) = \mathcal{O}\left(\frac{T}{J^{3/2}}\right) \xrightarrow{J \rightarrow \infty} 0.$$

In [1], the above convergence result was proven under the assumption that the Fourier transform of ψ_0 is supported in the ball of radius mc , a case where (A.3) becomes trivial, since

$$\begin{aligned} \|\psi_0\|_{\dot{H}^s(\mathbf{R}^d)}^2 &\approx \int_{p \in \mathbf{R}^d} |p|^{2s} |\widehat{\psi}_0(p)|^2 dp = \int_{|p| \leq mc} |p|^{2s} |\widehat{\psi}_0(p)|^2 dp \\ &\leq (mc)^{2s} \int_{|p| \leq mc} |\widehat{\psi}_0(p)|^2 dp = (mc)^{2s} \|\psi_0\|_{L^2}^2. \end{aligned}$$

The present extension is valid also for Gaussian wave packets

$$\psi_0(x) = \left(\frac{mc}{\hbar}\right)^{3/4} e^{-mc|x|^2/\hbar},$$

a case which was not covered in [1].

Proof. The Taylor formula yields

$$E - E_J = mc^2 \left(\frac{p}{mc}\right)^{2J+2} \frac{1}{(J+1)!} \int_0^1 f_{J+1} \left(\theta \left(\frac{p}{mc}\right)^2\right) (1-\theta)^J d\theta,$$

where

$$f_n(x) = \frac{d^n}{dx^n} (\sqrt{1+x}).$$

We infer

$$(A.4) \quad |E - E_J| \leq mc^2 \left(\frac{p}{mc}\right)^{2J+2} \alpha(J+1).$$

The functions ψ and ψ_J solve, respectively,

$$i\hbar \frac{\partial \psi}{\partial t} = E(-i\hbar \nabla_x) \psi; \quad i\hbar \frac{\partial \psi_J}{\partial t} = E_J(-i\hbar \nabla_x) \psi_J.$$

The difference $w_J = \psi - \psi_J$ satisfies $w_J|_{t=0} = 0$ and solves

$$i\hbar \frac{\partial w_J}{\partial t} = E(-i\hbar \nabla_x) w_J + r_J, \quad \text{where } r_J = (E(-i\hbar \nabla_x) - E_J(-i\hbar \nabla_x)) \psi_J.$$

Multiply the above equation by $\overline{w_J}$, integrate in space, and take the imaginary part: the term involving $E(-i\hbar \nabla_x) w_J$ disappears (because it is real), and we infer

$$(A.5) \quad \|w_J(t)\|_{L^2} \leq \frac{2}{\hbar} \int_0^t \|r_J(\tau)\|_{L^2} d\tau.$$

In view of the Plancherel formula, and since E and E_J are Fourier multipliers,

$$\|r_J(\tau)\|_{L^2} = \|\widehat{r}_J(\tau)\|_{L^2} = \left\| (E(p) - E_J(p)) \widehat{\psi}_J(\tau) \right\|_{L^2}.$$

As noticed in [1], we have the explicit formula (since E_J is a Fourier multiplier)

$$\widehat{\psi}_J(t, p) = \widehat{\psi}_0(p) e^{itE_J(p)},$$

hence

$$\|r_J(\tau)\|_{L^2} = \left\| (E(p) - E_J(p)) \widehat{\psi}_0(\tau) \right\|_{L^2}.$$

The inequality (A.4) and the Plancherel formula yield

$$\|r_J(\tau)\|_{L^2} \leq mc^2 \left(\frac{1}{mc}\right)^{2J+2} \|\psi_0\|_{\dot{H}^{2J+2}},$$

and the result follows (use (2.7) for the final equality). \square

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