Mathematical Models and Methods in Applied Sciences

Multi-Configuration Hartree–Fock Theory for Pseudorelativistic atoms: The Time Dependent Case

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In this paper, we study the Multi-Configuration Time-Dependent Hartree-Fock model for pseudorelativistic atoms with Coulomb interaction. We prove local-in-time existence and uniqueness of solutions under the technical hypothesis that the charge of the nucleus is smaller than a critical charge value Z_c. The global-in-time well-posedness is obtained under an assumption on the energy of the initial data. Also, we prove that in the attractive case, if the number of used orbitals is smaller than a critical value K_c then the system is globally well-posed.

Keywords: Well-posedness, Semi-relativistic, Cauchy problem, Hartree, Hartree-Fock, Multi-Configuration, density matrix

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1. Introduction and main result

The aim of this paper is to study the Cauchy problem for a set of coupled nonlinear PDEs and ODEs. The system generalizes the Hartree-Fock (HF in short) model that arises as quantum fermionic model for the dynamic of relativistic stars such white dwarf stars, neutron stars etc., [12,16]. More precisely, we establish existence and uniqueness of solutions to the Cauchy problem associated to the relativistic Multi-Configuration Hartree-Fock (MCHF in short).

The family of Multi-Configuration approximations such Multi-Configuration Time Dependent Hartree-Fock (MCTDHF in short) and Multi-Configuration Time Dependent Hartree (MCTDH in short, the equivalent model of MCTDHF without skew-symmetry) has to be seen as an extension and improvement of the well-known Hartree and Hartree-Fock models. Beyond the much more involved algebraic structure of these approximations, the associated equations of motion and the extra mathematical difficulties that appear compared to H and HF models (nonlinear coupling, singular density matrices etc.) requiring new mathematical arguments, the physical motivation of MC method resides in the fact that such models are able to catch the so-called *correlation* while the standard models fail, [6]. For instance, the HF model is considered as the degree zero of correlated dynamics. Improving the approximation by additional configurations systematically introduces correlation into the *ansatz* until, in the limit when the number of particle goes to infinity, the exact wave function is recovered. *Correlation* is obviously a key concept for many-particle systems even if its mathematical definition is still rather vague, [14,15].

From a purely mathematical point of view, in the non-relativistic setting, this model has been analyzed in the stationary case by Le Bris, [20] in a doubly excited configurations. Later on, Friesecke, [11] and Lewin [21], proved the existence of ground state solutions for the MC equations . In the time dependent framework, the mathematical analysis of MCTDHF equations was laid out in Ref. 3. Recently, Argaez and Melgaard, [1] extended the theory to the relativistic case and proved the existence of a ground state (see also Ref. 22).

Within the Born-Oppenheimer approximation, we consider an atom composed of N electrons and a space centered nucleus of charge Z. In order to take into account some relativistic effects, we introduce the following Hamiltonian in atomic units $\hbar = e = m = 1$

$$\begin{aligned} H_N &= \sum_{1\le i\le N} \left(\sqrt{-\alpha^2\,\Delta_{x_i} + \alpha^{-4}} - \alpha^{-2} - \frac{\alpha\, Z}{|x_i|} \right) + \sum_{1\le i<j\le N} \frac{1}{|x_i - x_j|} \\ &:= \alpha^{-1} \sum_{1\le i\le N} \left(\mathbf{H}_{x_i} - \alpha^{-1} \right) + V(x_1, \ldots, x_N) \end{aligned}$$

The operator $\mathbf{H}_{x_i}$ is then the sum of the kinetic energy operator $\sqrt{-\Delta + \alpha^{-2}}$, defined by its symbol $\sqrt{|p|^2+1}$ in Fourier domain, and the nucleus-i^{th}electron Coulomb interaction potential $\frac{\alpha\, Z}{|x_i|}$. Eventually, $\frac{1}{|x_i - x_j|}$ describes $i^{th} - j^{th}$ electronic interaction and $\alpha > 0$ is referred to as Sommerfeld's fine structure constant. The Hamiltonian H_N acts on a dense subspace of the N–particle Hilbert space $\wedge_{i=1}^N L^2(\mathbb{R}^3)$ of skew-symmetric functions[a]. In quantum mechanics, solving the lin-

[a]We voluntarily neglect the spin since it plays no role in our mathematical analysis.

ear N–particle Schrödinger equation

$$i\frac{\partial}{\partial t}\Psi = H_N\,\Psi, \quad \Psi(t=0) = \Psi_0 \in \wedge_{i=1}^N L^2(\mathbb{R}^3).$$

is merely impossible for more than a few particles. The retained strategy to solve this equation consists in resorting to approximations. The simplest approximation is the so called Hartree-Fock. It consists in forcing the approximate wavefunction Ψ_{HF} to evolve over the manifold

$$\mathcal{F}_N := \left\{\Psi = \phi_1 \wedge \ldots \wedge \phi_N, \quad \phi_i \in L^2(\mathbb{R}^3) \quad \int_{\mathbb{R}^3} \phi_i\,\bar{\phi}_j\,dx = \delta_{i,j}\right\}.$$

where $\phi_1 \wedge \ldots \wedge \phi_N = \frac{1}{\sqrt{N!}} det(\phi_p(x_q))_{p,q=1}^N$ and is referred to as *Slater determinant*. Then, the linear N–particle Schrödinger equation is replaced by the following nonlinear 1–particle coupled system of PDEs

$$\begin{aligned} i\,\frac{\partial}{\partial t}\,\phi_i(t,x) = H_{x_i}\,\phi_i(t,x) + \int_{\mathbb{R}^3} \frac{\sum_{j=1}^N\,|\phi_j(t,y)|^2}{|x-y|}\,dy\,\phi_i(t,x) \\ - \sum_{j=1}^N \int_{\mathbb{R}^3} \frac{\phi_i(t,y)\,\bar{\phi}_j(t,y)}{|x-y}\,dy\phi_j(t,x). \end{aligned}$$

The global-in-time existence and uniqueness of solutions in the energy space can be proved by combining the arguments of Chadam and Glassey in Ref. 8 and Lenzmann in Ref. 19 and further details can be found in Ref. 16. This observation can be stated as a Corollary of our main result since the HF model is a limiting case of the MCHF. Briefly speaking, in the MCHF, the wavefunction is forced to evolve on a set formed by linear combinations of Slater determinants which in turn means that in the MCHF, we use $K \geq N$ orthonormal functions in $L^2(\mathbb{R}^3)$ instead of only N in HF case. Obviously, when we set $K = N$ in MCHF, the model turns to be HF.

Let us now briefly introduce the MCTDHF method and equations. We refer the reader to Ref. 3 for a precise setting of these equations and associated algebraic properties that we shall strongly and tacitly use in the sequel.

Let $N, K \in \mathbb{N}^\star$ such that $N \leq K$ and let Σ_N^K be the $\binom{K}{N}$-set of increasing mappings $\sigma : \{1,\ldots,N\} \to \{1,\ldots,K\}$ of cardinal N. In other words, $\Sigma_N^K = \{\sigma = \{i_1 < i_1 < \ldots < i_N\},\, :\ 1 \leq i_k \leq K,\, 1 \leq k \leq N\}$ and $|\Sigma_N^K| = \binom{K}{N} := r$. Assume that Σ_N^K is lexicographically ordered and denote $\Sigma_N^K = \{\sigma_1,\ldots,\sigma_r\}$. Obviously, the notation $\sigma_i(j)$ will refers to the image of j by σ_i. Now, let us introduce the following sets

$$\mathcal{F}_N^K = \Big\{ (C,\Phi) = \Big((c_{\sigma_1},\ldots,c_{\sigma_r})_{\sigma_i\in\Sigma_N^K}, (\phi_1,\ldots,\phi_K)\Big) \in \mathbb{C}^r \times L^2(\mathbb{R})^K,$$
$$\sum_{i=1}^r |c_{\sigma_i}|^2 = 1,\ \int_{\mathbb{R}^3} \phi_i\,\bar{\phi}_j\,dx = \delta_{i,j} \Big\},$$
$$\mathcal{M}_N^K = \Big\{ \Psi \in L^2(\mathbb{R}^{3N}) \ : \ \Psi = \sum_{i=1}^r c_{\sigma_i}\,\phi_{\sigma_i(1)} \wedge \ldots \wedge \phi_{\sigma_i(N)},\ (C,\Phi)\in \mathcal{F}_N^K \Big\},$$

where $\delta_{i,j}$ denotes the Kronecker's delta. In the sequel, we will use the notation $\Phi_{\sigma_i} := \phi_{\sigma_i(1)} \wedge \ldots \wedge \phi_{\sigma_i(N)} = \frac{1}{\sqrt{N!}} det(\phi_{\sigma_i(p)}(x_q))_{p,q=1}^N$. Eventually, we define the mapping

$$\begin{aligned} \Psi:\ \mathcal{F}_N^K &\longrightarrow \mathcal{M}_N^K \\ (C,\Phi) &\longmapsto \Psi(C,\Phi) = \textstyle\sum_{i=1}^r c_{\sigma_i}\,\Phi_{\sigma_i}(x_1,\ldots,x_N) \end{aligned}$$

and we will write Ψ instead of $\Psi(C,\Phi)$ when there is no confusion. The mapping Ψ is clearly multi-linear with respect to the variables C and Φ, continuous and infinitely differentiable from $\mathcal{F}_N^K$ endowed with its natural topology into $L^2(\mathbb{R}^{3N})$. Let $\partial_C\Psi$ and $\partial_\Phi\Psi$ denote respectively the $\binom{K}{N}$-vector and K-vector of differentials of the mapping Ψ with respect to the coefficients and the functions. That is, $\partial_C\Psi = (\partial_{c_{\sigma_1}}\Psi,\ldots,\partial_{c_{\sigma_r}}\Psi)$ and $\partial_\Phi\Psi = (\partial_{\phi_1}\Psi,\ldots,\partial_{\phi_K}\Psi)$ where for all $\delta C \in \mathbb{C}^{\binom{K}{N}}$ and $\chi = (\chi_1,\ldots,\chi_K) \in (L^2(\mathbb{R}^3))^K$, we have

$$\partial_C\,\Psi\,[\delta C] = \sum_{i=1}^r (\partial_{c_{\sigma_i}}\Psi)\,\delta c_i = \sum_{i=1}^r \Phi_{\sigma_i}\,\delta c_i,$$

$$\partial_\Phi\,\Psi\,[\chi] = \sum_{i=1}^K (\partial_{\phi_i}\,\Psi)\,[\chi_i] = \sum_{i=1}^r c_{\sigma_i} \sum_{j=1}^K (\partial_{\phi_j}\,\Phi_{\sigma_i})[\chi_j],$$

and

$$(\partial_{\phi_k}\,\Phi_{\sigma_i})\,[\chi_j] = \sum_{i=1}^N \chi_j(x_i) \int_{\mathbb{R}^3} \Phi_{\sigma_i}(x_1,\ldots,x_N)\,\bar{\phi}_i(x_i)\,dx_i.$$

We refer the reader to Ref. 3 for further details concerning the definitions above. Now, let us introduce the $K\times K$ Hermitian matrix $\mathbf{\Gamma}$ defined *via* its entries as follows

$$\mathbf{\Gamma}_{i,j}\,\langle \xi,\chi\rangle_{L^2} = \big\langle (\partial_{\phi_j}\Psi)\,[\xi]\,,\,(\partial_{\phi_i}\Psi)\,[\chi]\big\rangle_{L^2(\mathbb{R}^{3N})} \quad \forall 1\le i,j\le K \quad \text{and} \quad \xi,\chi\in L^2(\mathbb{R}^3).$$

Eventually, we define for all $f \in L^2(\mathbb{R}^{3N})$, the operator $\partial_\Phi^\star\,\Psi$ as follows

$$\partial_\Phi^\star\,\Psi\,[f](x) = N \int_{\mathbb{R}^3} \phi_k(y) \left(\int_{\mathbb{R}^{3N}} f(x,x_2,\ldots,x_N)\,\bar{\Psi}(y,x_2,\ldots,x_N)\,dx_2,\ldots dx_N \right) dy.$$

In view of the algebraic structure of the MCHF method, there are some *inadmissible* cases. By *inadmissible* we mean a choice of $K := K(N)$ that leads systematically to a density matrix $\mathbf{\Gamma}$ of rank strictly less than K. In order to avoid these cases, we shall from now consider tacitly pairs (N, K) satisfying

$$K \begin{cases} \geq 1 & N = 1 \\ \geq 2 \ \text{ even} & N = 2 \\ \geq N \neq N+1 & N \geq 3 \end{cases}$$

This classification is due to Friesecke, [11] and based on purely algebraic considerations (see appendix of Ref. 21 as well). Now, we are able to present the MCTDHF system in a compact way, exhibiting the Hamiltonian nature of the MCTDHF approximation, as follows

$$\mathscr{S}\ : \quad \begin{cases} i\,\dfrac{d}{dt}\,C(t) = \ \langle H_N\,\Psi \mid \partial_C\,\Psi \rangle, \\[2ex] i\,\mathbf{\Gamma}(t)\,\dfrac{\partial}{\partial t}\,\Phi(t,x) = (I - \mathbf{P}_\Phi)\partial^\star_\Phi\,H_N\,\Psi, \\[2ex] (C(t=0), \Phi(t=0)) := (C^0, \Phi^0) \end{cases}$$

where the operator $\mathbf{P}_\Phi$ denotes the orthogonal projector onto the space spanned by the ϕ_i's. Therefore, we have to deal with a coupled nonlinear system of r first order ODEs and K PDEs.

Define the space $\mathscr{X} := \mathbb{C}^r \times (H^{\frac{1}{2}})^K$ equipped with the Euclidian norm $\|(C,\Phi)\|^2_{\mathcal{X}} = \|C\|^2 + \|\Phi\|^2_{H^{\frac{1}{2}}}$ and we shall use the Frobenuis norm for matrices. Also, we introduce the optimization problem

$$I_K = \inf_{\Psi \in \mathcal{M}_N^K} \langle H_N\,\Psi\,,\,\Psi\rangle\,. \tag{1.1}$$

Then, our main result is the following

Theorem 1.1. *Let $Z < \frac{2}{\alpha\,\pi}$ and $(C^0, \Phi^0) \in \mathcal{X}$ such that $\mathcal{E}(C^0, \Phi^0) < I_{K-1}$. Then, the system $\mathscr{S}$ has a unique solution $(C(t), \Phi(t)) \in \mathcal{F}_N^K$ satisfying*

$$C \in C^1([0, +\infty), \mathbb{C}^r)$$
$$\Phi \in C^0([0, +\infty);\, (H^{\frac{1}{2}}(\mathbb{R}^3))^K) \,\cap\, C^1([0, +\infty);\, (H^{-\frac{1}{2}}(\mathbb{R}^3))^K).$$

Moreover, the solution depends continuously on the initial data in $\mathbb{C}^r \times H^{\frac{1}{2}}(\mathbb{R}^3)^K$.

Theorem 1.1 establishes a global-in-time well-posedness of the pseudo relativistic MCTDHF equations in the energy space. This result is subjected to the necessary condition $Z < \frac{2}{\alpha\,\pi}$ and the sufficient condition $\mathcal{E}(C^0, \Phi^0) < I_{K-1}$. The first assumption is due to the nature of the 1–particle operator. Indeed, it is known that $\mathbf{H} - \alpha^{-1}$ is bounded from below if and only if $Z \leq \frac{2}{\alpha\,\pi}$ (see Ref. 18, 17). In particular, $\mathbf{H} - \alpha^{-1}$ is self-adjoint with domain $H^1(\mathbb{R}^3)$ when $Z < \frac{1}{2\,\alpha}$ since in this case, $\frac{Z\alpha}{|x|}$ is a small perturbation in the sense of operators of $\sqrt{-\Delta + \alpha^{-2}} - \alpha^{-1}$. However, when

$\frac{1}{2\,\alpha} \leq Z < \frac{2}{\alpha\,\pi}$, $\frac{Z\alpha}{|x|}$ is a small form perturbation of $\sqrt{-\Delta + \alpha^{-2}} - \alpha^{-1}$ following the Kato's inequality we shall present below. The second assumption is introduced in order to guarantee the global-in-time existence of the solution and was originally invented in Ref. 2, 3. The main difficulty one encounters in the MCTDHF framework is the possible loss of rank of the density matrix $\mathbf{\Gamma}(t)$. The assumption on the energy of the initial data is designed to force the dynamic to preserve the rank of $\mathbf{\Gamma}(t)$. The comparison with the ground state of the MCHF system when using $K-1$ orbital is rather intuitive. In some sense, this assumption tells us that if one can find a $(C^0, \Phi^0) \in \mathcal{F}_N^K$ approximating the MCHF ground state better than all pairs $(C, \Phi) \in \mathcal{F}_N^{K-1}$, then the flow of the MCTDHF system associated to such initial data preserves the rank of the density matrix.

In the particular setting $K = N$, the MCHF wavefunction becomes a single *Slater* determinant multiplied by a phase factor. Therefore, our result applies obviously to the TDHF case. Moreover, the density matrix $\mathbf{\Gamma}(t)$ reduces to the identity matrix I_N, hence there is no need to the second assumption of Theorem 1.1. It is rather clear that our result applies also when the Multi-Configuration is considered for symmetric wavefunctions or also for wavefunctions without symmetry, the Multi-Configuration Hartree for instance, [4]. Hence, our result is valid for Schrödinger-Poisson system and the simple Hartree approximation which consists in forcing the approximate wavefunction to evolve on the manifold of tensor products of the same function and therefore we recover the result of Ref. 19.

The paper is organized as follows. In the next section we state and prove some technical Lemmata. First of all, we prove the *formal* preservation in-time of the ortho-normalization constraints on the coefficients and the functions in Lemma 2.1. With the use of unitary transforms, for which we refer to Ref. 3, Lemma 2.1 allows us to reformulate the system $\mathscr{S}$ to a system $\mathscr{S}'$ better suited for our mathematical analysis in Lemma 2.3. Next, we prove the *formal* conservation of the total energy in Lemma 2.2 by the dynamic of the system $\mathscr{S}'$. Up to an unitary transformation, the property holds true for the system $\mathscr{S}$. Then, we state and prove Lemmata 2.4, 2.5, 2.6 where the local Lipschitz continuity character of the nonlinearities involved in the dynamic is shown. These terms are algebraically involved and for simplicity we split the proof on three Lemmata. The third section is devoted to the proof of our main result, namely Theorem 1.1. First we prove the local well-posedness, Lemma 3.1. Therefore, we prove the blow-up alternative and the existence of maximal time solution. The global-in-time existence is proved in Lemma 3.2. In section 4, we prove higher regularity result in Lemma 4.1. The last brief section is dedicated to extensions of Theorem 1.1 to the attractive case, in fact we show the existence of a critical value K_c such that if $K < K_c$, then the attractive system is still globally well-posed, thereby we recover the result of Ref. 19 and the existence of such critical value goes in the sense of Theorem 2.2 in Ref. 12. More precisely, we show

Theorem 1.2. *Under the same assumption of Theorem 1.1, there exists a critical* *value $K_c > 0$ such that if $K < K_c$, then the attractive MCTDHF system is globally-in-time well-posed in the energy space.*

2. Few technical Lemmata

Along this section, we shall perform some formal calculation. In order to justify them, we shall on the one hand assume the existence of a time $T > 0$ such that the density matrix $\mathbf{\Gamma}(t)$ is invertible on $[0,T]$. On the other hand, when the existence of solutions on $[0,T]$ is assumed, we mean tacitly regular enough or strong solutions, for instance $C \in C^1([0,T], \mathbb{C}^{\binom{K}{N}})$ and $\Phi \in C^0([0,T]; (H^1(\mathbb{R}^3))^K) \cap C^1([0,T]; (L^2(\mathbb{R}^3))^K)$. Now, we begin with

Lemma 2.1. *Let $(C^0, \Phi^0) \in \mathcal{F}_N^K$ be the initial data. If there exists a solution to the system $\mathscr{S}$ on $[0,T]$ such that rank$(\mathbf{\Gamma}(t)) = K$ for all $t \in [0,T]$, then*

$$\sum_{i=1}^{r} |c_{\sigma_i}(t)|^2 = 1 \quad \textit{and} \quad \int_{\mathbb{R}^3} \phi_i(t)\, \bar{\phi}_j(t)\, dt = \delta_{i,j} \quad \textit{for all} \quad 1 \le i,j \le K$$

for all $0 \le t \le T$.

Proof. The proof is based on the full rank assumption and the fact that $(I - \mathbf{P}_\Phi)$ defines a self-adjoint operator on $L^2(\mathbb{R}^3)$ and commutes with the matrix $\mathbf{\Gamma}(t)$. We refer the reader to Ref. 3 the detailed proof. □

Next, we prove that the dynamic of the system $\mathscr{S}$ conserves the total energy. More precisely, we have the following

Lemma 2.2. *Let $(C^0, \Phi^0) \in \mathcal{F}_N^K$ be the initial data. If there exists a solution to the system $\mathscr{S}$ on $[0,T]$ such that rank$(\mathbf{\Gamma}(t)) = K$ for all $t \in [0,T]$, then*

$$\begin{aligned} \mathcal{E}(C(t),\Phi(t)) &:= \langle \Psi(C(t),\Phi(t))\,, H_N\ \Psi(C(t),\Phi(t)) \rangle_{L^2(\mathbb{R}^{3N})} \\ &= \left\langle \Psi(C^0,\Phi^0)\,,\, H_N\,\Psi(C^0,\Phi^0) \right\rangle_{L^2(\mathbb{R}^{3N})}. \end{aligned}$$

Proof. The proof is based on the same calculation of Ref. 3 for the proof of the energy conservation if one changes $-\Delta_x$ in Ref. 3 by $\alpha^{-1}\sqrt{-\Delta_x + \alpha^{-2}}$. □

Since we are assuming the existence of strong solutions in the proof of Lemma 2.1 and Lemma 2.2, the calculation is formal but would be rigorous. In that calculation, we use products such $\left\langle \mathcal{R}(\Psi)\,,\, \frac{\partial}{\partial t}\Psi(t) \right\rangle$ involving (after expansion) products of $\partial_t \phi_i$ and $(I - \mathbf{P}_\Phi)(\mathbb{W}[C,\Phi]\,\Phi|)_i$ (see Ref. 3 and Appendix) which are obviously in $H^{-\frac{1}{2}}$ for solutions with functional part Φ with regularity $(H^{\frac{1}{2}}(\mathbb{R}^3))^K$. Such pairing is not well defined. In order to make the calculation rigorous for this class of solutions, one has to introduce a regularization argument as convolution with mollifiers (see Ref. 13) or by introducing the modified operator $(\epsilon\, H + 1)^{-1}$ for all $\epsilon > 0$ as in Ref. 19, 7 and proving that for all $t_1, t_2 \in [0,T]$, one has

$$\mathcal{E}(C(t_1), (\epsilon\, H + 1)^{-1}\Phi(t_1)) - \mathcal{E}(C(t_2), (\epsilon\, H + 1)^{-1}\Phi(t_2)) \xrightarrow[\epsilon \to 0]{} 0.$$

In order to prove this convergence, one uses the same kind of calculation given in the Appendix combined with the properties associated to the modified operator $(\epsilon H+1)^{-1}$ such $(\epsilon H+1)^{-1}\phi \xrightarrow[\epsilon\to 0]{} \phi$ for all ϕ in $\{\phi\in L^2(\mathbb{R}^3),\ \langle H\phi,\phi\rangle<+\infty\}\subset H^{\frac{1}{2}}(\mathbb{R}^3)$ and the fact that it commutes with H but as well the estimates we shall give in Lemma 2.4, Lemma 2.5 and Lemma 2.6 below and the dominated convergence Theorem. The proof would be very long to write it here but it is not very technical since it involves tedious but easy manipulations of the terms involved in the difference $\mathcal{E}(C(t_1),(\epsilon H+1)^{-1}\Phi(t_1))-\mathcal{E}(C(t_2),(\epsilon H+1)^{-1}\Phi(t_2))$. We refer to any textbook of analysis of PDEs for details on regularization arguments, [7] for instance.

The system $\mathscr{S}$ has the merit to be *compact* and has simple formulation. However, its form is not tractable for our mathematical analysis. Thanks to Lemma 2.1, we are able to recast $\mathscr{S}$ to an equivalent system $\mathscr{S}'$ which is the aim of the following

Lemma 2.3. *Let $(C^0,\Phi^0)\in\mathcal{F}_N^K$ be the initial data. If there exists a solution to the system $\mathscr{S}$ on $[0,T]$ such that $rank(\mathbf{\Gamma}(t))=K$ for all $t\in[0,T]$, then there exists a continuous mapping $\mathcal{U}:\mathcal{F}_N^K\to\mathcal{F}_N^K$, $(C,\Phi)\mapsto U(C,\Phi):=(C',\Phi')$ satisfying (omitting the prime for clarity) the system*

$$\mathscr{S}' : \begin{cases} i\,\dfrac{d}{dt}\,C(t)=\mathbb{K}(\Phi)(t)\,C(t), \\ i\,\mathbf{\Gamma}(t)\,\dfrac{\partial}{\partial t}\,\Phi(t,x)=\alpha^{-1}\,\mathbf{\Gamma}(t)\left(\sqrt{-\Delta_x+\alpha^{-2}}-\dfrac{\alpha\,Z}{|x|}\right)\Phi(t,x) \\ \qquad\qquad +(I-\mathbf{P}_\Phi)\mathbb{W}(C,\Phi)(t,x)\,\Phi(t,x) \\ (C(t=0),\Phi(t=0)):=(C^0,\Phi^0) \end{cases}$$

with $\mathbf{\Gamma}(t)$ being now

$$\mathbf{\Gamma}_{i,j}(t)=\sum_{\substack{k,l=1\,|\,i\in\sigma_k,\,j\in\sigma_l\\ \sigma_k\setminus\{i\}=\sigma_l\setminus\{j\}}}^{r}(-1)^{\sigma_k^{-1}(i)+\sigma_l^{-1}(j)}\,\overline{c}_{\sigma_k}(t)\,c_{\sigma_l}(t)$$

where $\sigma_k^{-1}(i)$ denotes the position of the element i in the set σ_k. The matrices $\mathbb{K}[\Phi]$

and $\mathbb{W}[C,\Phi]$ *are respectively* $r\times r$ *and* $K\times K$ *Hermitian matrices given as follows*

$$\begin{aligned}
\mathbb{K}(\Phi)_{\sigma_p,\sigma_q}(t) &= \frac{1}{2}\sum_{k,l\in\sigma_p,\, i,j\in\sigma_q,} \delta_{\sigma_p\setminus\{k,l\},\,\sigma_q\setminus\{i,j\},}\,(-1)^{\sigma_p}_{k,l}\,(-1)^{\sigma_q}_{i,j}\;\times\\
&\qquad\times\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\frac{\phi_i(t,x)\bar{\phi}_k(t,x)\;,\;\bar{\phi}_j(t,y)\phi_l(t,y)}{|x-y|}\,dx\,dy\\
\mathbb{W}(C,\Phi)_{ij}(t,x) &= 2\sum_{k,l=1}^{K}\gamma_{jkil}(t)\int_{\mathbb{R}^3}\frac{\phi_k(t,y)\overline{\phi}_l(t,y)}{|x-y|}\,dy\\
\gamma_{ijkl} &= \frac{1}{2}\,(1-\delta_{i,j})(1-\delta_{k,l})\sum_{\substack{p,q=1\,|\,i,j\in\sigma_p,\,k,l\in\sigma_q\\ \sigma_p\setminus\{i,j\}=\sigma_q\setminus\{k,l\}}}^{r}(-1)^{\sigma_p}_{i,j}(-1)^{\sigma_q}_{k,l}\,c_{\sigma_p}(t)\,\overline{c}_{\sigma_q}(t).
\end{aligned}$$

Finally,

$$(-1)^{\sigma_k}_{i,j} = \begin{cases}(-1)^{\sigma_k^{-1}(i)+\sigma_k^{-1}(j)+1} & \text{if } i<j,\\[2ex] (-1)^{\sigma_k^{-1}(i)+\sigma_k^{-1}(j)} & \text{if } i>j.\end{cases}$$

Proof. The proof is based on tedious but simple calculation and the *gauge* invariance property associated to the system $\mathscr{S}$. Again, we refer to Ref. 3 for precise details. □

The advantage of the system $\mathscr{S}'$ is that we see the nonlinear Schrödinger structure of the PDEs system with separate free and nonlinear parts. Moreover, it involves only 1–particle terms. Next, we prove the total energy conservation at a *formal* level using the formulation $\mathscr{S}'$. Observe that since the systems $\mathscr{S}$ and $\mathscr{S}'$ are equivalent, then the property holds for $\mathscr{S}$. We shall use for the energy the interchangeable notation $\mathcal{E}(C,\Phi), \mathcal{E}(\Psi(C,\Phi))$ and $\mathcal{E}(\Psi)$ depending on the context. Moreover, from this point onward, $\langle\cdot,\cdot\rangle$ will denote the $L^2(\mathbb{R}^3)$ scalar product unless specified. Now, the explicit expression of the energy reads

$$\begin{aligned}
\mathcal{E}(C(t),\Phi(t)) &:= \langle\Psi\,,\,H_N\,\Psi\rangle_{L^2(\mathbb{R}^{3N})}\\
&= \alpha^{-1}\sum_{i,j=1}^{K}\Big\langle(\mathbf{H}-\alpha^{-1})\,\mathbf{\Gamma}(t)\,\Phi\,,\;\Phi\Big\rangle + \frac{1}{2}\,\langle\mathbb{W}(C,\Phi)\,\Phi(t)\,,\,\Phi(t)\rangle\\
&= \alpha^{-1}\left\langle\left(\sqrt{-\Delta+\alpha^{-2}}-\frac{\alpha\,Z}{|x|}-\alpha^{-1}\right)\mathbf{\Gamma}(t)\,\Phi(t)\,,\,\Phi(t)\right\rangle\\
&\quad+\frac{1}{2}\sum_{i,j,k,l=1}^{K}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\gamma_{ijkl}\,\frac{\phi_i(t,x)\,\bar{\phi}_l(t,x)\,\phi_k(t,y)\,\bar{\phi}_j(t,y)}{|x-y|}\,dx\,dy.
\end{aligned}$$

Now, we are going to prove that the nonlinearities involved in the dynamic of the system $\mathscr{S}'$ are locally Lipschitz continuous in $(C,\Phi)\in\mathcal{X}$. The nonlinearities being rather complicated algebraically, we divide the proof into three separate Lemmata for clarity and future use of the estimates we shall use in the proofs. Our starting point is the definition of the following mapping

$$\begin{aligned} \mathscr{Q}\,:\,(H^{\frac{1}{2}}(\mathbb{R}^3))^3 \quad &\longrightarrow H^{\frac{1}{2}}(\mathbb{R}^3) \\ f:=(\psi,\phi,\chi) \;&\longmapsto\; \mathscr{Q}(f):=\left(\psi\bar{\phi}\star r^{-1}\right)\chi \end{aligned}$$

where the $\star$ denotes the convolution operator and r^{-1} the Coulomb potential. Also, we introduce the mapping

$$\begin{aligned} \mathscr{K}\,:\quad (H^{\frac{1}{2}}(\mathbb{R}^3))^4 \quad &\longrightarrow \mathbb{C} \\ f:=(\psi,\phi,\chi,\zeta) &\longmapsto \textstyle\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \frac{\psi(x)\,\bar{\phi}(x)\,\chi(y)\,\bar{\zeta}(y)}{|x-y|}\,dx\,dy. \end{aligned}$$

From this point onward, $\gamma\geq 0$ will denote variant constants that may change from line to line and never depend on (C,Φ) but on universal constants arising from functional estimates or norms equivalencies. Now, we claim

Lemma 2.4. *The mappings $\mathscr{Q}$ and $\mathscr{K}$ are well-defined and locally Lipschitz continuous respectively from $(H^{\frac{1}{2}}(\mathbb{R}^3))^3$ into $H^{\frac{1}{2}}(\mathbb{R}^3)$ and $(H^{\frac{1}{2}}(\mathbb{R}^3))^4$ into $\mathbb{C}$.*

Proof. Recall that for all $\psi\in H^{\frac{1}{2}}$, we have $\|\psi\|_{H^{\frac{1}{2}}}=\|(1+|\xi|^2)\,\mathcal{F}\,\psi\|_{L^2}$ with $\mathcal{F}$ being the Fourier transform. Thus, it is enough to prove that $\|\mathscr{Q}(f)\|_{L^2}+\|\sqrt[4]{-\Delta}\,\mathscr{Q}(f)\|_{L^2}$ is finite whenever $f=(\psi,\phi,\chi)\in(H^{\frac{1}{2}}(\mathbb{R}^3))^3$ to prove that the mapping $\mathscr{Q}$ is well defied. The proof relies on Kato's inequality $\frac{1}{|x|}\leq\frac{\pi}{2}\sqrt{-\Delta}$ (see Ref. 17, 18) in the sense of self-adjoint operators and the Leibniz fractional rule (see Ref. 19, Lemma 5) as a direct consequence of the Milhin multiplier Theorem (see Ref. 5). Indeed for all $f:=(\psi,\phi,\chi)\in(H^{\frac{1}{2}}(\mathbb{R}^3))^3$, we have on the one hand

$$\|\mathscr{Q}(f)\|_{L^2}=\|\left(\psi\bar{\phi}\star r^{-1}\right)\,\chi\|_{L^2}\leq\|\psi\bar{\phi}\star r^{-1}\,\|_{L^\infty}\,\|\chi\|_{L^2}.$$

The inequality $\frac{1}{|x|}\leq\frac{\pi}{2}\sqrt{-\Delta}$ implies that

$$\|\psi\bar{\phi}\star r^{-1}\,\|_{L^\infty}\leq\left|\sup_{\mathbb{R}^3}\int_{\mathbb{R}^3}\frac{\psi(x)\bar{\phi}(y)}{|x-y|}\,dx\right|\leq\frac{\pi}{2}\langle\psi\,,\,\sqrt{-\Delta}\,\psi\rangle_{L^2}^{\frac{1}{2}}\,\langle\phi\,,\,\sqrt{-\Delta}\,\phi\rangle_{L^2}^{\frac{1}{2}}.$$

Thus, we obtain

$$\|\mathscr{Q}(f)\|_{L^2}\leq\frac{\pi}{2}\,\|\sqrt[4]{-\Delta}\,\psi\|_{L^2}\,\|\sqrt[4]{-\Delta}\,\phi\|_{L^2}\,\|\chi\|_{L^2}\leq\frac{\pi}{2}\,\|\psi\|_{H^{\frac{1}{2}}}\,\|\phi\|_{H^{\frac{1}{2}}}\,\|\chi\|_{H^{\frac{1}{2}}}. \tag{2.1}$$

On the other hand, the fractional Leibniz rule gives

$$\|\sqrt[4]{-\Delta}\,\mathscr{Q}(f)\|_{L^2}\leq\|\sqrt[4]{-\Delta}\,(\psi\bar{\phi}\star r^{-1})\,\|_{L^6}\,\|\chi\|_{L^3}+\|\psi\bar{\phi}\star r^{-1}\,\|_{L^\infty}\,\|\sqrt[4]{-\Delta}\,\chi\|_{L^2} \tag{2.2}$$

The second term in the right hand side is then easily estimated by

$$\|\psi\bar{\phi}\star r^{-1}\,\|_{L^\infty}\,\|\sqrt[4]{-\Delta}\,\chi\|_{L^2}\leq\frac{\pi}{2}\,\|\psi\|_{H^{\frac{1}{2}}}\,\|\phi\|_{H^{\frac{1}{2}}}\,\|\chi\|_{H^{\frac{1}{2}}}. \tag{2.3}$$

In the sequel , we shall use the observation of Ref. 19 (following Ref. 23). For all $\alpha<3$ and function g in the Schwartz class $\mathcal{S}(\mathbb{R}^3)$, $\sqrt{-\Delta}^{\,-\alpha}g=G_\alpha\star g$ with

G_α being the Green's function of $\sqrt{-\Delta}^{-\alpha}$. In particular $G_\alpha = \frac{C_\alpha}{|x|^{3-\alpha}} \in L_w^{\frac{3}{3-\alpha}}(\mathbb{R}^3)$ where the subscript $\cdot_w$ stands for weak (Lorentz space) and C_α is a positive constant depending only on α. We shall in particular make use of the well known case $\alpha = 2$ corresponding to Poisson's equation and the case $\alpha = 3$. Thus

$$\begin{aligned} \| \sqrt[4]{-\Delta}\,(\psi\bar{\phi} \star r^{-1})\,\|_{L^6} \leq \| \sqrt[4]{-\Delta}^{-3}\,\psi\bar{\phi}\|_{L^6} &\leq \|\psi\bar{\phi} \star G_{\frac{3}{2}}\|_{L^6} \leq \|\psi\bar{\phi}\|_{L^{\frac{3}{2}}}\, \|G_{\frac{3}{2}}\|_{L^2_w} \\ &\leq C\, \|\psi\|_3\, \|\phi\|_{L^3}\, \|G_{\frac{3}{2}}\|_{L^2_w} \\ &\leq \|G_{\frac{3}{2}}\|_{L^2_w}\, \|\psi\|_{H^{\frac{1}{2}}}\, \|\phi\|_{H^{\frac{1}{2}}}. \end{aligned} \tag{2.4}$$

Eventually, combining (2.1–2.4) we get

$$\|\mathscr{Q}(f)\|_{H^{\frac{1}{2}}} \leq \gamma\, \|\psi\|_{H^{\frac{1}{2}}}\, \|\phi\|_{H^{\frac{1}{2}}}\, \|\chi\|_{H^{\frac{1}{2}}}. \tag{2.5}$$

This shows that the mapping $\mathscr{Q}$ is well-defined. It remains to show that $\mathscr{Q}$ is locally Lipschitz continuous. The proof is the same as in Ref. 19, with an extra term, and we write it here for the reader's convenience. We start by writing for all $f = (\psi, \phi, \chi), f' = (\psi', \phi', \chi') \in (H^{\frac{1}{2}}(\mathbb{R}^3))^3$

$$\mathscr{Q}(f) - \mathscr{Q}(f') = \mathscr{Q}(\psi - \psi', \phi, \chi) + \mathscr{Q}(\psi', \phi - \phi', \chi) + \mathscr{Q}(\psi', \phi', \chi - \chi').$$

Thus, using the estimate (2.5), we obtain

$$\begin{aligned} \|\mathscr{Q}(f) - \mathscr{Q}(f')\|_{H^{\frac{1}{2}}} &\leq \gamma\, \|\psi - \psi'\|_{H^{\frac{1}{2}}}\, \|\phi\|_{H^{\frac{1}{2}}}\, \|\chi\|_{H^{\frac{1}{2}}} \\ &+ \gamma\, \|\psi'\|_{H^{\frac{1}{2}}}\, \|\phi - \phi'\|_{H^{\frac{1}{2}}}\, \|\chi\|_{H^{\frac{1}{2}}} \\ &+ \gamma\, \|\psi'\|_{H^{\frac{1}{2}}}\, \|\phi'\|_{H^{\frac{1}{2}}}\, \|\chi - \chi'\|_{H^{\frac{1}{2}}} \\ &\leq \gamma\, (\|f\|_{H^{\frac{1}{2}}} + \|f'\|_{H^{\frac{1}{2}}})^2\, \|f - f'\|_{H^{\frac{1}{2}}} \\ &:= lip_{\mathscr{Q}}\, \|f - f'\|_{H^{\frac{1}{2}}}, \end{aligned} \tag{2.6}$$

where $lip_{\mathscr{Q}} := lip_{\mathscr{Q}}(\|f\|_{H^{\frac{1}{2}}}, \|f'\|_{H^{\frac{1}{2}}})$. Next, let $f := (\psi, \phi, \chi, \zeta) \in (H^{\frac{1}{2}})^4$ and observe that $\mathscr{K}(f) = \langle \mathscr{Q}(\psi, \phi, \chi)\,,\, \zeta\rangle_{L^2}$. Then, using Cauchy Schwarz inequality and (2.1) we have

$$|\mathscr{K}(f)| \leq \|\mathscr{Q}(\psi, \phi, \chi)\|_{L^2}\, \|\zeta\|_{L^2} \leq \frac{\pi}{2}\, \|f\|_{H^{\frac{1}{2}}}. \tag{2.7}$$

Moreover, we have for all $f := (\psi, \phi, \chi, \zeta), f' := (\psi', \phi', \chi', \zeta') \in H^{\frac{1}{2}}$

$$\mathscr{K}(f) - \mathscr{K}(f') = \langle \mathscr{Q}(\psi, \phi, \chi) - \mathscr{Q}(\psi', \phi', \chi')\,,\, \zeta\rangle_{L^2} + \langle \mathscr{Q}(\psi', \phi', \chi')\,,\, \zeta - \zeta'\rangle_{L^2}$$

Then, with (2.6), we have

$$\begin{aligned} |\mathscr{K}(f) - \mathscr{K}(f')| &\leq \gamma(\, \|f\|_{H^{\frac{1}{2}}} + \|f'\|_{H^{\frac{1}{2}}})^2\, \|f - f'\|_{H^{\frac{1}{2}}}\, \|\zeta\|_{L^2} \qquad (2.8) \\ &+ \|\mathscr{Q}(\psi', \phi', \chi')\|_{L^2}\, \|\zeta - \zeta'\|_{L^2} \\ &\leq \gamma(\, \|f\|_{H^{\frac{1}{2}}} + \|f'\|_{H^{\frac{1}{2}}})^3\, \|f - f'\|_{H^{\frac{1}{2}}} \\ &:= lip_{\mathscr{K}}\, \|f - f'\|_{H^{\frac{1}{2}}}, \end{aligned} \tag{2.9}$$

where $lip_{\mathscr{K}} := lip_{\mathscr{K}}(\|f\|_{H^{\frac{1}{2}}}, \|f'\|_{H^{\frac{1}{2}}})$ and the proof is finished.

□

Furthermore, we introduce the mapping

$$\mathscr{L}: \quad \mathcal{X} \longrightarrow (H^{\frac{1}{2}}(\mathbb{R}^3))^K$$

$$(C,\Phi) \longmapsto \mathscr{L}(C,\Phi) = \mathbf{\Gamma}^{-1}\,(I-\mathbf{P}_\Phi)\,\mathbb{W}(C,\Phi)\,\Phi.$$

Now, we claim

Lemma 2.5. *Assume that for all $(C,\Phi) \in \mathcal{X}$, there exists $\delta > 0$ such that $\|\mathbf{\Gamma}^{-1}\| \leq \delta$. Then, the mapping $\mathscr{L}$ is well-defined and locally Lipschitz continuous from $\mathcal{X}$ into $(H^{\frac{1}{2}}(\mathbb{R}^3))^K$.*

Proof. The proof relies strongly on Lemma 2.4, that we use implicitly, with the observation that for all $1 \leq i \leq K$, we have, thanks to Lemma 2.3

$$(\mathbb{W}(C,\Phi)\,\Phi)_i = 2\sum_{j,k,l=1}^{K} \gamma_{jkil}(t)\,\mathscr{Q}(\phi_k,\phi_l,\phi_i) \tag{2.10}$$

$$\mathbf{P}_\Phi\,(\mathbb{W}(C,\Phi)\,\Phi)_i = 2\sum_{p,j,k,l=1}^{K} \gamma_{jkil}(t)\,\mathscr{K}(\phi_k,\phi_l,\phi_i,\phi_p)\,\phi_p. \tag{2.11}$$

The most important fact is that $\mathbb{W}(C,\Phi)$ is quadratic with respect to the coefficients C and the functions Φ. Now, on the one side, for all $(C,\Phi) \in \mathcal{X}$ we have using $|\gamma_{ijkl}| \leq \|C\|^2$ and (2.5, 2.7, 2.10, 2.11)

$$\begin{aligned}
\|\mathscr{L}(C,\Phi)\|_{H^{\frac{1}{2}}} &\leq \|\mathbf{\Gamma}^{-1}\|(I-\mathbf{P}_\Phi)\,\mathbb{W}(C,\Phi)\,\|\Phi\|_{L^2}\\
&\leq \|\mathbf{\Gamma}^{-1}\|\left(\|\mathbb{W}(C,\Phi)\,\Phi\|_{H^{\frac{1}{2}}} + \|\,\mathbf{P}_\Phi\,\mathbb{W}(C,\Phi)\,\Phi\|_{H^{\frac{1}{2}}}\right)\\
&\leq \gamma\,\delta\,\|C\|^2\left(\|\Phi\|^3_{H^{\frac{1}{2}}} + \|\Phi\|^5_{H^{\frac{1}{2}}}\right).
\end{aligned}$$

On the other side, let $(C,\Phi), (C',\Phi') \in \mathcal{X}$, then

$$\begin{aligned}
\mathscr{L}(C,\Phi) - \mathscr{L}(C',\Phi') &= (\mathbf{\Gamma}^{-1} - \mathbf{\Gamma}'^{-1})\,(\mathbb{W}(C,\Phi)\,\Phi - \mathbf{P}_{\Phi'}\,\mathbb{W}(C',\Phi')\,\Phi')\\
&+ \mathbf{\Gamma}'^{-1}\,(\mathbb{W}(C,\Phi)\,\Phi - \mathbb{W}(C',\Phi')\,\Phi')\\
&+ \mathbf{\Gamma}^{-1}\,(\mathbf{P}_{\Phi'} - \mathbf{P}_\Phi)\,\mathbb{W}(C',\Phi')\,\Phi'\\
&+ \mathbf{\Gamma}^{-1}\,\mathbf{P}_\Phi\,(\mathbb{W}(C',\Phi')\,\Phi' - \mathbb{W}(C,\Phi)\,\Phi)\\
&:= \sum_{i=1}^{4} I_i.
\end{aligned}$$

The $(H^{\frac{1}{2}}(\mathbb{R}^3))^K$ norm of this difference is handled term by term for which we give the estimates and avoid explicit straightforward details. In particular, we shall use the following matrices and coefficients inequalities (see Ref. 3)

$$\mathbf{\Gamma}^{-1} - \mathbf{\Gamma}'^{-1} = \mathbf{\Gamma}'^{-1}\,(\mathbf{\Gamma}' - \mathbf{\Gamma})\,\mathbf{\Gamma}^{-1}, \qquad |\gamma_{\ldots} - \gamma'_{\ldots}| \leq (\|C\| + \|C'\|)\,\|C - C'\|, \tag{2.12}$$

so that $\|\mathbf{\Gamma}-\mathbf{\Gamma}'\| \leq (\|C\|+\|C'\|)\,\|C-C'\|$. Therefore, with (2.5–2.8) we get

$$\begin{aligned}
\|I_1\|_{H^{\frac12}} &\leq \gamma\,\delta^2\,\left(\|C\|^2\|\Phi\|^3_{H^{\frac12}} + \|C'\|^2\|\Phi\|^5_{H^{\frac12}}\right)(\|C\|+\|C'\|)\,\|C-C'\|\\
\|I_2\|_{H^{\frac12}} &\leq \gamma\,\delta\,\|\Phi\|^3_{H^{\frac12}}(\|C\|+\|C'\|)\,\|C-C'\|\\
&\quad + \gamma\,\delta\,\|C'\|^2\,(\|\Phi\|_{H^{\frac12}} + \|\Phi'\|_{H^{\frac12}})^2\,\|\Phi-\Phi'\|_{H^{\frac12}}\\
\|I_3\|_{H^{\frac12}} &\leq \gamma\,\delta\,\|C'\|^2\,(\|\Phi\|_{H^{\frac12}} + \|\Phi'\|_{H^{\frac12}})\|\Phi'\|^3_{H^{\frac12}}\,\|\Phi-\Phi'\|_{H^{\frac12}}\\
\|I_4\|_{H^{\frac12}} &\leq \gamma\,\delta\,\|\Phi\|^2_{H^{\frac12}}\|\Phi'\|^3_{H^{\frac12}}(\|C\|+\|C'\|)\,\|C-C'\|\\
&\quad + \gamma\,\delta\,\|C\|^2\,\|\Phi\|^2_{H^{\frac12}}(\|\Phi\|_{H^{\frac12}} + \|\Phi'\|_{H^{\frac12}})^2\,\|\Phi-\Phi'\|_{H^{\frac12}}
\end{aligned}$$

Eventually, summing up these estimates, we end up with

$$\|\mathscr{L}(C,\Phi)-\mathscr{L}(C',\Phi')\|_{H^{\frac12}} \leq lip_{\mathscr{L}}\,\|(C-C',\Phi-\Phi')\|_X, \tag{2.13}$$

where $lip_{\mathscr{L}} := lip_{\mathscr{L}}(\delta,\|C\|,\|C'\|,\|\Phi\|_{H^{\frac12}},\|\Phi'\|_{\frac12})$. This ends the proof. □

Now, we use Lemmata 2.4 and 2.5 in order to obtain the desired result concerning the local Lipschitz continuous character of the nonlinearities

Lemma 2.6. *Assume that for all* $(C,\Phi)\in\mathcal{X}$*, there exists* $\delta>0$ *such that* $\|\mathbf{\Gamma}^{-1}\|\leq\delta$*. Then the mapping*

$$\mathscr{M}\,:\,\mathcal{X}\,\to\,\mathcal{X},\,\begin{pmatrix}C\\ \\ \Phi\end{pmatrix}\mapsto\begin{pmatrix}\mathbb{K}(\Phi)\,C\\ \\ \mathbf{\Gamma}^{-1}\,(I-\mathbf{P}_\Phi)\,\mathbb{W}(C,\Phi)\,\Phi\end{pmatrix}$$

is well-defined and locally Lipschitz continuous from $\mathcal{X}$ *into itself.*

Proof. Observe that one has

$$\mathbb{K}[\Phi]_{\sigma_p,\sigma_q} = \frac12\sum_{k,l\in\sigma_p,\,i,j\in\sigma_q,}\delta_{\sigma_p\setminus\{k,l\},\,\sigma_q\setminus\{i,j\},}\,(-1)^{\sigma_p}_{k,l}\,(-1)^{\sigma_q}_{i,j}\,\mathscr{K}(\phi_i,\phi_k,\phi_j,\phi_l).$$

Then, it is rather obvious using Lemmata 2.4 and 2.5 to prove that for all $(C,\Phi),(C',\Phi')\in\mathcal{X}$ we have

$$\|\mathscr{M}(C,\Phi)-\mathscr{M}(C',\Phi')\|_{\mathcal{X}} \leq lip_{\mathscr{M}}\,\|(C,\Phi)-(C',\Phi')\|_{\mathscr{X}},$$

with $lip_{\mathscr{M}} := lip_{\mathscr{M}}(\delta,\|C\|,\|C'\|,\|\Phi\|_{H^{\frac12}},\|\Phi'\|_{H^{\frac12}})$. Therefore, $\mathscr{M}$ is well-defined and locally Lipschitz continuous from $\mathcal{X}$ into itself. □

3. Proof of Theorem 1.1

In this section we prove our main result, namely Theorem 1.1. This proof is divided into two steps. In the first step we prove Lemma 3.1 below where we show that starting with initial data of *full rank*, then there exists a maximal existence and uniqueness time $T^\star>0$. Let us mention that $T^\star$ is possibly equal to $+\infty$ since for the time being there is no rigorous argument proving that a loss of rank certainly occurs. In the second step, we prove Lemma 3.2 where we prove that the assumption on the initial data provides a control on the rank of the density matrix. Thereby, we obtain the global-in-time well-posedness of the system $\mathscr{S}'$, hence $\mathscr{S}$.

3.1. *Local well-posedness*

We begin with

Lemma 3.1. *Let $Z < \frac{2}{\alpha\,\pi}$ and $(C^0, \Phi^0) \in \mathcal{X}$ such that rank$(\mathbf{\Gamma}(t=0)) = K$. Then, there exists a maximal existence time $T^\star > 0$ (possibly $+\infty$) such that the system $\mathscr{S}'$ has a unique solution $(C(t), \Phi(t)) \in \mathcal{F}_N^K$ satisfying*

$$C \in C^1([0, T^\star), \mathbb{C}^r)$$
$$\Phi \in C^0([0, T^\star);\, (H^{\frac{1}{2}}(\mathbb{R}^3))^K) \,\cap\, C^1([0, T^\star);\, (H^{-\frac{1}{2}}(\mathbb{R}^3))^K).$$

Moreover $(C(t), \Phi(t))$ depends continuously on the initial data in $\mathbb{C}^r \times H^{\frac{1}{2}}(\mathbb{R}^3)^K$ and when $T^\star < +\infty$, then $\lim_{t \to T^\star} \|\mathbf{\Gamma}^{-1}(t)\| = +\infty$.

Proof. Our starting point is Kato's inequality $\frac{1}{|x|} \leq \frac{\pi}{2}\sqrt{-\Delta}$ in the sense of self-adjoint operators. In other words, we have for all $\psi \in H^{\frac{1}{2}}$

$$\||\psi|^2 \star \frac{1}{|x|}\|_{L^\infty} \leq \frac{\pi}{2}\,\langle \psi\,,\, \sqrt{-\Delta}\,\psi\rangle_{L^2}.$$

Therefore, we deduce immediately that the multiplicative Coulomb operator $\frac{\alpha\,Z}{|x|}$ is $(\sqrt{-\Delta + \alpha^{-2}})$– form bounded as soon as $\frac{1}{2\alpha} < Z < \frac{2}{\alpha\,\pi}$ with relative bound less than 1. Moreover, when $Z < \frac{1}{2\alpha}$, then $\frac{\alpha\,Z}{|x|}$ is $(\sqrt{-\Delta + \alpha^{-2}})$–bounded with relative bound 2. Then, the operator $\mathbf{H} := \sqrt{-\Delta + \alpha^{-2}} - \frac{\alpha\,Z}{|x|}$ gives rise to a self-adjoint operator on L^2 with domain H^1 when $Z < \frac{1}{2\alpha}$ and form domain $H^{\frac{1}{2}}(\mathbb{R}^3)$ when $\frac{1}{2\alpha} < Z < \frac{2}{\alpha\,\pi}$. Moreover, $\mathbf{H}$ can be extended to $H^{\frac{1}{2}}$ so that its extension (we still denote it $\mathbf{H}$ by abuse of notation) $\mathbf{H}\ :\ H^{\frac{1}{2}} \to H^{-\frac{1}{2}}$ generates a C^0–semigroup of isometries $\{\mathscr{U}(t)\}_{t\in\mathbb{R}} := \{e^{-it\mathbf{H}}\}_{t\in\mathbb{R}}$ acting on $\mathbf{H}^{\frac{1}{2}}$.

The matrix $\mathbf{\Gamma}$ being explicitly dependent on the coefficients *via* the formula (2.3), it is clear that one can construct a unit coefficient vector C^0 such that $\mathbf{\Gamma}(t=0) = \mathbf{\Gamma}(C^0)$ is of maximal rank K, hence invertible. Since invertible matrices form an open subset of $\mathcal{M}_{K\times K}$ and the mapping $C \mapsto \mathbf{\Gamma}^{-1}$ being locally Lipschitz continuous (see (2.12)), we expect that by continuity of the dynamic of the system $\mathscr{S}'$ (equivalently the system $\mathscr{S}$), this property will be propagated in time at least up to a certain time $T^\star > 0$ for which $rank(\mathbf{\Gamma}(T^\star)) < K$. Therefore, for all $t \in [0, T^\star)$, there exists $\delta > 0$ such that $\|\mathbf{\Gamma}^{-1}(t)\| \leq \delta$.

With the Lemma 2.3, we have the equivalence (up to *gauge* transformation) of the system $\mathscr{S}$ and the system $\mathscr{S}'$. Fom now on, we shall use them in an interchangeable way. Let $0 \leq T \leq T^\star$, we shall apply a fixed point argument in order to prove the existence and uniqueness of a solution to the system $\mathscr{S}$. We denote by $\mathcal{Y} = C([0,T],\mathcal{X})$ endowed with the norm $\sup_{t\in[0,T]} e^{-\lambda\, t}\|(C(t),\Phi(t))\|_{\mathcal{X}}$ for all $(C,\Phi)\in\mathcal{Y}$ and $\lambda>0$ to be fixed hereafter. The solution of $\mathscr{S}'$ is obtained as a mild solution, that is a solution of the integral equation

$$\pi((C(t),\Phi(t))) := \begin{pmatrix} C(t) \\ \\ \Phi(t) \end{pmatrix} = \begin{pmatrix} C^0 \\ \\ \mathscr{U}(t)\,\Phi^0 \end{pmatrix} - i\int_0^t \begin{pmatrix} \mathbb{K}(\Phi(s))\,C(s) \\ \\ \mathscr{U}(t-s)\,\mathscr{L}(C(s),\Phi(s)) \end{pmatrix} ds.$$

We are going to show, that this equation has a unique solution in $\mathcal{Y}$ by proving that the mapping π defined above has a unique fixed point in the closed ball $B_R = \{(C,\Phi)\in\mathcal{Y};\ \|(C,\Phi)\|_{\mathcal{Y}}\le R\}$ for a convenient R to be chosen. Now, $\mathscr{U}(t)$ being an isometry for all $t\in\mathbb{R}$, we have obviously $\|\mathscr{U}(t)\psi\|_{\mathcal{X}}\le\|\psi\|_{\mathcal{X}}$ for all $\psi\in\mathcal{X}$.

On the one side, thanks to Lemmata 2.4 and 2.5 we have for all $(C,\Phi)\in B_R$ the existence of $0<\gamma_1$ such that

$$\begin{aligned}\|(\mathbb{K}(\Phi(s))\,C(s),\mathscr{L}(C(s),\Phi(s)))\|_{\mathcal{X}} &\le \gamma_1\|\Phi(s)\|^4_{H^{\frac12}}\,\|C(s)\| \\ &\quad + \gamma_1\delta\|C(s)\|^2\left(\|\Phi(s)\|^3_{H^{\frac12}}+\|\Phi(s)\|^5_{H^{\frac12}}\right)\end{aligned}$$

Then, we chooe $\lambda > 2\gamma_1\,R^4(1+\delta+R^2)$ and get

$$\begin{aligned}\|\pi(C(t),\Phi(t))\|_{\mathcal{X}} &\le \|(C^0,\mathscr{U}(t)\Phi^0)\|_{\mathcal{X}} + \int_0^t \|(\mathbb{K}(\Phi(s))\,C(s),\mathscr{L}(C(s),\Phi(s)))\|_{\mathcal{X}}\,ds \\ &\le \|(C^0,\Phi^0)\|_{\mathcal{X}} + \frac{\gamma_1\,R^5\,(1+\delta+R^2)}{\lambda}\,e^{\lambda t}.\end{aligned}$$

Thus, we have

$$\|\pi(C(t),\Phi(t))\|_{\mathcal{Y}} \le \|(C^0,\Phi^0\|_{\mathcal{X}} + \frac{\gamma_1\,R^5\,(1+\delta+R^2)}{\lambda}.$$

Therefore, if we choose R such that $R>2\,\|(C^0,\Phi^0\|_{\mathcal{X}}$, then π maps B_R into itself. On the opposite side, thanks to Lemma 2.6 we have for all $(C,\Phi),(C',\Phi')\in B_R$

$$\begin{aligned}\|\pi((C(t),\Phi(t))-(C'(t),\Phi'(t)))\|_{\mathcal{X}} &= -i\int_0^t \mathscr{U}(t-s)\mathscr{M}(C(s),\Phi(s))\,ds \\ &\quad + i\int_0^t \mathscr{U}(t-s)\mathscr{M}(C'(s),\Phi'(s))\,ds \\ &\le \frac{lip_{\mathscr{M}}(\delta,R,R,R,R)}{\lambda}\,e^{\lambda t}\,\|(C,\Phi)-(C',\Phi')\|_{\mathcal{Y}} \\ \|\pi((C(t),\Phi(t))-(C'(t),\Phi'(t)))\|_{\mathcal{Y}} &\le \frac{lip_{\mathscr{M}}(\delta,R,R,R,R)}{\lambda}\,\|(C,\Phi)-(C',\Phi')\|_{\mathcal{Y}}\end{aligned}$$

Thus, if we set now $\lambda > \max(2\gamma_1\,R^4(1+\delta+R^2), lip_{\mathscr{M}}(\delta,R,R,R,R))$, then π is a strict contraction from B_R into itself and therefore has a unique fixed point, yielding the solution of the system $\mathscr{S}'$ (equivalently $\mathscr{S}$) in $\mathcal{Y}$ for all $t\in[0,T]$.

The continuous dependence on the initial data is straightforward in view of our choice of R and λ. Let $(C,\Phi),(C',\Phi')\in B_R$ be two fixed points of the mapping π associated to two different initial data $(C^0,\Phi^0),({C'}^0,{\Phi'}^0)\in\mathcal{X}$, then we have

$$\|((C(t),\Phi(t))-(C'(t),\Phi'(t)))\|_{\mathcal{Y}}\leq\frac{\lambda}{\lambda-lip_{\mathscr{M}}(\delta,R,R,R,R)}\|((C^0,\Phi^0),({C'}^0,{\Phi'}^0))\|_{\mathcal{Y}}.$$

Let us precise that by continuous dependence of the solution $(C(t),\Phi(t))$ of the system $\mathscr{S}'$ on the initial data, we mean that the mapping $(C^0,\Phi^0)\mapsto(C(t),\Phi(t))\in C^1([0,T^\star),\mathbb{C}^{\binom{K}{N}})\times C^0([0,T^\star),(H^{\frac12}(\mathbb{R}^3))^K)$ is continuous for all closed and bounded intervals of $[0,T^\star)$. Eventually, standard arguments (see Ref. 7 for instance) allow to show the equivalence between the mild formulation $\pi((C(t),\Phi(t)))$ and the strong formulation namely the system of ODEs and PDEs $\mathscr{S}'$.

3.2. *Global well-posedness*

This section is devoted to the proof of global-in-time well-posedness of the system $\mathscr{S}'$ (equivalently $\mathscr{S}$). More precisely, we shall extend the existence time of the solution $(C(t),\Phi(t))$ beyond T. Observe that if $T=T^\star$, then Lemma 3.1 is proved. Therefore, we assume that $T<T^\star$.

In order to achieve this aim, we need *a priori* estimates on the solution $(C(t),\Phi(t))$ in $\ell^2(\mathbb{C}^{\binom{K}{N}})\times H^{\frac12}(\mathbb{R}^3)^K$. We shall obtain these estimates using the conservation laws associated to the system $\mathscr{S}'$ (equivalently $\mathscr{S}$). Indeed, on the one side, thanks to Lemma 2.1 we have conservation of mass. More precisely, we have $\|C(t)\|=1$ and $\int_{\mathbb{R}^3}\phi_i(t,x)\,\bar\phi_j(t,x)\,dx=\delta_{i,j}$ for all $t\in[0,T]$. In particular, we obtain a uniform control on the ℓ^2 norm of the coefficients and the L^2 norm of functions. On the opposite side, thanks to Lemma 2.2, we have the conservation of the total energy for all $t\in[0,T]$. This property will allows us to control the $H^{\frac12}(\mathbb{R}^3)$ norm of the ϕ_i's which amounts to control the Frobenuis norm of the inverse of the density matrix $\mathbf{\Gamma}(t)$.

Let $T^\star$ denote the maximal existence time of the solution $(C(t),\Phi(t))$ and assume $T^\star<+\infty$. Arguing by contradiction as in Ref. 3, we show that $\limsup_{t\to T^\star}\|\mathbf{\Gamma}^{-1}\|=+\infty$. Hence, there exists a constant $\kappa>0$ such that for all $t\in[0,T^\star)$ we have $\|\mathbf{\Gamma}^{-1}\|\leq\kappa$. Now, the total semi-relativistic multi-configuration Hartree-Fock energy reads for all $t\in[0,T]$

$$\begin{aligned}
&\mathcal{E}(C^0, \Phi^0) = \mathcal{E}(C(t), \Phi(t)) \\
&= \alpha^{-1} \left\langle \left(\sum_{i=1}^{N} \left(\sqrt{-\Delta_{x_i} + \alpha^{-2}} - \frac{\alpha Z}{|x_i|} - \alpha^{-1} \right) \right) \Psi(t)\,,\, \Psi(t) \right\rangle \\
&+ \left\langle \left(\sum_{1 \le i < j \le N} \frac{1}{|x_i - x_j|} \right) \Psi(t)(t)\,,\, \Psi(t) \right\rangle \\
&\ge \alpha^{-1} \left\langle \left(\sum_{i=1}^{N} \left(\sqrt{-\Delta_{x_i} + \alpha^{-2}} - \frac{\alpha Z}{|x_i|} - \alpha^{-1} \right) \right) \Psi(t)\,,\, \Psi(t) \right\rangle \\
&= \alpha^{-1} \left\langle \left(\sqrt{-\Delta + \alpha^{-2}} - \frac{\alpha Z}{|x|} - \alpha^{-1} \right) \mathbf{\Gamma}(t)\, \Phi(t)\,,\, \Phi(t) \right\rangle
\end{aligned}$$

where we used the positivity of $V = \sum_{1 \le i < j \le N} |x_i - x_j|^{-1}$. With the equivalence of $\|\Phi\|_{H^{\frac12}}$ and $\|(\sqrt{-\Delta + \alpha^{-2}} - \frac{\alpha Z}{|x|})\, \Phi\|_{H^{\frac12}}$ by Kato's inequality (and the mass conservation) we obtain the existence of a positive constant γ independent of time such that

$$\|\sqrt{\mathbf{\Gamma}}\, \Phi\|_{H^{\frac12}} \le \gamma. \tag{3.1}$$

The matrix $\mathbf{\Gamma}$ being invertible on $[0, T^\star)$, we denote its lowest eigenvalue by $\mu(t)$ and obtain $\frac{1}{\sqrt{\mu(t)}} \le \|\sqrt{\mathbf{\Gamma}^{-1}}\| \le \frac{\sqrt[4]{K}}{\sqrt{\mu(t)}}$ for all $t \in [0, T^\star)$. We refer to Ref. 3 for further details, especially for the factor $\sqrt[4]{K}$ appearing in the last inequality. Therefore

$$\|\Phi\|_{H^{\frac12}} \le \frac{\sqrt[4]{K}}{\sqrt{\mu(t)}}\, \|\sqrt{\mathbf{\Gamma}(t)}\, \Phi\|_{H^{\frac12}} \;\le \gamma\, \sqrt[4]{K}\, \sqrt{\|\mathbf{\Gamma}(t)\|} \le \gamma\, \sqrt{\kappa}\, \sqrt[4]{K}.$$

Therefore, the solution can be extended to the whole interval of time $[0, T^\star)$ by the classical iteration argument in intervals $[t, t+T]$ for $t > 0$ and since t is arbitrary close to $T^\star$ we reach a contradiction with the definition of $T^\star$. This proves the existence of maximal solution to the system $\mathscr{S}'$, thus to the system $\mathscr{S}$ in the energy space on the time interval $[0, T^\star)$ where $T^\star$ is the time for which at least one rank's loss holds for the density matrix $\mathbf{\Gamma}(t)$. □

The last point to prove is the global-in-time existence and uniqueness of solution under the hypothesis on the energy of the initial data. For that purpose, we need the following

Lemma 3.2. *Let $(C^0, \Phi^0) \in \mathcal{F}_{N,K} \cap H^{\frac12}$ and $(C(t), \phi(t))$ be the associated solution to the system $\mathscr{S}'$ (equivalently $\mathscr{S}$). If $T^\star < +\infty$, then*

$$\mathcal{E}(C^0, \Phi^0) \ge I_{K-1}.$$

Proof. The proof is in the spirit of Ref. 2, 3 with different functional spaces. By Lemma 3.1, we have the existence and uniqueness of a maximal solution $(C(t), \Phi(t))$ in the class

$$C \in C^1([0,T^\star), \mathbb{C}^r)$$
$$\Phi \in C^0([0,T^\star);\, (H^{\frac{1}{2}}(\mathbb{R}^3))^K) \,\cap\, C^1([0,T^\star);\, (H^{-\frac{1}{2}}(\mathbb{R}^3))^K).$$

Moreover, we have $\|\mathbf{\Gamma}(t)\| \xrightarrow[t\to T^\star]{} +\infty$. The energy being invariant under *gauge* transformations, then we can assume without loss of generality that the matrix $\mathbf{\Gamma}(t) = diag\{0 \le \mu_K(t) \le \ldots \le \mu_1(t) \le 1\}$ and still use the notation $(C(t), \Phi(t))$ instead of $\mathcal{U}(t)\,(C(t), \Phi(t))$. In fact we have even an explicit expression for the $\mu_k(t)$ that reads

$$\mu_k(t) = \sum_{i=1}^r \mathbb{1}_{\{k\in\sigma_i\}}\, |c_{\sigma_i}(t)|^2. \tag{3.2}$$

Therefore $\|\mathbf{\Gamma}(t)\| \xrightarrow[t\to T^\star]{} +\infty$ is equivalent to $\mu_K(t) \xrightarrow[t\to T^\star]{} 0$. In particular, a loss of rank of the density matrix $\mathbf{\Gamma}(t)$ occurs at $T^\star$. Let us mention that it is trivial that the density matrix cannot loose more that $K - N$ rank. Indeed, in the case when $K = N$ the whole wavefunction Ψ reduces to a single *Slater* determinant and the matrix $\mathbf{\Gamma}(t)$ turns to be I_N. We mention also, that it is proved in Ref. 1 equivalently to the relativistic case, [21], that at $T^\star$, the density matrix looses at most one rank so that $rank\mathbf{\Gamma}(T^\star) = K - 1$. Therefore, there exists a sequence of times $t_n \xrightarrow[n\to+\infty]{} T^\star$ and a positive real γ such that $\mu_K(t_n) \xrightarrow[n\to+\infty]{} 0$ and $0 < \gamma < \mu_k(t_n))$ for all $1 \le k \le K-1$. Thus, in view of (3.2), we have obviously $c^n_{\sigma_i} \xrightarrow[n\to+\infty]{} 0$ for all σ_i such that $K \in \sigma_i$ and $\sum_{i=1}^r \mathbb{1}_{\{K\notin\sigma_i\}}\, |c^n_{\sigma_i}|^2 \xrightarrow[n\to+\infty]{} 1$. Thus, since $\Psi_n = \sum_{i=1}^r \mathbb{1}_{\{K\notin\sigma_i\}}\, c^n_{\sigma_i}\, \Phi^n_{\sigma_i} + \sum_{i=1}^r \mathbb{1}_{\{K\in\sigma_i\}}\, c^n_{\sigma_i}\, \Phi^n_{\sigma_i}$, we have obviously

$$\Big\|\sum_{i=1}^r \mathbb{1}_{\{K\in\sigma_i\}}\, c^n_{\sigma_i}\, \Phi^n_{\sigma_i}\Big\|_{L^2(\mathbb{R}^{3N})} \xrightarrow[n\to+\infty]{} 0,$$
$$\Big\|\Psi_n - \sum_{i=1}^r \mathbb{1}_{\{K\notin\sigma_i\}}\, c^n_{\sigma_i}\, \Phi^n_{\sigma_i}\Big\|_{L^2(\mathbb{R}^{3N})} \xrightarrow[n\to+\infty]{} 0 \tag{3.3}$$

Now, recall that we have the conservation of the energy on $[0, T^\star)$ and

$$\begin{aligned}
\mathcal{E}(C^0,\Phi^0) &= \alpha^{-1}\,\mathcal{E}(C^n(t),\Phi^n(t))\\
&= \sum_{i=1}^K \mu_i^n\, \left\langle \left(\sqrt{-\Delta+\alpha^{-2}} - \frac{\alpha\, Z}{|x|} - \frac{1}{\alpha}\right) \phi_i^n(t)\,,\, \phi_i^n(t)\right\rangle\\
&+ \sum_{i,j,k,l=1}^K \gamma_{ijkl}\, \mathscr{K}(\phi_l^n,\phi_i^n,\phi_k^n,\phi_j^n)\\
&\ge \alpha^{-1} \sum_{i=1}^K \mu_i^n\, \left\langle \left(\sqrt{-\Delta+\alpha^{-2}} - \frac{\alpha\, Z}{|x|} - \frac{1}{\alpha}\right) \phi_i^n(t)\,,\, \phi_i^n(t)\right\rangle.
\end{aligned}$$

Therefore, again using Kato's inequality, we get the existence of a positive γ independent of n such that

$$\sum_{i=1}^{K} \sqrt{\mu_i^n}\, \| - \sqrt[4]{\Delta}\phi_i^n \| \leq \gamma.$$

Thus, for all $1 \leq i \leq K$, we have $\sqrt{\mu_i^n}\,\phi_i$ is bounded in $H^{\frac{1}{2}}$. Therefore, we deduce that up to extraction of subsequences if necessary (we keep the same notation) ϕ_i^n is bounded in $H^{\frac{1}{2}}$ for all $1 \leq i \leq K-1$ and $\sqrt{\mu_K^n}\,\phi_K$ converges to 0 weakly in $H^{\frac{1}{2}}$ and strongly in L^2. The next step consists in proving the following

$$\alpha^{-1} \liminf_{n\to+\infty} \sum_{i=1}^{K-1} \mu_i^n \left\langle \left(\sqrt{-\Delta+\alpha^{-2}} - \frac{\alpha\, Z}{|x|} - \frac{1}{\alpha} \right) \phi_i^n(t)\,,\, \phi_i^n(t) \right\rangle$$
$$+ \liminf_{n\to+\infty} \sum_{i,j,k,l=1}^{K-1} \gamma_{ijkl}^n\, \mathscr{K}(\phi_l^n, \phi_i^n, \phi_k^n, \phi_j^n) \leq \liminf_{n\to=+\infty} \mathcal{E}(C^n, \Phi^n) \tag{3.4}$$

The main difficulty here as pointed out by Lewin, [21] is that the potential $\frac{Z\,\alpha}{|x|}$ term is not continuous with respect to $H^{\frac{1}{2}}$ weak topology , that is the operator $\sqrt[-4]{1-\Delta}\,|x|^{-1}\, \sqrt[-4]{1-\Delta}$ is not compact and hence the weak convergence of the ϕ_i^n to the ϕ_i's is not enough in order to conclude that $\int_{\mathbb{R}^3} \frac{|\phi_i^n|^2}{|x|}\, dx \xrightarrow[n\to+\infty]{} \int_{\mathbb{R}^3} \frac{|\phi_i|^2}{|x|}\, dx$. However, following the argument of Ref. 10, as soon as $Z < \frac{2}{\pi\,\alpha}$, we can decompose the free-one body operator $\frac{1}{\alpha}\sqrt{-\Delta+\alpha^{-2}} - \frac{\alpha\, Z}{|x|} - \frac{1}{\alpha}$ as follows

$$\frac{1}{\alpha}\sqrt{-\Delta+\alpha^{-2}} - \frac{\alpha\, Z}{|x|} - \frac{1}{\alpha} = \left(\frac{1}{\alpha}\sqrt{-\Delta+\alpha^{-2}} - \frac{\alpha\, Z}{|x|} - \frac{1}{\alpha} \right)_{-}$$
$$+ \left(\frac{1}{\alpha}\sqrt{-\Delta+\alpha^{-2}} - \frac{\alpha\, Z}{|x|} - \frac{1}{\alpha} \right)_{+}$$

with the first part defining a compact operator and the second part positive operator on $H^{\frac{1}{2}}$ and we refer to Ref. 10 for further details. Therefore, we obtain

$$\liminf_{n\to+\infty} \sum_{i=1}^{K} \mu_i^n \left\langle \left(\sqrt{-\Delta+\alpha^{-2}} - \frac{\alpha\, Z}{|x|} - \frac{1}{\alpha} \right) \phi_i^n(t)\,,\, \phi_i^n(t) \right\rangle$$
$$\geq \liminf_{n\to+\infty} \sum_{i=1}^{K-1} \mu_i^n \left\langle \left(\sqrt{-\Delta+\alpha^{-2}} - \frac{\alpha\, Z}{|x|} - \frac{1}{\alpha} \right) \phi_i(t)\,,\, \phi_i(t) \right\rangle.$$

The second term is easier to handle. Indeed, recall that

$$\gamma_{ijkl} = \frac{1}{2}\,(1-\delta_{i,j})(1-\delta_{k,l}) \sum_{\substack{p,q=1 \,|\, i,j\in\sigma_p,\, k,l\in\sigma_q \\ \sigma_p\setminus\{i,j\}=\sigma_q\setminus\{k,l\}}}^{r} (-1)_{i,j}^{\sigma_p}(-1)_{k,l}^{\sigma_q}\, c_{\sigma_p}\, \overline{c}_{\sigma_q}.$$

Then, observe that since the eigenvalues of $\mathbf{\Gamma}^n$ are between 0 and 1 we have

$$|\gamma_{ijkl}| \leq \min\left(\sqrt{\mu_i^n}, \sqrt{\mu_i^n}\right)\, \min\left(\sqrt{\mu_i^n}, \sqrt{\mu_i^n}\right) \leq \min(\mu_i^n, \mu_k^n, \mu_j^n, \mu_l^n)^{\frac{1}{2}}.$$

Thus, if $K \in \{i,j,k,l\}$ then $\gamma_{ijkl} \xrightarrow[n\to+\infty]{} 0$. Now, using Lemma 2.4, we have clearly

$$\begin{aligned}|\gamma_{ijkl}\,\mathscr{K}(\phi_l^n,\phi_i^n,\phi_k^n,\phi_j^n)| &\le \frac{\pi}{2}\,\sqrt{\mu_i^n}\,\sqrt{\mu_k^n}\,\|\sqrt[4]{-\Delta}\,\phi_l^n\|_{L^2}\,\|\sqrt[4]{-\Delta}\,\phi_i^n\|_{L^2}\,\|\phi_k^n\|_{L^2}\,\|\phi_j^n\|_{L^2}\\ &\le \gamma\,\sqrt{\mu_k^n}\end{aligned}$$

by conservation of mass and uniform boundedness of $\sqrt{\mu_k}\,\phi_K^n$ in $H^{\frac12}$. Thus, we end with

$$\sum_{i,j,k,l=1}^{K} \mathbb{1}_{\{K\in\{i,j,k,l\}\}}\,\gamma_{ijkl}^n\,\mathscr{K}(\phi_l^n,\phi_i^n,\phi_k^n,\phi_j^n) \xrightarrow[n\to+\infty]{} 0.$$

This shows (3.4). Let us now introduce $(\tilde{C}^n,\tilde{\Phi}^n)$ where $\tilde{C}^n$ denotes the vector of all $c_{\sigma_i}^n$ for $i=1,\dots,r$ such that $K \notin \sigma_i^n$ and $\tilde{\Phi} = (\phi_1^n,\dots,\phi_{K-1}^n)$. Of course the vector $\tilde{C}$ is not normalized in $\mathbb{C}^{\binom{K-1}{N}}$ point-wise but only asymptotically and this issue will be fixed in the end of the proof. Thus, we have

$$\sum_{i=1}^{r} \mathbb{1}_{\{K\notin\sigma_i\}}\,c_{\sigma_i}^n\,\Phi_{\sigma_i}^n = \tilde{\Psi}_n(\tilde{C},\tilde{\Phi}) = \sum_{i=1}^{\binom{K-1}{N}} \tilde{c}_{\sigma_i}^n\,\tilde{\Phi}_{\sigma_i}^n.$$

The new matrix $\tilde{\mathbf{\Gamma}}^n$ is no longer diagonal and is now defined via its entries for all $1\le i,j\le K-1$

$$\tilde{\mathbf{\Gamma}}_{i,j}^n = \mu_i^n\delta_{i,j} + \sum_{\substack{k,l=1 \mid i\in\sigma_k,\, j\in\sigma_l, K\in\sigma_i\cup\sigma_j\\ \sigma_k\setminus\{i\}=\sigma_l\setminus\{j\}}}^{\binom{K-1}{N}} (-1)^{\sigma_k^{-1}(i)+\sigma_l^{-1}(j)}\,\overline{c}_{\sigma_k}^n\,c_{\sigma_l}^n.$$

Obviously, we have $\tilde{\mathbf{\Gamma}}_{i,j}^n - \mu_i^n\delta_{i,j} \xrightarrow[n\to+\infty]{} 0$. Furthermore, we have

$$\begin{aligned}&\sum_{i=1}^{K-1} \mu_i^n\,\Big\langle \Big(\sqrt{-\Delta+\alpha^{-2}} - \frac{\alpha\,Z}{|x|} - \frac{1}{\alpha}\Big)\,\phi_i^n(t)\,,\,\phi_i^n(t)\Big\rangle\\ &= \sum_{i,j=1}^{K-1} \tilde{\mathbf{\Gamma}}_{i,j}^n\,\Big\langle \Big(\sqrt{-\Delta+\alpha^{-2}} - \frac{\alpha\,Z}{|x|} - \frac{1}{\alpha}\Big)\,\tilde{\phi}_i^n(t)\,,\,\tilde{\phi}_j^n(t)\Big\rangle + o(1)\end{aligned}$$

since each term of the form $\Big\langle \Big(\sqrt{-\Delta+\alpha^{-2}} - \frac{\alpha\,Z}{|x|} - \frac{1}{\alpha}\Big)\,\phi_i^n(t)\,,\,\phi_i^n(t)\Big\rangle$ is uniformly bounded. In the same way, since each term of the form $\mathscr{K}(\phi_l^n,\phi_i^n,\phi_k^n,\phi_j^n)$ is uniformly bounded and for all $1\le i,j,k,l\le K-1$, we have $|\gamma_{ijkl}^n - \tilde{\gamma}_{ijkl}| \xrightarrow[n\to+\infty]{} 0$ since the difference involves coefficients c_{σ_i} where $K\notin\sigma_i$, then

$$\sum_{i,j,k,l=1}^{K-1} \gamma_{ijkl}^n\,\mathscr{K}(\phi_l^n,\phi_i^n,\phi_k^n,\phi_j^n) = \sum_{i,j,k,l=1}^{K-1} \tilde{\gamma}_{ijkl}^n\,\mathscr{K}(\tilde{\phi}_l^n,\tilde{\phi}_i^n,\tilde{\phi}_k^n,\tilde{\phi}_j^n) + o(1)$$

Now, recall that $\tilde{C}^n \notin \mathbb{S}^{\binom{K-1}{N}-1}$, thus $(\tilde{C}^n,\tilde{\Phi}^n) \notin \mathcal{F}_N^{K-1}$, therefore it is not sure that $\mathcal{E}(\tilde{\Psi}_n) \ge I_{K-1}$. However, since $\|\tilde{\Psi}_n\| \xrightarrow[n\to+\infty]{} 1$ and the energy is quadratic in

Ψ, we have

$$\mathcal{E}(\tilde{\Psi}_N) = \|\tilde{\Psi}_n\|^2\, \mathcal{E}\left(\frac{\tilde{\Psi}_n}{\|\tilde{\Psi}_N\|}\right) \geq \|\tilde{\Psi}_n\|^2\, I_{K-1}.$$

Eventually, we end up with

$$\liminf_{n\to+\infty} \mathcal{E}(C^n,\Phi^n) \geq \liminf_{n\to+\infty} \mathcal{E}(\tilde{C}^n,\tilde{\Phi}^n) = \liminf_{n\to+\infty} \mathcal{E}(\tilde{\Psi}_n) \geq \|\tilde{\Psi}_N\|^2\, I_{K-1}.$$

That is

$$\liminf_{n\to+\infty} \mathcal{E}(C^n,\Phi^n) \geq\ I_{K-1},$$

which is the desired result. □

Finally, combing Lemma 3.1 and Lemma 3.2 we obtain Theorem 1.1.

We mention that the assumption on the initial data is well-defined in the sense that one can always find a (C^0,Φ^0) such that $\mathcal{E}(C^0,\Phi^0) < I_{K-1}$. Indeed, with the assumption $N-1 < Z$, it is known, [9] that we have $I_K < I_{K-2}$ so that our assumption can always be satisfied by changing K into $K-1$ if necessary.

4. Higher regularity

In this section we extend Theorem 1.1 as follows

Theorem 4.1. *Let $s \geq \frac{1}{2}, Z < \frac{2}{\alpha\,\pi}$ and $(C^0,\Phi^0) \in \mathcal{F}_N^K \cap (H^s(\mathbb{R}^3))^K$ such that $\mathcal{E}(C^0,\Phi^0) < I_{K-1}$. Then, the system $\mathscr{S}$ has a unique solution $(C(t),\Phi(t)) \in \mathcal{F}_N^K$ satisfying*

$$\begin{aligned} &C \in C^1(\mathbb{R},\mathbb{C}^r)\\ &\Phi \in C^0(\mathbb{R};\, (H^s(\mathbb{R}^3))^K)\, \cap\, C^1(\mathbb{R};\, (H^{s-1}(\mathbb{R}^3))^K). \end{aligned}$$

Moreover, the solution depends continuously on the initial data in $\mathbb{C}^r \times H^s(\mathbb{R}^3)^K$.

Proof. The squeleton of the proof is similar to the proof of Theorem 1.1. The steps are the following:

1. Prove Lemma 2.6 in H^s for all $s \geq \frac{1}{2}$.
2. Prove the equivalent of Lemma 3.1 in H^s for all $s \geq \frac{1}{2}$.
3. Establish *a priori* estimate for the H^s norm of the local solution for all $s \geq \frac{1}{2}$.

The remaining part of the proof as the blow-up alternative and the global existence is merely the same.

4.1. *Step 1.*

This step is based on the generalized Leibniz rule. We shall only prove bounds for $\mathscr{Q}$ and $\mathscr{K}$. The proof of the bound on $\mathscr{Q}$ is given in Ref. 19 and we write it here for completeness with different functions which simplifies the proof of the local Lipschitz continuous property. Also, for further purpose, we shall use the less norm order as possible. Let $\psi, \phi, \chi \in H^s$ and note $1/p + 1/p' = 1/2$ for all $1 < p$ and $p' \leq \infty$ and a generic constant γ, then, on the one hand, we have

$$\begin{aligned}
\|\mathscr{Q}(\psi,\phi,\chi)\|_{H^s} &= \|\mathscr{Q}(\psi,\phi,\chi)\|_{L^2} + \|\sqrt{-\Delta}^s\,\mathscr{Q}(\psi,\phi,\chi)\|_{L^2}\\
&\leq \frac{\pi}{2}\,\|\sqrt[4]{-\Delta}\,\psi\|_{L^2}\,\|\sqrt[4]{-\Delta}\,\phi\|_{L^2}\,\|\chi\|_{L^2} + \|\sqrt{-\Delta}^s((-\Delta^{-1})\psi\bar{\phi})\chi\|_{L^2}\\
&\leq \frac{\pi}{2}\,\|\sqrt[4]{-\Delta}\,\psi\|_{L^2}\,\|\sqrt[4]{-\Delta}\,\phi\|_{L^2}\,\|\chi\|_{L^2} + \|\sqrt{-\Delta}^{s-2}\psi\bar{\phi}\|_{L^p}\,\|\chi\|_{L^{p'}}\\
&+ \|(-\Delta)\,\psi\phi\|_{L^\infty}\,\|\sqrt{(-\Delta)}^s\chi\|_{L^2}\\
&\leq \frac{\pi}{2}\,\|\sqrt[4]{-\Delta}\,\psi\|_{L^2}\,\|\sqrt[4]{-\Delta}\,\phi\|_{L^2}\,\|\chi\|_{L^2} + \|\sqrt{-\Delta}^{s-2}\psi\bar{\phi}\|_{L^p}\,\|\chi\|_{L^{p'}}\\
&+ \frac{\pi}{2}\,\|\sqrt[4]{-\Delta}\,\psi\|_{L^2}\,\|\sqrt[4]{-\Delta}\,\phi\|_{L^2}\,\|\chi\|_{H^s}.
\end{aligned}$$

We treat the middle term of the right-hand side as follows with $r := max(s-1, \frac{1}{2})$

$$\begin{aligned}
\|\sqrt{-\Delta}^{s-2}\psi\bar{\phi}\|_{L^{\frac{3}{s}}}\,\|\chi\|_{L^{\frac{6}{3-2s}}} &\leq \|G_{2-s}\|_{L_w^{\frac{3}{1+s}}}\,\|\psi\bar{\phi}\|_{L^{\frac{3}{2}}}\,\|\chi\|_{H^s}, \quad \frac{1}{2} \leq s < \frac{3}{2}, \quad p_1 = \frac{3}{s}\\
&\leq \gamma\,\|\psi\|_{H^{\frac{1}{2}}}\,\|\phi\|_{H^{\frac{1}{2}}}\,\|\chi\|_{H^s}\\
&\leq \gamma\,\|\psi\|_{H^r}\,\|\phi\|_{H^r}\,\|\chi\|_{H^s}.\\
\|\sqrt{-\Delta}^{s-2}\psi\bar{\phi}\|_{L^6}\,\|\chi\|_{L^3} &\leq \|\sqrt{-\Delta}^{s-1}\psi\bar{\phi}\|_{L^2}\,\|\chi\|_{L^3}, \quad \frac{3}{2} \leq s, \quad p = 6\\
&\leq \|\sqrt{-\Delta}^s\psi\|_{L^2}\,\|\phi\|_{L^3}\,\|\chi\|_{L^3} \quad \left(\|\psi\|_{L^3}\,\|\sqrt{-\Delta}^s\phi\|_{L^2}\,\|\chi\|_{L^3}\right)\\
&\leq \|\psi\|_{H^s}\,\|\phi\|_{H^r}\,\|\chi\|_{H^r} \quad (\|\psi\|_{H^r}\,\|\phi\|_{H^s}\,\|\chi\|_{H^r}).
\end{aligned}$$

Therefore

$$\begin{aligned}
\|\mathscr{Q}(\psi,\phi,\chi)\|_{H^s} &\leq \gamma\,\|\psi\|_{H^{\frac{1}{2}}}\,\|\phi\|_{H^s}\,\|\chi\|_{L^2} + \gamma\,\|\psi\|_{H^s}\,\|\phi\|_{H^r}\,\|\chi\|_{H^r}.\\
\|\mathscr{Q}(\psi,\phi,\chi)\|_{H^s} &\leq \gamma\,\|\psi\|_{H^{\frac{1}{2}}}\,\|\phi\|_{H^s}\,\|\chi\|_{L^2} + \gamma\,\|\psi\|_{H^r}\,\|\phi\|_{H^s}\,\|\chi\|_{H^r}.
\end{aligned}$$

On the other hand, $P_\Phi \mathbb{W}(C,\phi)\Phi$ part involves terms of the form

$$\begin{aligned}
\|\mathscr{K}(\psi,\phi,\chi,\zeta)\,\theta\|_{H^s} &\leq |\mathscr{K}(\psi,\phi,\chi,\zeta)|\,\|\theta\|_{H^s}\\
&\leq \|\mathscr{Q}(\psi,\phi,\chi)\|_{L^2}\,\|\zeta\|_{L^2}\,\|\theta\|_{H^s} \leq \gamma\,\|\psi\|_{H^{\frac{1}{2}}}\,\|\phi\|_{H^{\frac{1}{2}}}\,\|\chi\|_{H^{\frac{1}{2}}}\,\|\theta\|_{H^s}.
\end{aligned}$$

4.2. *Step 2.*

The operator $\mathbf{H} : H^s \to H^{-s}$ still generates a C^0–semigroup of isometries $\{\mathscr{U}(t)\}_{t\in\mathbb{R}^3}$ acting on H^s. Then, a fixed point argument in the space $C([0,T], \mathbb{C}^r \times (H^s(\mathbb{R}^3))^K)$ leads to the local-in-time existence and uniqueness of a solution in the time interval $[0,T]$.

4.3. *Step 3.*

We are kept with the proof of *a priori* bound on the local solution. First of all we still have the conservation of mass, that is for all $t \in [0,T]$ we have $\|C(t)\| = 1$ and $\int_{\mathbb{R}^3} \phi_i(t,x)\,\bar{\phi}_j(t,x)\,dx = \delta_{i,j}$. Now, we estimate the H^s norm of the functional part of the solution. We start by writing the integral formulation of the PDEs equations of the system $\mathscr{S}'$

$$\Phi(t) = \mathscr{U}(t)\,\Phi^0 - i\int_0^t \mathscr{U}(t-s)\,\mathbf{\Gamma}^{-1}(s)\,(I - \mathbf{P}_\Phi)\,\mathbb{W}(C(s),\Phi(s))\,\Phi(s)\,ds$$

Now, we consider the H^s norm of this equation. The main point will be the estimates obtained in Step 1 where only one H^s norm appears on the right-hand sides. This is precisely the argument that allows for Gronwall's inequality invocation. Indeed

$$\begin{aligned}
\|\Phi(t)\| &\leq \|\Phi^0\|_{H^s} + \int_0^t \|\,\mathbf{\Gamma}^{-1}(s)\,(I - \mathbf{P}_\Phi)\,\mathbb{W}(C(s),\Phi(s))\,\Phi(s)\|_{H^s}\,ds \\
&\leq \|\Phi^0\|_{H^s} \\
&+ \int_0^t \|\mathbf{\Gamma}^{-1}(s)\|\,\|C\|^2\,\Big(\|\Phi(s)\|^2_{H^{\max(s-1,1/2)}} + \|\Phi(s)\|^2_{H^{\frac{1}{2}}}\,\|\Phi(s)\|^2_{L^2}\Big)\,\|\Phi(s)\|_{H^s}\,ds \\
&\leq \|\Phi^0\|_{H^s} \\
&+ \sup_{s\in[0,T]}\Big(\|\mathbf{\Gamma}^{-1}(s)\|\,\Big(\|\Phi(s)\|^2_{H^{\max(s-1,1/2)}} + K\,\|\Phi(s)\|^2_{H^{\frac{1}{2}}}\Big)\Big)\int_0^t \|\Phi(s)\|_{H^s}\,ds.
\end{aligned}$$

Eventually, using Gronwall's inequality we obtain

$$\|\Phi\|_{H^s} \leq \|\Phi^0\|_{H^s}\,e^{\gamma\,T}, \qquad \gamma := \sup_{s\in[0,T]}\Big(\|\mathbf{\Gamma}(s)\|\,\Big(\|\Phi\|^2_{H^{\max(s-1,1/2)}} + K\,\|\Phi\|^2_{H^{\frac{1}{2}}}\Big)\Big).$$

Then, with iterations on time argument we extend the result up to $T^\star$. Eventually, Lemma 3.2 applies in H^s and leads to the global existence. Theorem 4.1 is now proved. □

5. Extensions and Conclusion

In order to prove Theorem 1.2, let us introduce the attractive Hamiltonian

$$H_N = \sum_{1\leq i\leq N}\left(\sqrt{-\,\alpha^2\,\Delta_{x_i} + \alpha^{-4}} - \alpha^{-2} - \sum_{j=1}^{M}\frac{\alpha\,Z_j}{|x_i - R_j|}\right) - \sum_{1\leq i<j\leq N}\frac{1}{|x_i - x_j|}$$

The proof of Theorem 1.2 follows the same lines of the proof of Theorem 1.1. The only change is that we need an *a priori* estimate of the norm of the local-in-time solution using the new energy expression without using the positivity of the Coulomb electronic interaction. Recall, that the energy can be written as follows after diagonalization of $\mathbf{\Gamma}$

$$\mathcal{E}(C,\Phi) = \alpha^{-1}\sum_{i=1}^{K}\mu_i\,\left\langle\left(\sqrt{-\Delta+\alpha^{-2}}-\frac{\alpha\,Z}{|x|}-\frac{1}{\alpha}\right)\phi_i(t)\,,\,\phi_i(t)\right\rangle - \sum_{i,j,k,l=1}^{K}\gamma_{ijkl}\,\mathscr{K}(\phi_l,\phi_i,\phi_k,\phi_j).$$

Then, since we have $\|\Phi\|_{L^2} = \sqrt{K}$ and $\|C\| = 1$, then we can write for all time $t\in[0,T]$

$$\mathcal{E}(C^0,\Phi^0) \geq \delta\left(\frac{\alpha^{-1}}{2}\,\|\sqrt[4]{-\Delta}\,\Phi\|_{L^2}^2 - \frac{K}{\alpha^2}\right) - \frac{\pi\,K}{4}\,\|\sqrt[4]{-\Delta}\,\Phi\|_{L^2}^2 = \left(\frac{\delta}{2\,\alpha}-\frac{\pi\,K}{4}\right)\|\sqrt[4]{-\Delta}\,\Phi\|_{L^2}^2 - \frac{K}{\alpha^2}.$$

where $\delta = \inf_{0\leq t\leq T}\{\mu_i,\ 1\leq i\leq K\}$ which is time-independent and $\delta>0$ since the matrix $\mathbf{\Gamma}$ is invertible on $[0,T]$. Physically, we know that $\alpha\simeq 1/137.036$, then certainly $\frac{\delta}{2\,\alpha}-\frac{\pi\,K}{4}\geq 0$ for reasonable K (depending on δ as well). That is for all $t\in[0,T]$, we have the bound

$$\|\sqrt[4]{-\Delta}\,\Phi\|_{L^2}^2 \leq \left(\mathcal{E}(C^0,\Phi^0)+\frac{K}{\alpha^2}\right)\left(\frac{\delta}{2\,\alpha}-\frac{\pi\,K}{4}\right)^{-1}.$$

Therefore our Theorem 1.1 is still valid in the case of attractive electronic interaction for $K<K_c := \frac{2\,\delta}{\alpha\pi}$ (now minimizing the new attractive energy). This recover the result of Ref. 19 since in that case $K=N=1$ then $\delta=1$ and obviously $1<\frac{2}{\alpha\,\pi}$. In the case of Hartree-Fock $K=N$ ($\delta=1$) we show the existence of a critical particle number N_c such that for system composed for more than N_c electrons, the associated Cauchy problem is not necessarily well-posed and our observation goes in the sense of Theorem 2.2 in Ref. 12.

Let us mention that our result holds true when extra particular potentials are added. For instance adding to the coulomb potential in both nuclear-electronic and electronic-electronic interaction a second potential $W(|x|)\in C^\infty[0,\infty)$ such that $|x|\,|W(|x|)|$ and $(1+|x|^{1+\epsilon})\,|W'(|x|)|$ are uniformly bounded do not change the proofs and Theorem 1.1 is still valid in this case.

Appendix

This appendix is dedicated to the proof of the energy conservation directly on the system $\mathscr{S}'$ for completeness. The equivalent proof given in Ref. 3 is based on the formulation $\mathscr{S}$, the variational principle and the unitary group action on the flow. Let $(C^0,\Phi^0)\in\mathcal{F}_N^K$ be the initial data and assume that there exists a strong solution to the system $\mathscr{S}$ on $[0,T]$ such that $rank(\mathbf{\Gamma}(t)) = K$ for all $t\in[0,T]$. For all $\Psi\in\mathcal{M}_N^K$, let $\Psi_i^{(k)} = \int_{\mathbb{R}^3}\Psi\bar{\phi}_i(x_k)dx_k := \langle\Psi\,,\,\phi_i\rangle_{-k}$. Thus, $\Psi_i^{(k)}$ is a skew-symmetric function that depends on time and all space variables except x_k and for every $1 \leq k \leq K$, we have $\Psi = \sum_{i=1}^{K} \phi_i(x_k)\, \Psi_i^{(k)}$. It is rather easy to see that for any $1 \leq l \leq N$ and $l \neq k$

$$\langle \Psi_j^{(k)} \big| \Psi_i^{(k)} \rangle_{L^2(\mathbb{R}^{3(N-1)})} = N^{-1}\, \mathbf{\Gamma}_{i,j}, \tag{5.1}$$

$$\Big\langle \Psi_j^{(k)} \Big| \frac{1}{|x_k - x_l|} \Big| \Psi_i^{(k)} \Big\rangle_{L^2(\mathbb{R}^{3(N-1)})} = \frac{1}{N(N-1)}\, \mathbb{W}[C,\Phi]_{i,j}(t, x_k). \tag{5.2}$$

The calculation above is justified by the fact that if $(C(t), \Phi(t))$ satisfies the MCT-DHF system $\mathscr{S}'$, then it belongs to $\mathcal{F}_{N,K}$ for all $t \in [0,T]$. Next, we show that the PDEs system for the ϕ_i's and the ODEs system for the coefficients C are equivalent to the following PDE on the $N-$particle space

$$i\frac{\partial \Psi}{\partial t} - H_N \Psi = -(I - \mathcal{P}_\Phi)\,[V\,\Psi] + \sum_{k=1}^{N}\sum_{i=1}^{K} \Psi_i^{(k)}\, \mathbf{P}_\Phi\, \left[\mathbf{\Gamma}^{-1}\mathbb{W}(C,\Phi)\,\Phi\right]_i := \mathcal{R}(\Psi), \tag{5.3}$$

where we have denoted by $\mathcal{P}_\Phi$ the projector onto the space spanned by all the Slater determinants that may be formed from the ϕ_i's, that is $\mathcal{P}_\Phi = \sum_{i=1}^{r} \langle \cdot \big| \Phi_{\sigma_i} \rangle_{L^2(\mathbb{R}^{3N})}\, \Phi_{\sigma_i}$ and set $V := V(x_1, \ldots, x_N)$. In order to construct (5.3), we use the decomposition of Ψ above and observe that $\frac{\partial}{\partial t}\,\Psi = \sum_{i=1}^{r} \left[\frac{d}{dt}\, c_{\sigma_i}\right]\, \Phi_{\sigma_i} + \sum_{k=1}^{N}\sum_{i=1}^{K} \frac{\partial \phi_i(x_k)}{\partial t}\, \Psi_i^{(k)}$. Then, we insert the MCTDHF equations that compose $\mathscr{S}'$ in (**??**) and observe that, by construction,

$$\sum_{i=1}^{K}\sum_{k=1}^{N} \left(\sqrt{-\Delta_{x_k} + \alpha^{-2}} - \frac{\alpha\, Z}{|x_k|}\right) \phi_i(x_k)\, \Psi_i^{(k)} = \left(\sum_{k=1}^{N} \left(\sqrt{-\Delta_{x_k} + \alpha^{-2}} - \frac{\alpha\, Z}{|x_k|}\right)\right) \Psi, \tag{5.4}$$

whereas, by the ODE of the coefficients and the skew-symmetry,

$$i \sum_{i=1}^{r} \left[\frac{d}{dt}\, c_{\sigma_i}\right]\, \Phi_{\sigma_i} = \sum_{i=1}^{r} \langle \Psi \big| V \big| \Phi_{\sigma_i} \rangle_{L^2(\mathbb{R}^{3N})}\, \Phi_{\sigma_i} = \mathcal{P}_\Phi[V\,\Psi]. \tag{5.5}$$

We conclude by using the definition of the Hamiltonian H_N. Next, the time derivative of the total energy for all $t \in [0,T]$ is clearly given by $\frac{d}{dt}\, \mathcal{E}_{N,K}(t) = -2\,\Im \left\langle \mathcal{R}(\Psi)\,,\, \frac{\partial}{\partial t}\, \Psi(t) \right\rangle$. Now, according to (5.3), $\mathcal{R}(\Psi)$ is a difference of two terms, that we now treat separately. First, we have

$$\begin{aligned}
\Re\langle (I-\mathcal{P}_\Phi)\,[V\Psi]\Big|\frac{\partial \Psi}{\partial t}\rangle &= \sum_{k=1}^{N}\sum_{i=1}^{K}\Re\langle \Psi\big|V\big|(I-\mathcal{P}_\Phi)\,[\frac{\partial \phi_i(x_k)}{\partial t}\ \Psi_i^{(k)}]\rangle \\
&= \sum_{k=1}^{N}\sum_{i,j=1}^{K}\Re\langle \Psi_j^{(k)}\,\phi_j\big|V\big|\Psi_i^{(k)}\,(I-\mathbf{P}_\Phi)\,\frac{\partial \phi_i}{\partial t}\rangle, \qquad (5.6)\\
&= \sum_{k=1}^{N}\sum_{\substack{l=1\\ l\neq k}}^{N}\sum_{i,j=1}^{K}\Re\langle \Psi_j^{(k)}\,\phi_j\Big|\frac{1}{|x_k-x_l|}\Big|\Psi_i^{(k)}\,(I-\mathbf{P}_\Phi)\,\frac{\partial \phi_i}{\partial t}\rangle, \qquad (5.7)\\
&= \sum_{k=1}^{N}\sum_{\substack{l=1\\ l\neq k}}^{N}\sum_{i,j=1}^{K}\frac{1}{N(N-1)}\,\Re\langle \mathbb{W}(C,\Phi)_{i,j}\phi_j\Big|(I-\mathbf{P}_\Phi)\,\frac{\partial \phi_i}{\partial t}\rangle, \qquad (5.8)\\
&= \Re\langle \mathbb{W}(C,\Phi)\,\Phi\Big|(I-\mathbf{P}_\Phi)\,\frac{\partial \Phi}{\partial t}\rangle, \qquad (5.9)
\end{aligned}$$

where we have used $\mathcal{P}_\Phi[\Psi_i^{(k)}\frac{\partial \phi_i}{\partial t}] = \Psi_i^{(k)}\mathbf{P}_\Phi[\frac{\partial \phi_i}{\partial t}]$ and the decomposition of Ψ in (5.6), the orthogonality conditions on the ϕ_i's in (5.7) and finally (5.2) in (5.8). For the second term we proceed as follows

$$\begin{aligned}
&\sum_{k=1}^{N}\sum_{i=1}^{K}\Re\langle \Psi_i^{(k)}\,(I-\mathbf{P}_\Phi)[\mathbf{\Gamma}^{-1}\mathbb{W}(C,\Phi)\Phi]_i\Big|\frac{\partial \Psi}{\partial t}\rangle \\
&= \sum_{k=1}^{N}\sum_{i,j=1}^{K}\Re\langle \Psi_i^{(k)}\,(I-\mathbf{P}_\Phi)[\mathbf{\Gamma}^{-1}\mathbb{W}(C,\Phi)\Phi]_i\Big|\Psi_j^{(k)}\,\frac{\partial \phi_j}{\partial t}\rangle, \qquad (5.10)\\
&= \sum_{i,j=1}^{K}\Re\left(\overline{\mathbf{\Gamma}}_{i,j}\,\langle\,[\mathbf{\Gamma}^{-1}\mathbb{W}(C,\Phi)\Phi]_i\Big|(I-\mathbf{P}_\Phi)\,\frac{\partial \phi_j}{\partial t}\rangle\right), \qquad (5.11)\\
&= \sum_{i=1}^{K}\Re\langle [\mathbf{\Gamma}^{-1}\mathbb{W}(C,\Phi)\Phi]_i\Big|(I-\mathbf{P}_\Phi)\,[\mathbf{\Gamma}\frac{\partial}{\partial t}\Phi]_i\rangle,\\
&= \sum_{k,l=1}^{K}\Re\left(\left[\mathbf{\Gamma}\,\mathbf{\Gamma}^{-1}\right]_{l,k}\langle [\mathbb{W}(C,\Phi)\Phi]_k\Big|(I-\mathbf{P}_\Phi)\,\frac{\partial \phi_l}{\partial t}\rangle\right).\\
&= \sum_{i=1}^{K}\Re\langle [\mathbb{W}(C,\Phi)\Phi]_i\Big|(I-\mathbf{P}_\Phi)\frac{\partial \phi_i}{\partial t}\rangle. \qquad (5.12)
\end{aligned}$$

In (5.10) we used expression of the time derivative of Ψ, the equation of the MCTDHF system and the definition $I-\mathbf{P}_\Phi$, and in (5.11) we used (5.1). If we now compare (5.9) and (5.12) with the definition of $\mathcal{R}(\Psi)$ in (5.3), we infer that $\langle \mathcal{R}(\Psi), \frac{\partial}{\partial t}\Psi\rangle_{L^2(\mathbb{R}^{3N})} = 0$. Therefore, we have $\mathcal{E}_{N,K}(t) = \mathcal{E}_{N,K}(t=0)$. This leads to the total energy conservation in $[0,T]$ and ends the proof.

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