



HAL
open science

L^2 Analysis of the Multi-Configuration Time-Dependent Hartree-Fock Equations

Norbert J. Mauser, Saber Trabelsi

► **To cite this version:**

Norbert J. Mauser, Saber Trabelsi. L^2 Analysis of the Multi-Configuration Time-Dependent Hartree-Fock Equations. 2008. hal-00453962

HAL Id: hal-00453962

<https://hal.science/hal-00453962>

Preprint submitted on 6 Feb 2010

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

L^2 ANALYSIS OF THE MULTI-CONFIGURATION TIME-DEPENDENT HARTREE-FOCK EQUATIONS

NORBERT J. MAUSER AND SABER TRABELSI

ABSTRACT. The multiconfiguration methods are widely used by quantum physicists and chemists for numerical approximation of the many electron Schrödinger equation. Recently, first mathematically rigorous results were obtained on the time-dependent models, e.g. short-in-time well-posedness in the Sobolev space H^2 for bounded interactions [20] with initial data in H^2 , in the energy space for Coulomb interactions with initial data in the same space [25, 5], as well as global well-posedness under a sufficient condition on the energy of the initial data [4, 5]. The present contribution extends the analysis by setting an L^2 theory for the MCTDHF for general interactions including the Coulomb case. This kind of results is also the theoretical foundation of ad-hoc methods used in numerical calculation when modification ("regularization") of the density matrix destroys the conservation of energy property, but keeps invariant the mass.

1. INTRODUCTION

The Multi-Configuration Time-Dependent Hartree-Fock (MCTDHF in short) system aims to describe the time-evolution of systems composed of fermions (e.g. electrons), that is, particles with half integer spin. More precisely, it represents a hierarchy of approximations of the linear N particle (fermion) Schrödinger equation.

$$(1) \quad i \frac{\partial}{\partial t} \Psi(t, x_1, \dots, x_N) = H_N \Psi(t, x_1, \dots, x_N),$$

where Ψ is the N -particle wavefunction which we normalize to one in $L^2(\mathbb{R}^{3N}; \mathbb{C})$ since $|\Psi(t, x_1, \dots, x_N)|^2$ is interpreted as the probability density of finding the i^{th} particle in the position x_i at time t for all $1 \leq i \leq N$. In order to account for the Pauli exclusion principle which feature the fermionic nature of the particles we are dealing with, an antisymmetry condition is imposed to the wavefunction Ψ *i.e.*

$$\Psi(t, x_1, \dots, x_N) = \epsilon(\tau) \Psi(x_{\tau(1)}, \dots, x_{\tau(N)}),$$

for every permutation of $\{1, \dots, N\}$ with signature $\epsilon(\tau)$. The N -body Hamiltonian of the system is then the self-adjoint operator H_N acting on the Hilbert space $L^2(\mathbb{R}^{3N}; \mathbb{C})$ given by

$$(2) \quad H_N = \sum_{1 \leq i \leq N} \left(-\frac{1}{2} \Delta_{x_i} + U(x_i) \right) + \sum_{1 \leq i < j \leq N} V(|x_i - x_j|).$$

The subscript x_i of Δ_{x_i} means that the derivation is with respect to the space position of the i^{th} particle and $U(x)$ is the "external potential", created, e.g. by nuclei localized at fixed positions R_m with charges $z_m > 0$ for $1 \leq m \leq M$. The last term of H_N is the interaction potential between the electrons, which is fundamentally given by the Coulomb interaction. Hence we have

$$(3) \quad U(x) = - \sum_{m=1}^M \frac{z_m}{|x - R_m|} \quad \text{and} \quad V(|x - y|) = \frac{1}{|x - y|}.$$

We use the so-called atomic units for writing the Hamiltonian H_N and the N -particle Schrödinger equation; hence the Planck constant \hbar , the mass of the electrons, the elementary charge and the factor $\frac{1}{4\pi\epsilon_0}$ are all set

to one with ϵ_0 denotes the dielectric constant of the vacuum. For the sake of simple notation we omit the spin variable, taking the spin into account does not add any mathematical difficulties.

A particular advantage over the simple Time-Dependent Hartree-Fock (TDHF) method (see e.g. [23, 13, 6, 5]) is that MCTDHF can handle "correlation", an essential concept of many electron systems that vanishes (by definition) for TDHF. We refer the reader to [18, 19] for more details.

MCTDHF methods are widely used for numerical calculation of the dynamics of few electron systems in quantum physics/chemistry (see e.g. [1, 2, 3, 10] and references therein, also [7, 8, 9, 15] for the MCTDH case). From a theoretical point of view, excellent results were obtained for the stationary case [21, 14, 22]. However, the time-dependent case still poses serious open problems for the mathematical analysis. In fact, even the global-in-time existence of solutions without recourse to extra assumption as in [4, 5] is not proved yet.

The MCTDHF system for the approximate wavefunction $\Psi_{\text{MC}}(t, x_1, \dots, x_N)$ is composed of $K \geq N$ non-linear Schrödinger-type evolution equations (for "the orbitals", as a dynamic basis for an expansion by "Slater determinants") coupled with $r := \binom{K}{N}$ first order differential equations (for "the coefficients" C). The many particle wavefunction Ψ can be well approximated by such linear combinations of Slater determinants, much better than by the simple TDHF method that corresponds to the limiting case $K = N$. In principle, for fixed N , the MCTDHF equations yield a hierarchy of models with increasing accuracy with increasing K , in the sense that many particle wavefunction constructed from the solution of MCTDHF converges (in some sense) toward the exact solution Ψ with increasing K . However, especially in the time-dependent case, there is no proof for this seemingly "obvious" property.

Let us now formulate the MCTDHF equations which are much more complicated to write down than the "usual NLS" like cubic NLS or "Schrödinger-Poisson". For a short and readable introduction to the multiconfiguration time-dependent Hartree-Fock system, we refer the reader to [20, 25, 4, 5], or [21, 14, 22] focussed on the stationary case. First of all, we introduce the set $\mathcal{F}_{N,K}$ of "coefficients and orbitals" (C, Φ)

$$(4) \quad \mathcal{F}_{N,K} = \left\{ C = (C_\sigma)_{\sigma \in \Sigma_{N,K}} \in \mathbb{C}^r, \quad \sum_{\sigma \in \Sigma_{N,K}} |C_\sigma|^2 = 1 \right\} \times$$

$$(5) \quad \left\{ \Phi = (\phi_1, \dots, \phi_K) \in L^2(\mathbb{R}^3)^K, \quad \int_{\mathbb{R}^3} \phi_i \bar{\phi}_j dx = \delta_{i,j} \right\},$$

with $\delta_{i,j}$ being the Kronecker delta, the bar denotes the complex conjugation and

$$\Sigma_{N,K} = \left\{ \sigma = \{\sigma(1) < \dots < \sigma(N)\} \subset \{1, \dots, K\} \right\}, \quad |\Sigma_{N,K}| = \binom{K}{N} := r.$$

That is, the range of the family of increasing mappings $\sigma : \{1, \dots, N\} \rightarrow \{1, \dots, K\}$ for $1 \leq N \leq K$ with integers N and K and we shall not make difference between mappings and sets σ for simplicity. Now, given $\sigma \in \Sigma_{N,K}$, we define the associated *Slater determinant* as follows

$$\Phi_\sigma(x_1, \dots, x_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_{\sigma(1)}(x_1) & \dots & \phi_{\sigma(1)}(x_N) \\ \vdots & & \vdots \\ \phi_{\sigma(N)}(x_1) & \dots & \phi_{\sigma(N)}(x_N) \end{vmatrix}.$$

That is, the determinant built from the ϕ_i 's such that $i \in \sigma$. The ϕ_i 's being an orthonormal family, the factor $\frac{1}{\sqrt{N!}}$ ensures then the normalization $\|\Phi_\sigma\|_{L^2(\mathbb{R}^{3N})} = 1$. The MCTDHF wavefunction reads now

$$(6) \quad \Psi_{\text{MC}}(t, x_1, \dots, x_N) := \Psi_{\text{MC}}(C(t), \Phi(t)) = \sum_{\sigma \in \Sigma_{N,K}} C_\sigma(t) \Phi_\sigma(t, x_1, \dots, x_N).$$

In the sequel, we shall use the same notation for operators acting on $L^2(\mathbb{R}^3)$ and diagonal matrices of operators acting on vectors in $L^2(\mathbb{R}^3)^K$. The equations of motion associated to the *ansatz* (6) correspond to a variational procedure combined with space rotations thanks to the gauge invariance of the system we are dealing with. We refer to [7, 20] and particularly to [5]. In our formulation we obtain the following coupled system :

$$(7) \quad \mathcal{S} : \begin{cases} i \frac{d}{dt} C(t) = \mathbb{K}[\Phi](t) C(t), \\ i \mathbf{\Gamma}[C(t)] \frac{\partial}{\partial t} \Phi(t, x) = \mathbf{\Gamma}[C(t)] \left[-\frac{1}{2} \Delta_x + U(x) \right] \Phi(t, x) + (I - \mathbf{P}_\Phi) \mathbb{W}[C, \Phi](t, x) \Phi(t, x). \end{cases}$$

Let us now define the different operators and matrices involved in the system \mathcal{S} . First, $\mathbb{K}[\Phi]$ denotes an $r \times r$ Hermitian matrix depending only on the orbitals ϕ_i and the binary interaction V and is indexed by the sets $\sigma, \tau \in \Sigma_{N,K}$ as follows

$$(8) \quad \mathbb{K}[\Phi]_{\sigma, \tau}(t) = \frac{1}{2} \sum_{i, j \in \tau, k, l \in \sigma} (1 - \delta_{i, j})(1 - \delta_{k, l}) \delta_{\tau \setminus \{i, j\}, \sigma \setminus \{k, l\}} (-1)_{i, j}^\tau (-1)_{k, l}^\sigma \times$$

$$(9) \quad \times \int_{\mathbb{R}^3 \times \mathbb{R}^3} \phi_i(t, x) \bar{\phi}_k(t, x) V(|x - y|) \phi_j(t, y) \bar{\phi}_l(t, y) dx dy,$$

where the symbols $(-1)_{k, l}^\sigma = \pm 1$ are not relevant for analysis and are given by

$$(10) \quad (-1)_{k, l}^\sigma = \begin{cases} (-1)^{\sigma^{-1}(k) + \sigma^{-1}(l) + 1} & \text{if } k < l, \\ (-1)^{\sigma^{-1}(k) + \sigma^{-1}(l)} & \text{if } k > l, \end{cases}$$

with $\sigma^{-1}(k)$ being the position of the entry k in the set σ .

The matrix $\mathbf{\Gamma}[C(t)]$ is a $K \times K$ Hermitian "density matrix" depending only on the coefficients as follows

$$(11) \quad \mathbf{\Gamma}[C(t)]_{i, j} = \sum_{\substack{\sigma, \tau \in \Sigma_{N, K} \\ \sigma \setminus \{i\} = \tau \setminus \{j\}}} (-1)^{\sigma^{-1}(i) + \tau^{-1}(j)} \bar{C}_\sigma(t) C_\tau(t).$$

The projection operator \mathbf{P}_Φ is given by

$$(12) \quad \mathbf{P}_\Phi(\psi) = \sum_{i=1}^K \int_{\mathbb{R}^3} \psi(t, x) \bar{\phi}_i(t, x) dx \phi_i(t, x),$$

for all $\psi \in L^2(\mathbb{R}^3)$. That is the orthogonal projector onto the space spanned by the ϕ_i 's. Finally, the $K \times K$ Hermitian matrix $\mathbb{W}[C, \Phi](t, x)$ is given by the entries

$$(13) \quad \mathbb{W}[C, \Phi]_{ij}(x) = 2 \sum_{k, l=1}^K \gamma_{jkil} \int_{\mathbb{R}^3} \phi_k(y) V(|x - y|) \bar{\phi}_l(y) dy,$$

with

$$(14) \quad \gamma_{ijkl} = \frac{1}{2} (1 - \delta_{i, j})(1 - \delta_{k, l}) \sum_{\substack{\sigma, \tau \mid i, j \in \sigma, k, l \in \tau \\ \sigma \setminus \{i, j\} = \tau \setminus \{k, l\}}} (-1)_{i, j}^\sigma (-1)_{k, l}^\tau C_\sigma \bar{C}_\tau.$$

Observe that the potential V appears in the definition of $\mathbb{W}[C, \Phi]$ and $\mathbb{K}[\Phi]$, but that neither the kinetic energy operator nor the interaction U appear in $\mathbb{K}[\Phi]$ and hence in the equation for the $C(t)$. We refer the reader to [5] for more details on this formulation that corresponds to a carefully chosen gauge. Hence we have to deal with a strongly non-linear coupled system of $r = \binom{K}{N}$ first order ODEs and K Schrödinger-type PDEs.

A preliminary result on the existence and uniqueness of solutions to the MCTDH system \mathcal{S} (i.e. the adequate version of the multiconfiguration models for bosons) has been established in [20] under the drastic simplification of bounded and smooth interaction potential V (and $U \equiv 0$), where H^2 regularity for a solution associated to initial data in the Sobolev space H^2 was shown to hold up to a certain positive time. Indeed, for such potentials it should be straightforward to get L^2 solutions, too.

For the case of the Coulomb potential, some results have recently been obtained in [25, 5] with less regularity of initial data, namely in H^1 . However, all these results are local-in-time in the sense that the existence, uniqueness and regularity persist only as long as the density operator associated to the system remains of full rank K . That is, the matrix $\mathbf{\Gamma}[C(t)]$ remains invertible. In case of a “loss of rank” at a certain time T^* , the well-posedness holds only locally-in-time, until T^* . However, in [5, 4] it is shown how the global-in-time existence can be assured under an assumption on the energy of the initial state $\Psi_{\text{MC}}(C(t=0), \Phi(t=0))$.

The purpose of this contribution is, essentially, to establish an L^2 existence and uniqueness result of solutions for the Cauchy problem associated to the MCTDHF equations, the system \mathcal{S} . For the binary interaction V and the external potential U we allow for a large class including the Coulomb potential :

$$(15) \quad U(|x|), V(|x|) \in L^{p_1}(\mathbb{R}^3, \mathbb{R}) + L^{p_2}(\mathbb{R}^3, \mathbb{R}), \quad p_1, p_2 > \frac{3}{2}.$$

In order to make the proofs less technical, we shall take from now on $U, V \in L^p(\mathbb{R}^3, \mathbb{R})$ with $p > \frac{3}{2}$ omitting the decomposition in two parts. One can easily see that the same proof holds *mutatis mutandis* in the decomposed case, for the price of technically heavier and longer formulation of the estimates. One more simplification will be used in the sequel, we will usually write $U, V \in L^p(\mathbb{R}^3)$ with $p > \frac{3}{2}$, however, this has to be understood in the sense that $U \in L^p(\mathbb{R}^3, \mathbb{R})$ and $V \in L^q(\mathbb{R}^3, \mathbb{R})$ with different p and q satisfying $p, q > 3/2$.

Observe that the assumptions above hold true in the Coulomb case (3), as can be seen using the following cut-off

$$(16) \quad \chi(r) \begin{cases} = 1 & \text{for } 0 \leq r \leq 1 \\ \in [0, 1] & \text{for } 1 \leq r \leq 2 \\ = 0 & \text{for } 2 \leq r \end{cases} \quad \text{and set} \quad \begin{cases} V_1(|x|) = \frac{\chi(|x|)}{|x|} \in L^p(\mathbb{R}^3) \\ V_2(|x|) = \frac{1-\chi(|x|)}{|x|} L^\infty(\mathbb{R}^3) \end{cases}$$

with

$$\frac{3}{2} \leq p < 3.$$

Now, let us introduce

$$(17) \quad \partial\mathcal{F}_{N,K} = \left\{ (C, \Phi) \in \mathcal{F}_{N,K} \quad : \quad \text{rank}(\mathbf{\Gamma}[C]) = K \right\}.$$

With these definitions, we are able to recall a result from [25, 5] that will be useful in the sequel.

Theorem 1.1. *Let $(C^0, \Phi^0) \in \partial\mathcal{F}_{N,K} \cap H^1(\mathbb{R}^3)^K$ be an H^1 initial data, $U, V \in L^d(\mathbb{R}^3)$ with $d > \frac{3}{2}$. Then, there exists a time $T^* > 0$ such that the MCTDHF system \mathcal{S} admits a unique maximal solution $(C(t), \Phi(t))$ in*

$$C^1([0, T^*]; \mathbb{C})^r \times \left(C^1([0, T^*]; H^{-1}(\mathbb{R}^3))^K \cap C^0([0, T^*]; H^1(\mathbb{R}^3))^K \right)$$

depending continuously on the initial data (C^0, Φ^0) . Moreover, for all $0 \leq t < T^*$, we have

- $(C(t), \Phi(t)) \in \partial\mathcal{F}_{N,K}$,
- $\langle \Psi_{\text{MC}}(C(t), \Phi(t)) | H_N | \Psi_{\text{MC}}(C(t), \Phi(t)) \rangle_{L^2(\mathbb{R}^{3N})} = \langle \Psi_{\text{MC}}(C^0, \Phi^0) | H_N | \Psi_{\text{MC}}(C^0, \Phi^0) \rangle_{L^2(\mathbb{R}^{3N})}$.

Finally, either $T^* = +\infty$ or $T^* < +\infty$ and $\int_0^{T^*} \|\Gamma[C(t)]^{-1}\|^{3/2} dt = +\infty$. In particular

$$\limsup_{t \rightarrow T^*} \|\Gamma[C(t)]^{-1}\|^{3/2} = +\infty.$$

This Theorem then yields a local well-posedness result to the MCTDHF system. However, observe that the result is possibly global since, for the time being, there is no indication that T^* is necessarily finite [25, 4, 5]. As noticed before, the special case $N = K$ corresponds to a single Slater determinant *ansatz*. In particular, the set $\mathcal{F}_{N,N}$ coincides with $\partial\mathcal{F}_{N,N}$ and becomes a smooth manifold actually. In other words, the matrix $\Gamma[C]$ reduces to a globally invertible matrix since it becomes the $N \times N$ identity matrix. Therefore, Theorem 1.1 ensures the global existence of a unique solution to the TDHF system, that is, $T^* = +\infty$ and it improves then previous results obtained in [13]. Actually, the proof of the energy conservation presented in [5] is much more readable than the one there.

Finally, recall that this result (and the one we shall present in the next section) is valid in the case of the MCTDH. The so-called Schrödinger-Poisson system (SPS), which coincides with the Hartree system in the special case of "Bose Einstein condensation" when Coulombic interaction is used, can be also obtained as a limiting case of the MCTDH and our result applies obviously to this model, too.

2. MAIN RESULT

In [29], an L^2 -Theory to a TDHF type model is established. However, that model is a peculiar mixed state formulation. Usually, Hartree-Fock is characterized by a finite number of N equations with occupation numbers equal to 1 which is, of course, a completely different paradigm than a mixed state for a one particle model. That is, the eigenvalues of $\Gamma[C(t)]$ are one for all time $t \geq 0$. However, the result obtained in [29] obviously also holds for finite N (even if the author does not explicitly remark that) and can obviously be adapted to the usual TDHF setting. In our work this TDHF result is improved.

Independently, Castella established an L^2 theory of the mixed state Schrödinger-Poisson system [11]. More precisely, he studied a system of infinitely coupled Schrödinger equations with self-consistent Coulomb potential. The initial data needs only an L^2 bound, so the initial kinetic energy can possibly be infinite. Moreover, he obtained a blow-up (resp. decay) estimates for the solution as time goes to zero (resp. infinity).

Our work is inspired by Castella's results and Strichartz techniques. Our result on MCTDHF applies also to the TDHF and the TDH "pure state" case. We prove the following

Theorem 2.1. *Let the potentials $U, V \in L^d(\mathbb{R}^3)$ with $d > \frac{3}{2}$ in the sense of (15) and let $(C^0, \Phi^0) \in \partial\mathcal{F}_{N,K}$ be an L^2 initial data with full rank (cf (4), (17)).*

Then there exists a time $T^ > 0$ (possibly $T^* = +\infty$) such that the MCTDHF system \mathcal{S} (7) admits solutions $(C(t), \Phi(t))$ satisfying*

- $C \in C^1([0, T^*], \mathbb{C})^r$ and $\Phi \in C^0([0, T^*], L^2(\mathbb{R}^3))^K$.

Moreover, for all $2 \leq q < 6$

- i) $\Phi(t) \in L^{\frac{4q}{3(q-2)}}([0, T], L^q(\mathbb{R}^3))^K$.

- ii) *The solution $(C(t), \Phi(t))$ is unique in the class*

$$L^\infty([0, T], \mathbb{C})^r \times L^\infty([0, T], L^2(\mathbb{R}^3))^K \cap L^{\frac{4q}{3(q-2)}}([0, T], L^q(\mathbb{R}^3))^K,$$

for all $T < T^$.*

- iii) $(C(t), \Phi(t)) \in \partial\mathcal{F}_{N,K}$ for all $t \in [0, T^*)$.

Hence, this result establishes an L^2 theory for the solution $\Psi_{\text{MC}}(C(t), \Phi(t))$ (6) of the MCTDHF equations as long as the density matrix $\Gamma[C(t)]$ remains of full rank. Note that our theorem yields a global L^2 theory for the TDHF and the TDH models (the "pure state" versions of the models studied in [29, 11] as mentioned above).

The paper is structured as follows. In the next section, we collect some well-known tools, like Strichartz estimates and the properties associated to the semigroup $\mathbf{U}(t)$ generated by $i\frac{1}{2}\Delta$ on $L^2(\mathbb{R}^3)$. Moreover, we prove a local existence result using a standard contraction argument in an adequate space $\mathcal{X}_{T'}^{p,q}$ for a given reals p, q and a nonnegative time T' . In section 3, we prove that this local solution satisfies an *a priori* estimate which will be crucial in order to prolongate the solution beyond T' . Section 4 is dedicated to the proof of the main result 2.1. Finally, we make some comments and application of this Theorem.

3. A FEW TECHNICAL LEMMATA

First of all, let us specify the notation we will use throughout this paper and recall some well known tools. The real p' will be the conjugate of p with $1 \leq p \leq \infty$, that is, $\frac{1}{p} + \frac{1}{p'} = 1$. By abuse of notation, we denote $L^p = L^p(\mathbb{R}^3, \mathbb{C})$ but also $L^p = L^p(\mathbb{R}^3, \mathbb{R})$ when there is no confusion. The same notation will be used for $L^p(\mathbb{R}^3, \mathbb{C})^K$ and will be specified explicitly when necessary. The associated norms will be denoted $\|\cdot\|_{L^p}$. The same conventions are adopted for the Sobolev spaces H^1 . $(\mathbf{U}(t))_{t \in \mathbb{R}}$ is the group of isometries $(e^{i\frac{1}{2}t\Delta})_{t \in \mathbb{R}}$ generated by $\frac{1}{2}\Delta$ on $L^2(\mathbb{R}^3, \mathbb{C})$. Finally, κ will be an auxiliary positive constant depending on N and K . Also "const." will denote generic constants depending on quantities that will be indicated explicitly when necessary. Next, for a given $V(|x|)$, let for all $1 \leq i, j \leq K$

$$\mathbb{V}[\Phi]_{i,j}(t, x) := \int_{\mathbb{R}^3} \phi_i(t, y) V(|x - y|) \bar{\phi}_j(t, y) dy$$

and

$$D_V[f, \bar{g}](t) = \int_{\mathbb{R}^3 \times \mathbb{R}^3} f(t, x) V(|x - y|) \bar{g}(t, y) dx dy.$$

From this point onward, we shall omit the dependence on t and x when the context is clear. Finally, for a given $T > 0$ we denote $L_T^{p,q} = L^p([0, T], L^q)$. Now,

Definition 3.1. *The pair of reals (p, q) is said to be admissible, we denote $(p, q) \in \mathcal{A}$, if and only if the following relation holds true.*

$$\frac{2}{3p} = \left(\frac{1}{2} - \frac{1}{q}\right) \quad \text{and} \quad 2 \leq q < 6.$$

Then, we are able to recall

Lemma 3.2. *Let $0 < t \leq T$, then for all $(a, b), (p, q) \in \mathcal{A}$, $\phi \in L^2$ and $\varphi \in L_T^{a', b'}$, there exists $\rho(a)$ and $\rho(a, p)$ such that*

$$(18) \quad \|\mathbf{U}(t) \phi\|_{L_T^{p,q}} \leq \rho(p) \|\phi\|_{L^2} \quad \text{and} \quad \left\| \int_0^t \mathbf{U}(t-s) \varphi(s) ds \right\|_{L_T^{p,q}} \leq \rho(p, a) \|\varphi\|_{L_T^{a', b'}}.$$

Proof. This is a classical Lemma and we refer the reader to [16, 17, 24, 12]. □

The first inequality appearing in (18) describes a notable smoothing effect. In particular it tell us that for all $t \in \mathbb{R}$ and $\phi \in L^2$, we have obviously $\mathbf{U}(t) \phi \in L^p$. The second inequality is crucial when dealing with non-linearities in the framework of Schrödinger type equations. Indeed, without loss of generality we write the following generic Duhamel formula

$$\psi(t) = \mathbf{U}(t) \phi - i \int_0^t \mathbf{U}(t-s) f(\psi(s)),$$

for a given functional f . Then, the first inequality of (18) allows to control the L^2 norm of $\mathbf{U}(t) \phi$ in terms of the L^2 norm of ϕ . However, it is merely impossible to control the L^2 norm of $\int_0^t \mathbf{U}(t-s) f(\psi(s)) ds$ in terms of the one of ψ for general non-linearities f . The second inequality of (18) will, then, enable us to control the $L_T^{p,q}$ norm of $\int_0^t \mathbf{U}(t-s) f(\psi(s)) ds$ for a given $T > 0$ and a couple of reals $(p, q) \in \mathcal{A}$ in terms of the $L_T^{p',q'}$ norm of f and allows to conclude.

The Duhamel formula associated to the MCTDHF system \mathcal{S} for a given initial data (C^0, Φ^0) is written as follows for all time t such that $\mathbf{\Gamma}[C(t)]$ is invertible,

$$(19) \quad \begin{bmatrix} C(t) \\ \Phi(t) \end{bmatrix} = \begin{bmatrix} C^0 \\ \mathbf{U}(t) \Phi^0 \end{bmatrix} - i \int_0^t \begin{bmatrix} \mathbb{K}[\Phi(s)] C(s) \\ \mathbf{U}(t-s) \left[U \Phi(s) + \mathbf{\Gamma}[C(s)]^{-1} (I - \mathbf{P}_\Phi) \mathbb{W}[C(s), \Phi(s)] \Phi(s) \right] \end{bmatrix} ds.$$

Remark 3.3. *The potential U being time-independent, we chose for simplicity to add it to the non-linear part. An alternative way to proceed consists in considering the linear PDE $i \frac{\partial}{\partial t} u(t, x) = -\frac{1}{2} \Delta u(t, x) + U(x)u(t, x)$ and find adequate real p for $U \in L^p$ such that one can associate to this flow a propagator that satisfies Strichartz-type estimates (18). We refer the reader to, e.g., [28].*

Next, formal functional analysis calculation leads to

Lemma 3.4. *Let $U, V \in L^d$, $(p, q), (p_i, q_i) \in \mathcal{A}$ for $i = 1, \dots, 4$ and $T > 0$. Then,*

$$(20) \quad \|U \phi_1\|_{L_T^{p',q'}} \leq T^{\frac{3}{2}(\frac{1}{q} + \frac{1}{q_1}) - \frac{1}{2}} \|U\|_{L^d} \|\phi_1\|_{L_T^{p_1, q_1}}, \quad \frac{1}{q} + \frac{1}{q_1} = 1 - \frac{1}{d},$$

$$(21) \quad \|\mathbb{V}[\Phi]_{1,2} \phi_3\|_{L_T^{p',q'}} \leq T^{\frac{3}{2}(\frac{1}{q} + \sum_{k=1}^3 \frac{1}{q_k}) - 2} \|V\|_{L^d} \prod_{i=1}^3 \|\phi_i\|_{L_T^{p_i, q_i}}, \quad \frac{1}{q} + \sum_{i=1}^3 \frac{1}{q_i} = 2 - \frac{1}{d},$$

$$(22) \quad \left| \int_0^T D_V(\phi_1(t) \bar{\phi}_2(t), \phi_3(t) \bar{\phi}_4(t)) dt \right| \leq T^{\frac{3}{2} \sum_{k=1}^4 \frac{1}{q_k} - 2} \|V\|_{L^d} \prod_{i=1}^4 \|\phi_i\|_{L_T^{p_i, q_i}},$$

$$\sum_{i=1}^4 \frac{1}{q_i} = 2 - \frac{1}{d}.$$

Proof. The proof is nothing but a straightforward calculation based on the well-known Hölder and Young inequalities in space and time and we refer to [29] for similar estimates. \square

An immediate corollary of Lemma 3.4 is the following

Corollary 3.5. *Let $U, V \in L^d, d > \frac{3}{2}$ and $(p, q = \frac{2d}{d-1}) \in \mathcal{A}$. Then, for all $T > 0$, we have*

$$(23) \quad \|U \Phi\|_{L_T^{p', q'}} \leq \kappa T^{\frac{3}{q} - \frac{1}{2}} \|U\|_{L^d} \|\Phi\|_{L_T^{p, q}},$$

$$(24) \quad \left| \int_0^T \mathbb{K}[\Phi(t)] dt \right| \leq \kappa T^{\frac{3}{q} - \frac{1}{2}} \|V\|_{L^d} \|\Phi\|_{L_T^{\infty, 2}}^2 \|\Phi\|_{L_T^{p, q}}^2,$$

$$(25) \quad \|\mathbb{W}[C, \Phi] \Phi\|_{L_T^{p', q'}} \leq \kappa T^{\frac{3}{q} - \frac{1}{2}} \|V\|_{L^d} \|C\|_{\mathbb{C}^r}^2 \|\Phi\|_{L_T^{\infty, 2}}^2 \|\Phi\|_{L_T^{p, q}},$$

$$(26) \quad \|\mathbf{P}_\Phi \mathbb{W}[C, \Phi] \Phi\|_{L_T^{1, 2}} \leq \kappa T^{\frac{3}{q} - \frac{1}{2}} \|V\|_{L^d} \|\Phi\|_{L_T^{\infty, 2}}^3 \|\Phi\|_{L_T^{p, q}}^2.$$

Proof. The proof relies on the estimates (21) and (22) of Lemma 3.4. The assertion (23) is easy, in fact one sets $(p_1, q_1) = (p, q) \in \mathcal{A}$ and gets the result. Next, given a potential $V \in L^d$, the matrix \mathbb{K} involves elements of type $D_V(\phi_i \bar{\phi}_j, \phi_k \bar{\phi}_l)$ for which one use the estimate (22) by setting, for instance, $(p_3, q_3) = (p_4, q_4) = (\infty, 2) \in \mathcal{A}$ and $(p_1, q_1) = (p_2, q_2) = (p, q) \in \mathcal{A}$. Also, the vector $\mathbb{W}[C, \Phi] \Phi$ involves terms of type $\mathbb{V}[\Phi]_{i,j} \phi_k$ that can be handled using the estimate (21). In fact, we set for instance $(p_2, q_2) = (p_3, q_3) = (\infty, 2) \in \mathcal{A}$ and $(p_3, q_3) = (p, q) \in \mathcal{A}$. Finally, the vector $\mathbf{P}_\Phi \mathbb{W}[C, \Phi] \Phi$ involves terms of type $D_V(\phi_i \bar{\phi}_j, \phi_k \bar{\phi}_l) \phi_l$. Observe that $D_V(\phi_i \bar{\phi}_j, \phi_k \bar{\phi}_l)$ is a time-dependent scalar, thus, estimating the left hand side in an $L_T^{p', q'}$ leads automatically to an $L_x^{q'}$ norm on ϕ_l in the right hand side. For convenience, we estimate this term in $L_T^{1, 2}$ in order to get an $\|\phi_l\|_{L_T^{\infty, 2}}$ and use the same choice as in (24). \square

Remark 3.6. *From the one side, observe that for $d > \frac{3}{2}$, we have obviously $2 \leq q = \frac{2d}{d-1} < 6$. Moreover, the estimates of Corollary 3.5 involve T^α with power $\alpha > 0$ so that $T^\alpha \rightarrow 0$ as $T \rightarrow 0$. Indeed, since $2 \leq q < 6$, we have $0 < \frac{3}{q} - \frac{1}{2} \leq 1$. This observation will be crucial in the sequel. From the opposite side, assume V bounded, that is, $d = \infty$, then, the estimates of the Corollary 3.5 are valid with $q = 2$ and α , the power of T , equal to 1.*

Next, given $T > 0$ and $(p, q) \in \mathcal{A}$, we define the spaces

$$\mathcal{Z}_T^{p, q} = L_T^{\infty, 2} \cap L_T^{p, q}, \quad \mathcal{X}_T^{p, q} = \mathbb{C}^r \times \mathcal{Z}_T^{p, q},$$

endowed with the norms

$$\|\phi\|_{\mathcal{Z}_T^{p, q}} = \|\phi\|_{L_T^{2, \infty}} + \|\phi\|_{L_T^{p, q}}, \quad \|C, \Phi\|_{\mathcal{X}_T^{p, q}} = \|C\|_{\mathbb{C}^r} + \|\Phi\|_{\mathcal{Z}_T^{p, q}}.$$

A topology on $\mathcal{Z}_T^{p, q}$ and $\mathcal{X}_T^{p, q}$ being defined, we are able to prove the following

Lemma 3.7. *Let $U, V \in L^d, d > \frac{3}{2}, (p, q) \in \mathcal{A}$ such that $q = \frac{2d}{d-1}$. Then, for all $T > 0$, we have*

$$(27) \quad \|\mathbb{K}[\Phi(t)] C(t) - \mathbb{K}[\Phi'(t)] C'(t)\|_{L^1([0, T])} \leq \text{const}_1 T^{\frac{3}{q} - \frac{1}{2}} \|(C, \Phi) - (C', \Phi')\|_{\mathcal{X}_T^{p, q}},$$

$$(28) \quad \|U(\Phi - \Phi')\|_{L_T^{p', q'}} \leq \kappa T^{\frac{3}{q} - \frac{1}{2}} \|U\|_{L^d} \|\Phi - \Phi'\|_{\mathcal{Z}_T^{p, q}},$$

$$(29) \quad \|\mathbb{W}[C, \Phi] \Phi - \mathbb{W}[C', \Phi'] \Phi'\|_{L_T^{p', q'}} \leq \text{const}_2 T^{\frac{3}{q} - \frac{1}{2}} \|(C, \Phi) - (C', \Phi')\|_{\mathcal{X}_T^{p, q}},$$

$$(30) \quad \|\mathbf{P}_\Phi \mathbb{W}[C, \Phi] \Phi - \mathbf{P}_{\Phi'} \mathbb{W}[C', \Phi'] \Phi'\|_{L_T^{1, 2}} \leq \text{const}_3 T^{\frac{3}{q} - \frac{1}{2}} \|(C, \Phi) - (C', \Phi')\|_{\mathcal{X}_T^{p, q}},$$

with $\text{const}_1, \text{const}_2$ and const_3 depending on

$$N, K, \|U\|_{L^d}, \|V\|_{L^d}, \|\Phi\|_{L_T^{\infty, 2}}, \|\Phi'\|_{L_T^{\infty, 2}}, \|C\|_{\mathbb{C}^r}, \|C'\|_{\mathbb{C}^r}, \|\Phi\|_{L_T^{p, q}} \text{ and } \|\Phi'\|_{L_T^{p, q}}.$$

Proof. For a given V , observe that the difference $\mathbb{K}[\Phi] - \mathbb{K}[\Phi']$ involves terms of type $D_V(\phi_i \bar{\phi}_j, \phi_k \bar{\phi}_l) - D_V(\phi'_i \bar{\phi}'_j, \phi'_k \bar{\phi}'_l)$ that we manage as follows

$$\begin{aligned} |D_V(\phi_i \bar{\phi}_j, \phi_k \bar{\phi}_l) - D_V(\phi'_i \bar{\phi}'_j, \phi'_k \bar{\phi}'_l)| &\leq |D_V([\phi_i - \phi'_i] \bar{\phi}_j, \phi_k \bar{\phi}_l)| + |D_V(\phi'_i [\bar{\phi}_j - \bar{\phi}'_j], \phi_k \bar{\phi}_l)| \\ &+ |D_V(\phi'_i \bar{\phi}'_j, [\phi_k - \phi'_k] \bar{\phi}_l)| + |D_V(\phi'_i \bar{\phi}'_j, \phi'_k [\bar{\phi}_l - \bar{\phi}'_l])|. \end{aligned}$$

Thus, thanks to (24), we get

$$\begin{aligned} \|\mathbb{K}[\Phi] C - \mathbb{K}[\Phi'] C'\|_{L^1([0,T])} &\leq \|\mathbb{K}[\Phi]\|_{L^1([0,T])} \|C - C'\|_{C^r} + \|\mathbb{K}[\Phi] - \mathbb{K}[\Phi']\|_{L^1([0,T])} \|C'\|_{C^r}, \\ &\leq \kappa T^{\frac{3}{q}-\frac{1}{2}} \|V\|_{L^d} \|\Phi\|_{L_T^{\infty,2}}^2 \|\Phi\|_{L_T^{p,q}}^2 \|C - C'\|_{C^r} \\ &+ \kappa T^{\frac{3}{q}-\frac{1}{2}} \|V\|_{L^d} \|C'\|_{C^r} \left[\|\Phi\|_{L_T^{\infty,2}} \|\Phi\|_{L_T^{p,q}}^2 + \|\Phi'\|_{L_T^{\infty,2}} \|\Phi'\|_{L_T^{p,q}}^2 \right] \|\Phi - \Phi'\|_{L_T^{\infty,2}} \\ &+ \kappa T^{\frac{3}{q}-\frac{1}{2}} \|V\|_{L^d} \|C'\|_{C^r} \left[\|\Phi\|_{L_T^{\infty,2}}^2 \|\Phi'\|_{L_T^{p,q}} + \|\Phi'\|_{L_T^{\infty,2}}^2 \|\Phi\|_{L_T^{p,q}} \right] \|\Phi - \Phi'\|_{L_T^{p,q}}^2. \end{aligned}$$

The proof of the estimate (27) follows then by setting, for instance

$$\begin{aligned} \text{const}_1 &= \kappa \|V\|_{L^d} \|\Phi\|_{L_T^{\infty,2}}^2 \|\Phi\|_{L_T^{p,q}}^2 + \kappa \|V\|_{L^d} \|C'\|_{C^r} \left[\|\Phi\|_{L_T^{\infty,2}} \|\Phi\|_{L_T^{p,q}}^2 + \|\Phi'\|_{L_T^{\infty,2}} \|\Phi'\|_{L_T^{p,q}}^2 \right] \\ &+ \kappa \|V\|_{L^d} \|C'\|_{C^r} \left[\|\Phi\|_{L_T^{\infty,2}}^2 \|\Phi'\|_{L_T^{p,q}} + \|\Phi'\|_{L_T^{\infty,2}}^2 \|\Phi\|_{L_T^{p,q}} \right]. \end{aligned}$$

Proving the inequality (28) is obviously a straightforward application of (23). Now, one has

$$\begin{aligned} \|\mathbb{W}[C, \Phi] \Phi - \mathbb{W}[C', \Phi'] \Phi'\|_{L_T^{p',q'}} &\leq \|\mathbb{W}[C, \Phi] (\Phi - \Phi')\|_{L_T^{p',q'}} \\ &+ \|\mathbb{W}[C - C', \Phi] \Phi'\|_{L_T^{p',q'}} \\ &+ \|\mathbb{W}[C', \Phi - \Phi'] \Phi'\|_{L_T^{p',q'}}. \end{aligned}$$

Observe that $\mathbb{W}[C, \Phi]$ is quadratic in C and Φ . Then, by (25), we obtain

$$\begin{aligned} \|\mathbb{W}[C, \Phi] \Phi - \mathbb{W}[C', \Phi'] \Phi'\|_{L_T^{p',q'}} &\leq \kappa T^{\frac{3}{q}-\frac{1}{2}} \|V\|_{L^d} \|C\|_{C^r}^2 \|\Phi\|_{L_T^{\infty,2}}^2 \|\Phi - \Phi'\|_{L_T^{p',q'}} \\ &+ \kappa T^{\frac{3}{q}-\frac{1}{2}} \|V\|_{L^d} [\|C\|_{C^r} + \|C'\|_{C^r}] \|\Phi\|_{L_T^{\infty,2}}^2 \|\Phi'\|_{L_T^{p,q}} \|C - C'\|_{C^r} \\ &+ \kappa T^{\frac{3}{q}-\frac{1}{2}} \|V\|_{L^d} \|C'\|_{C^r}^2 \left[\|\Phi\|_{L_T^{\infty,2}} + \|\Phi'\|_{L_T^{\infty,2}} \right] \|\Phi'\|_{L_T^{p,q}} \|\Phi - \Phi'\|_{L_T^{\infty,2}}. \end{aligned}$$

Next, setting

$$\begin{aligned} \text{const}_2 &= \kappa \|V\|_{L^d} \left[\|C\|_{C^r}^2 \|\Phi\|_{L_T^{\infty,2}}^2 + \|C'\|_{C^r}^2 \left[\|\Phi\|_{L_T^{\infty,2}} + \|\Phi'\|_{L_T^{\infty,2}} \right] \|\Phi'\|_{L_T^{p,q}} \right] \\ &+ \kappa \|V\|_{L^d} [\|C\|_{C^r} + \|C'\|_{C^r}] \|\Phi\|_{L_T^{\infty,2}}^2 \|\Phi'\|_{L_T^{p,q}}. \end{aligned}$$

for instance, finish the proof of (29). It remains to estimate the projection part in $L_T^{1,2}$. For that purpose, we estimate first $[\mathbf{P}_\Phi - \mathbf{P}_{\Phi'}] \xi$ in $L_T^{1,2}$ for a given function $\xi(t, x) \in L_T^{p',q'}$ and all $(p, q) \in \mathcal{A}$. This can be achieved thanks to Hölder inequality in space and time as follows

$$\begin{aligned} \|\mathbf{P}_\Phi - \mathbf{P}_{\Phi'}\| \xi\|_{L_T^{1,2}} &\leq \sum_{k=1}^K \left[\|\langle \xi, \phi_k \rangle\|_{L^1([0,T])} \|\phi_k - \phi'_k\|_{L_T^{\infty,2}} + \|\langle \xi, \phi_k - \phi'_k \rangle\|_{L^1([0,T])} \|\phi'_k\|_{L_T^{\infty,2}} \right], \\ (31) \quad &\leq \kappa \|\xi\|_{L_T^{p',q'}} \|\Phi\|_{L_T^{p,q}} \|\Phi - \Phi'\|_{L_T^{\infty,2}} + \kappa \|\xi\|_{L_T^{p',q'}} \|\Phi'\|_{L_T^{\infty,2}} \|\Phi - \Phi'\|_{L_T^{p,q}}. \end{aligned}$$

Now, we have

$$\begin{aligned}
\|\mathbf{P}_\Phi \mathbb{W}[C, \Phi] \Phi - \mathbf{P}_{\Phi'} \mathbb{W}[C', \Phi'] \Phi'\|_{L_T^{1,2}} &\leq \|\mathbf{P}_\Phi [\mathbb{W}[C, \Phi] \Phi - \mathbb{W}[C', \Phi'] \Phi']\|_{L_T^{1,2}} \\
&+ \|\mathbf{P}_\Phi - \mathbf{P}_{\Phi'}\| \mathbb{W}[C', \Phi'] \Phi'\|_{L_T^{1,2}}, \\
&\leq \kappa \|\mathbb{W}[C, \Phi] \Phi - \mathbb{W}[C', \Phi'] \Phi'\|_{L_T^{p',q'}} \|\Phi\|_{L_T^{p,q}} \|\Phi\|_{L_T^{\infty,2}} \\
&+ \kappa \|\mathbb{W}[C', \Phi'] \Phi'\|_{L_T^{p',q'}} [\|\Phi\|_{L_T^{p,q}} + \|\Phi'\|_{L_T^{\infty,2}}] \|\Phi - \Phi'\|_{\mathcal{Z}_T^{p,q}}.
\end{aligned}$$

The estimate above is an application of (31), first with $\Phi' \equiv 0$, $\xi \equiv \mathbb{W}[C, \Phi] \Phi - \mathbb{W}[C', \Phi'] \Phi'$ and second with $\xi \equiv \mathbb{W}[C', \Phi'] \Phi'$. Finally, Let $q = \frac{2d}{d-1}$ and recall that $V \in L^d$ with $d > \frac{3}{2}$. Then following (29), we get the desired estimate by setting for instance

$$\text{const}_3 = \text{const}_2 \|\Phi\|_{L_T^{p,q}} \|\Phi\|_{L_T^{\infty,2}} + \kappa \|V\|_{L^d} \|C'\|_{\mathbb{C}^r}^2 \|\Phi'\|_{L_T^{p,q}} \|\Phi'\|_{L_T^{\infty,2}} [\|\Phi\|_{L_T^{p,q}} + \|\Phi'\|_{L_T^{\infty,2}}],$$

which achieves the proof. \square

Now, let $R, T > 0$ be arbitrary reals to be fixed later on. Moreover let $(C^0, \Phi^0) \in \mathcal{F}_{N,K}$ and introduce the closed ball

$$(32) \quad \tilde{\mathcal{X}}_T^{p,q}(R) = \left\{ (C, \Phi) \in \mathcal{X}_T^{p,q} : \|C, \Phi\|_{\mathcal{X}_T^{p,q}} \leq R \right\}.$$

This defines a complete metric space equipped with the distance induced by the norm of $\mathcal{X}_T^{p,q}$. Finally, introduce the following mapping

$$(33) \quad \pi_{C^0, \Phi^0} : \begin{bmatrix} C(\cdot) \\ \Phi(\cdot) \end{bmatrix} \mapsto \begin{bmatrix} C^0 \\ \mathbf{U}(\cdot) \Phi^0 \end{bmatrix} - i \int_0^\cdot \begin{bmatrix} \mathbb{K}[\Phi(s)] C(s) \\ \mathbf{U}(\cdot - s) [U \Phi(s) + \mathbb{L}[C(s), \Phi(s)]] \end{bmatrix} ds,$$

with

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

This formulation is then well defined as long as the matrix $\mathbf{\Gamma}[C(t)]$ is invertible. From now on, we will consider initial data $(C^0, \Phi^0) \in \partial \mathcal{F}_{N,K}$, that is, the associated first order density operator is of full rank. Thus, the quadratic dependence of $\mathbf{\Gamma}[C]$ on the coefficients C_σ and the continuity of the MCTDHF's flow guarantees the propagation of this property up to a certain time $T^* > 0$, at least infinitesimal but possibly infinite. That is, $\mathbf{\Gamma}[C(t)]$ is of rank K for all $t \in [0, T^*)$, hence invertible and we refer the reader to [5] for more details on this point.

Now, we claim the following

Lemma 3.8. *Let $U, V \in L^d$, $d > \frac{3}{2}$, $(p, q = \frac{2d}{d-1}) \in \mathcal{A}$ and $(C^0, \Phi^0) \in \partial \mathcal{F}_{N,K}$ with $\|(C^0, \Phi^0)\|_{\mathbb{C}^r \times L^2} \leq \beta$. Then, there exist a radius $R > 0$ and a time T with $0 < T < T^*$ such that the mapping π is a strict contraction on $\tilde{\mathcal{X}}_T^{p,q}(R)$. Moreover, given $(C'^0, \Phi'^0) \in \partial \mathcal{F}_{N,K}$ with $\|(C'^0, \Phi'^0)\|_{\mathbb{C}^r \times L^2} \leq \beta$, then*

$$(34) \quad \|(C, \Phi) - (C', \Phi')\|_{\mathcal{X}_T^{p,q}} \leq \text{const} \|(C^0, \Phi^0) - (C'^0, \Phi'^0)\|_{\mathbb{C}^r \times L^2},$$

where (C, Φ) and (C', Φ') denote the fixed points of π associated with (C^0, Φ^0) and (C'^0, Φ'^0) respectively.

Proof. The proof is based on the Lemma 3.7. By abuse of notation, $\pi_{C^0, \Phi^0}(C, \Phi)$ will be used instead of the vertical notation (33). Moreover for notation's lightness, we set

$$S(\phi)(t) := \int_0^t \mathbf{U}(t-s) \phi(s) ds.$$

Next, let $(a, b) \in \mathcal{A}$, $(C, \Phi), (C', \Phi') \in \mathcal{X}_T^{p,q}$, $T > 0$ to be fixed later on and $t \in [0, T]$. Finally we set $(p = \frac{4d}{3}, q = \frac{2d}{d-1}) \in \mathcal{A}$. Then

$$\begin{aligned}
(35) \quad & \|\pi_{C^0, \Phi^0}(C(t), \Phi(t)) - \pi_{C'^0, \Phi'^0}(C'(t), \Phi'(t))\|_{\mathbb{C}^r \times L_T^{a,b}} \leq \\
& (1 + \rho(a)) \|(C^0, \Phi^0) - (C'^0, \Phi'^0)\|_{\mathbb{C}^r \times L^2} \\
& + \left\| \int_0^t [\mathbb{K}[\Phi(s)] C(s) - \mathbb{K}[\Phi'(s)] C'(s)] ds \right\|_{\mathbb{C}^r} + \|S(U\Phi - U\Phi')(t)\|_{L_T^{a,b}} \\
& + \|S(\mathbb{L}[C, \Phi] - \mathbb{L}[C', \Phi'])(t)\|_{L_T^{a,b}} := \mathcal{T}_1 + \dots + \mathcal{T}_4.
\end{aligned}$$

The term \mathcal{T}_1 is due to the Lemma 3.2. More precisely, the first assertion of (18). Next, thanks to the inequality (27) of Lemma 3.7, we have

$$(36) \quad \mathcal{T}_2 \leq \text{const}_1 T^{\frac{3}{q} - \frac{1}{2}} \|(C, \Phi) - (C', \Phi')\|_{\mathcal{X}_T^{p,q}}.$$

Now, we use the second assertion of (18) in order to estimate \mathcal{T}_3 and \mathcal{T}_4 . We start with

$$\begin{aligned}
(37) \quad \mathcal{T}_3 & \leq \rho(a, p) \|U\Phi - U\Phi'\|_{L_T^{p',q'}}, \\
& \leq \rho(a, p) \kappa T^{\frac{3}{q} - \frac{1}{2}} \|U\|_{L^d} \|(C, \Phi) - (C', \Phi')\|_{\mathcal{X}_T^{p,q}}.
\end{aligned}$$

The second line above is due to (28) where we upper-bounded obviously the $\mathcal{Z}_T^{p,q}$ norm by the $\mathcal{X}_T^{p,q}$ one. Finally

$$\begin{aligned}
\mathcal{T}_4 & \leq \|S(\Gamma[C]^{-1} \mathbb{W}[C, \Phi] \Phi - \Gamma[C']^{-1} \mathbb{W}[C', \Phi'] \Phi')(t)\|_{L_T^{a,b}} \\
& + \|S(\mathbf{P}_\Phi \Gamma[C]^{-1} \mathbb{W}[C, \Phi] \Phi - \mathbf{P}_{\Phi'} \Gamma[C']^{-1} \mathbb{W}[C', \Phi'] \Phi')(t)\|_{L_T^{a,b}}, \\
& \leq \rho(a, p) \|\Gamma[C]^{-1} \mathbb{W}[C, \Phi] \Phi - \Gamma[C']^{-1} \mathbb{W}[C', \Phi'] \Phi'\|_{L_T^{p',q'}} \\
& + \rho(a, p) \|\mathbf{P}_\Phi \Gamma[C]^{-1} \mathbb{W}[C, \Phi] \Phi - \mathbf{P}_{\Phi'} \Gamma[C']^{-1} \mathbb{W}[C', \Phi'] \Phi'\|_{L_T^{1,2}}.
\end{aligned}$$

Next, observe the trivial algebraic relation

$$\begin{aligned}
\|\Gamma[C]^{-1} - \Gamma[C']^{-1}\| & \leq \|\Gamma[C]^{-1}(\Gamma[C'] - \Gamma[C])\Gamma[C']^{-1}\|, \\
& \leq \kappa \|\Gamma[C]^{-1}\| \|\Gamma[C']^{-1}\| (\|C\| + \|C'\|) \|C - C'\|_{\mathbb{C}^r}.
\end{aligned}$$

Thus, by the mean of (25,26,29,30), we get

$$(38) \quad \mathcal{T}_4 \leq \rho(a, p) \text{const}_4 T^{\frac{3}{q} - \frac{1}{2}} \|(C, \Phi) - (C', \Phi')\|_{\mathcal{X}_T^{p,q}}.$$

More precisely

$$\begin{aligned}
\text{const}_4 & = \kappa \|V\|_{L^d} \|\Gamma[C]^{-1}\| \|\Gamma[C']^{-1}\| \|C'\|_{\mathbb{C}^r}^2 [\|C\|_{\mathbb{C}^r} + \|C'\|_{\mathbb{C}^r}] [1 + \|\Phi'\|_{L_T^{\infty,2}} \|\Phi'\|_{L_T^{p,q}}] \times \\
& \times \|\Phi'\|_{L_T^{\infty,2}}^2 \|\Phi'\|_{L_T^{p,q}} + \|\Gamma[C]^{-1}\| [\text{const}_2 + \text{const}_3].
\end{aligned}$$

Summing (36-38) and adding the sum to the first line of (35) leads to

$$\begin{aligned}
(39) \quad & \|\pi_{C^0, \Phi^0}(C(t), \Phi(t)) - \pi_{C'^0, \Phi'^0}(C'(t), \Phi'(t))\|_{\mathbb{C}^r \times L_T^{a,b}} \leq (1 + \rho(a)) \|(C^0, \Phi^0) - (C'^0, \Phi'^0)\|_{\mathbb{C}^r \times L^2} \\
& + [\text{const}_1 + \rho(a, p) \text{const}_4 + \rho(a, p) \kappa \|U\|_{L^d}] T^{\frac{3}{q} - \frac{1}{2}} \|(C, \Phi) - (C', \Phi')\|_{\mathcal{X}_T^{p,q}}.
\end{aligned}$$

Now, the inequality (39) holds for any admissible pair $(a, b) \in \mathcal{A}$. Therefore, we write it in the special case $(a, b) = (p, q) \in \mathcal{A}$ and then in the case $(a, b) = (\infty, 2) \in \mathcal{A}$. Moreover, we set $(C^0, \Phi^0) \equiv (C'^0, \Phi'^0)$ and use $\|C, \Phi\|_{\mathcal{X}_T^{p,q}}, \|C', \Phi'\|_{\mathcal{X}_T^{p,q}} \leq R$ since $(C, \Phi), (C', \Phi') \in \mathcal{X}_T^{p,q}(R)$. Recall that $T < T^*$ since the initial data is in $\partial \mathcal{F}_{N,K}$, that is, the matrix $\Gamma[C]$ and $\Gamma[C']$ are invertible thus there exists $\theta > 0$ such that

$\|\mathbf{I}[C]^{-1}\|_{L^\infty(0,T^*)}, \|\mathbf{I}[C']^{-1}\|_{L^\infty(0,T^*)} \leq \theta$. This procedure leads to

$$(40) \quad \begin{aligned} \|\pi_{C^0, \Phi^0}(C(t), \Phi(t)) - \pi_{C^0, \Phi^0}(C'(t), \Phi'(t))\|_{\mathcal{X}_T^{p,q}} &\leq \text{const}_5(\kappa, R, \theta, p) T^{\frac{3}{q}-\frac{1}{2}} \times \\ &\times \|(C, \Phi) - (C', \Phi')\|_{\mathcal{X}_T^{p,q}}. \end{aligned}$$

Equivalently, if we set $(C', \Phi') \equiv (0, 0)$ and use the fact that $\|C^0, \Phi^0\|_{\mathbb{C}^r \times L^2} \leq \beta$. Again, after summation

$$(41) \quad \|\pi_{C^0, \Phi^0}(C(t), \Phi(t))\|_{\mathcal{X}_T^{p,q}} \leq \text{const}_6(\kappa, R, \theta, \beta, p) T^{\frac{3}{q}-\frac{1}{2}}.$$

More precisely

$$\begin{aligned} \text{const}_5 &= 2\kappa R^4 \|V\|_{L^d} [5 + \rho(p)(2\theta^2 R^4 + (2\theta + 7)\theta R^2 + 5\theta)] + \rho(p)\kappa \|U\|_{L^d}, \\ \text{const}_6 &= 2(1 + \rho(p)) + 2\kappa R^5 [\|V\|_{L^d} + \rho(p)\theta \|V\|_{L^d}(1 + R^2)] + 2R\rho(p)\kappa \|U\|_{L^d}. \end{aligned}$$

Thus, we choose R and T such that

$$(42) \quad T < \inf \left\{ T^*, \left[\frac{R}{\text{const}_6} \right]^{\frac{2q}{6-q}} \right\}, \quad R \text{const}_5 - \text{const}_6 < 0.$$

That is

$$(43) \quad \text{const}_6 T^{\frac{3}{q}-\frac{1}{2}} < R \quad \text{and} \quad \text{const}_5 T^{\frac{3}{q}-\frac{1}{2}} < 1.$$

Hence, by (40, 41), π_{C^0, Φ^0} is a strict contracting map on $\tilde{\mathcal{X}}_T^{p,q}$. Eventually, it remains to prove the continuous dependence on the initial data (34). Again, the essence is the inequality (39). Let (C, Φ) and (C', Φ') be the fixed points of π_{C^0, Φ^0} and $\pi_{C'^0, \Phi'^0}$ respectively. Let us write again the inequality for $(a, b) = (p, q)$ and then in the case $(a, b) = (\infty, 2)$ and sum up. One obtains

$$\begin{aligned} \|\pi_{C^0, \Phi^0}(C(t), \Phi(t)) - \pi_{C'^0, \Phi'^0}(C'(t), \Phi'(t))\|_{\mathcal{X}_T^{p,q}} &= \|(C, \Phi) - (C', \Phi')\|_{\mathcal{X}_T^{p,q}} \\ &\leq 2(1 + \rho(p)) \|(C^0, \Phi^0) - (C'^0, \Phi'^0)\|_{\mathbb{C}^r \times L^2} + \text{const}_5(\kappa, R, \theta, p) T^{\frac{3}{q}-\frac{1}{2}} \|(C, \Phi) - (C', \Phi')\|_{\mathcal{X}_T^{p,q}}. \end{aligned}$$

Finally, the estimate above with (43) proves the continuous dependence on the initial data (34). \square

Now, we propose the following crucial proposition

Proposition 3.9. *Let $(C^0, \Phi^0) \in \partial\mathcal{F}_{N,K}, U, V \in L^d(\mathbb{R}^3)$ with $d > \frac{3}{2}$ and $(p, q = \frac{2d}{d-1}) \in \mathcal{A}$. Then there exists a $T(p, \|C\|_{\mathbb{C}^r}, \|\Phi\|_{L^2}, \|\Phi^0\|_{L^2}) > 0$ and a unique solution $(C(t), \Phi(t)) \in \mathcal{X}_T^{p,q}$ to*

$$(44) \quad \begin{bmatrix} C(t) \\ \Phi(t) \end{bmatrix} = \begin{bmatrix} C^0 \\ \mathbf{U}(t) \Phi^0 \end{bmatrix} - i \int_0^t \begin{bmatrix} \mathbb{K}[\Phi(s)] C(s) \\ \mathbf{U}(t-s) [U \Phi(s) + \mathbb{L}[C(s), \Phi(s)]] \end{bmatrix} ds.$$

In particular, the function part of the solution satisfies

$$(45) \quad \|\Phi\|_{L_T^{p,q}} \leq 2\rho(p) \|\Phi^0\|_{L^2}.$$

Proof. Thanks to Lemma 3.8, there exists a $T' > 0$ for which the integral formulation (44) associated to the MCTDHF admits a unique solution $(C(t), \Phi(t)) \in \mathcal{X}_{T'}^{p,q}$. The main point then is to characterize $0 < T \leq T'$ for which the property (45) holds. The function part of the solution satisfies

$$\Phi(t) = \mathbf{U}(t)\Phi^0 - iS(\mathbb{L}[C, \Phi])(t)$$

Let $0 < \tau \leq T \leq T'$ where T is to be fixed later on and recall that $\|\mathbf{\Gamma}[C(t)]^{-1}\|_{L^\infty(0, T^*)} \leq \theta$. Next, we estimate the $L_\tau^{p, q}$ of the right hand side and get using the estimate (18) of Lemma 3.2.

$$\begin{aligned}
\|\Phi\|_{L_\tau^{p, q}} &\leq \rho(p) \|\Phi^0\|_{L^2} + \|S(U \Phi)(t)\|_{L_\tau^{p, q}} + \|S(\mathbf{\Gamma}[C]^{-1} \mathbb{W}[C, \Phi] \Phi)(t)\|_{L_\tau^{p, q}} \\
&+ \|S(\mathbf{\Gamma}[C(s)]^{-1} \mathbf{P}_\Phi \mathbb{W}[C, \Phi] \Phi)(t)\|_{L_\tau^{p, q}}, \\
&\leq \rho(p) \|\Phi^0\|_{L^2} + \|U \Phi\|_{L_\tau^{p', q'}} + \|\mathbf{\Gamma}[C]^{-1}\| \|\mathbb{W}[C, \Phi] \Phi\|_{L_\tau^{p', q'}} \\
&+ \|\mathbf{\Gamma}[C]^{-1}\| \|\mathbf{P}_\Phi \mathbb{W}[C, \Phi] \Phi\|_{L_\tau^{1, 2}}, \\
&\leq \rho(p) \|\Phi^0\|_{L^2} + \kappa \theta T^{\frac{3}{q}-\frac{1}{2}} \|U\|_{L^d} \|\Phi\|_{L_\tau^{p, q}} + \kappa \theta T^{\frac{3}{q}-\frac{1}{2}} \|V\|_{L^d} \|C\|_{\mathbb{C}^r}^2 \|\Phi\|_{L_\tau^{\infty, 2}}^2 \|\Phi\|_{L_\tau^{p, q}} \\
(46) \quad &+ \kappa \theta T^{\frac{3}{q}-\frac{1}{2}} \|V\|_{L^d} \|C\|_{\mathbb{C}^r}^2 \|\Phi\|_{L_\tau^{\infty, 2}}^3 \|\Phi\|_{L_\tau^{p, q}}^2.
\end{aligned}$$

Next, we follow the argument of Tsutsumi in [27]. That is, we choose T so small so that there exists a positive number η satisfying

$$\begin{cases} f(\eta, T) := \rho(p) \|\Phi^0\|_{L^2} - \eta + \kappa \theta \eta T^{\frac{3}{q}-\frac{1}{2}} \left(\|U\|_{L^d} + \|V\|_{L^d} \|C\|_{\mathbb{C}^r}^2 \|\Phi\|_{L_\tau^{\infty, 2}}^2 \left[1 + \eta \|\Phi\|_{L_\tau^{\infty, 2}} \right] \right) < 0 \\ 0 < \eta \leq 2 \rho(p) \|\Phi^0\|_{L^2}. \end{cases}$$

For that purpose, it is sufficient to choose $T > 0$ such that

$$(47) \quad T < \inf \left\{ \left(2 \kappa \theta \left[\|U\|_{L^d} + \|V\|_{L^d} \|C\|_{\mathbb{C}^r}^2 \|\Phi\|_{L_\tau^{\infty, 2}}^2 \left[1 + 2 \rho(p) \|\Phi^0\|_{L^2} \|\Phi\|_{L_\tau^{\infty, 2}} \right] \right) \right]^{\frac{2q}{q-6}}, T' \right\}.$$

Then, let

$$(48) \quad \eta_0 = \min_{\eta} \{ 0 < \eta \leq 2 \rho(p) \|\Phi^0\|_{L^2} \quad ; \quad f(\eta, T) = 0 \}.$$

Now, let $\mathcal{Y}(\tau) = \|\Phi\|_{L_\tau^{p, q}}$. Then, by (46), we have for $0 \leq \tau \leq T$

$$(49) \quad \begin{cases} \mathcal{Y}(\tau) \leq \rho(p) \|\Phi^0\|_{L^2} + \kappa \theta \mathcal{Y}(\tau) T^{\frac{3}{q}-\frac{1}{2}} \left(\|U\|_{L^d} + \|V\|_{L^d} \|C\|_{\mathbb{C}^r}^2 \|\Phi\|_{L_\tau^{\infty, 2}}^2 \left[1 + \mathcal{Y}(\tau) \|\Phi\|_{L_\tau^{\infty, 2}} \right] \right), \\ \mathcal{Y}(\tau = 0) = 0. \end{cases}$$

Then, if T is chosen such that (47) holds, then by (48, 49), we get

$$\mathcal{Y}(\tau) \leq \eta_0 \leq 2 \rho(p) \|\Phi^0\|_{L^2}, \quad \text{for all } \tau \in [0, T].$$

Thus, passing to the limit as $\tau \rightarrow T$, we get by Fatou's Lemma

$$\|\Phi\|_{L_T^{p, q}} \leq 2 \rho(p) \|\Phi^0\|_{L^2},$$

which is the desired inequality. \square

4. PROOF OF THEOREM 2.1

This section is devoted to the proof of the main result Theorem 2.1. It relies mainly on proposition 3.9 and Theorem 1.1 which assures the existence and uniqueness of a solution, in short time, to the MCTDHF system with function part in the Sobolev space H^1 .

From the one side, let $(C^0, \Phi^0) \in \partial\mathcal{F}_{N,K}$ by proposition 3.9, there exists a certain time $T_0 > 0$ such that the integral formulation (44) admits a unique solution $(C(t), \Phi(t))$ in the space $\mathcal{X}_{T_0}^{p,q}$.

Now, one writes one more time the Duhamel formula associated to the function part of the system \mathcal{S} , more precisely, the second component of (19). Next, one uses the estimates (23,25,26) of Corollary 3.5, as in (35) with $(C', \Phi') \equiv (0, 0)$, and gets thanks to continuous embedding

$$L^{q'}(\mathbb{R}^3) \hookrightarrow H^{-1}(\mathbb{R}^3), \quad \text{for all } (p, q) \in \mathcal{A}$$

and the absolute continuity of the integral (the Duhamel formulation) that

$$\Phi \in C([0, T_0], H^{-1}) \quad \text{thus} \quad \Phi \in C_w([0, T_0], L^2)$$

where the subscript w stands for weak.

From the opposite side, let $(C^{0,n}, \Phi^{0,n}) \in \partial\mathcal{F}_{N,K} \cap H^1(\mathbb{R}^3)^K$ be a sequence of initial data for $n \in \mathbb{N}$ such that

$$(50) \quad \|C^{0,n}, \Phi^{0,n}\|_{\mathbb{C}^r \times L^2} \leq \|C^0, \Phi^0\|_{\mathbb{C}^r \times L^2}, \quad (C^{0,n}, \Phi^{0,n}) \xrightarrow{n \rightarrow +\infty} (C^0, \Phi^0) \quad \text{in } \mathbb{C}^r \times L^2.$$

The Theorem 1.1 guarantees the existence of a time $\tilde{T}_n > 0$, the existence and uniqueness of a solution in the interval of time $t \in [0, \tilde{T}_n)$ such that

$$(51) \quad C^n \in C^1([0, \tilde{T}_n), \mathbb{C})^r, \quad \Phi^n \in C^0([0, \tilde{T}_n), H^1(\mathbb{R}^3))^K.$$

This solution satisfies the following conservation laws

$$\|C^n(t)\|_{\mathbb{C}^r} = \|C^{0,n}\|_{\mathbb{C}^r}, \quad \|\Phi^n(t)\|_{L^2} = \|\Phi^{0,n}\|_{L^2}, \quad \forall t \in [0, \tilde{T}_n),$$

for all $n \in \mathbb{N}$. Moreover, the solutions (C^n, Φ^n) being continuously depending on the initial data, one can assume (up to the extraction of a subsequence) that the sequence \tilde{T}_n converges towards T^* where T^* denotes the maximal time of wellposedness of the Cauchy problem associated to the system \mathcal{S} with initial data (C^0, Φ^0) .

Then, by (50), (C^0, Φ^0) and $(C^{0,n}, \Phi^{0,n})$ are fixed points of the functions π_{C^0, Φ^0} and $\pi_{C^{0,n}, \Phi^{0,n}}$ respectively on the same closed ball of $\mathcal{X}_{T_0}^{p,q}$ for all $(p, 2 \leq q = \frac{2d}{d-1} < 6) \in \mathcal{A}$. Thus, one can pass to the limit as $n \rightarrow +\infty$ using the continuous dependence on the initial data (34) and (50). We get

$$(52) \quad \|C(t)\|_{\mathbb{C}^r} = \|C^0\|_{\mathbb{C}^r}, \quad \|\Phi(t)\|_{L^2} = \|\Phi^0\|_{L^2}, \quad \text{for all } 0 \leq t < \inf \{T_0, T^*\}.$$

Hence, (52) with $\Phi \in C_w([0, \inf \{T_0, T^*\}), L^2)$ leads to $\Phi \in C([0, \inf \{T_0, T^*\}), L^2)$. Moreover, the fact that $C \in C^1([0, \inf \{T_0, T^*\}), \mathbb{C})^r$ follows from the continuity of $t \mapsto \mathbb{K}[\Phi(t)]$ for all $t \in [0, \inf \{T_0, T^*\})$ which is a consequence of the continuity of the ϕ'_i s.

Eventually, recall that the function part of this solution satisfies the *a priori* estimate (45). In particular, the time T_0 depends only on the constants $N, K, p, \|C^0\|_{\mathbb{C}^r}$ and $\|\Phi^0\|_{L^2}$. Thus, one can reiterate the argument with initial data $(C(\inf \{T_0, T^*\}), \Phi(\inf \{T_0, T^*\})), (C(2 \inf \{T_0, T^*\}), \Phi(2 \inf \{T_0, T^*\})), \dots$ up to T^{*-} . We now check the uniqueness of the solution to the integral formulation associated to the MCTDHF, namely (19). The uniqueness on $[0, \inf \{T_0, T^*\})$ is given for free by the contraction argument. Again, one can reiterate up to T^{*-} and get the uniqueness on the whole interval $[0, T^*)$. The points i) and ii) are straightforward and the last point

to make clear before finishing the proof of the Theorem 2.1, is the equivalence between the MCTDHF as an integral formulation and in the distributional sense. For that purpose, we refer, for instance, to [11] (paragraph 4: Proof of Theorem 2.2, more precisely, the uniqueness part of the proof).

Recall that the Coulomb potential satisfies after cut-off $\frac{1}{|x|} \in L^d + L^\infty$ with $d \in [\frac{3}{2}, 3[$. Thus, for $p = \frac{2d}{d-1}$, we have obviously (omitting the case $d = \frac{3}{2}$) $3 < q < 6$ which is the result obtained by Castella in [11] for the SPS system. Moreover, notice that the estimates of the Lemma 3.7 hold true for bounded potentials. In particular in such case one can show that the mapping

$$\begin{bmatrix} C \\ \Phi \end{bmatrix} \mapsto \begin{bmatrix} \mathbb{K}[\Phi] C \\ U \Phi + \mathbb{I}[C]^{-1} (I - \mathbf{P}_\Phi) \mathbb{W}[C, \Phi] \Phi(s) \end{bmatrix} ds,$$

is locally lipschitz in $\mathbb{C}^r \times L^2$. This shows in particular the restriction of the results obtained in [20] since in this configuration we need only to prove the preservation of $\mathcal{F}_{N,K}$ by the MCTDHF flow as long as the density matrix is of full rank.

5. SOME COMMENTS AND CONCLUSION

For the time being, all the well-posedness results on the multiconfiguration models [20, 25, 4, 5] hold up to a certain time T^* , possibly infinite, for which $\text{rank}(\mathbb{I}[C(T^*)]) < K$. In [4, 5], we obtained with C. Bardos and I. Catto a sufficient condition that ensures the global well-posedness. More precisely, starting with initial data $(C^0, \Phi^0) \in \mathcal{F}_{N,K} \cap H^1(\mathbb{R}^3)^K$ satisfying

$$\left\langle \Psi_{\text{MC}}(C^0, \Phi^0) | H_N | \Psi_{\text{MC}}(C^0, \Phi^0) \right\rangle_{L^2(\mathbb{R}^{3N})} < \min_{(C, \Phi) \in \mathcal{F}_{N, K-1}} \left\langle \Psi_{\text{MC}}(C, \Phi) | H_N | \Psi_{\text{MC}}(C, \Phi) \right\rangle_{L^2(\mathbb{R}^{3N})},$$

then, the MCTDHF system \mathcal{S} admits a unique global-in-time solution $(C(t), \Phi(t))$ in the class

$$C^1([0, +\infty); \mathbb{C})^r \times \left(C^1([0, +\infty); H^{-1}(\mathbb{R}^3))^K \cap C^0([0, +\infty); H^1(\mathbb{R}^3))^K \right).$$

However, such a condition is not possible for an L^2 theory since the energy of the initial data is not well-defined for $(C^0, \Phi^0) \in \mathcal{F}_{N,K}$. In order to remediate this problem in practice in numerical simulations, physicists and chemists use to perturb the density matrix [7, 10] (see also [20]). In order to illustrate their method we use, without loss of generality, the following perturbation

$$\mathbb{I}_\epsilon[C] = \mathbb{I}[C] + \epsilon I_K,$$

with I_K being the $K \times K$ identity matrix. The MCTDHF system \mathcal{S} (7) with $\mathbb{I}_\epsilon[C]$ instead of $\mathbb{I}[C]$ is then ϵ -dependent. Then, observe that the L^2 theory we proved in the present paper is also global for \mathcal{S}_ϵ since the time T of the Proposition 3.9 depends only on quantities that the flow \mathcal{S}_ϵ conserves. Consequently, one can iterate the argument in time and cover the whole real line. Notice that \mathcal{S}_ϵ does not conserve the total energy because of the perturbation. We are then able to claim the following corollary for \mathcal{S}_ϵ

Corollary 5.1. *Let $U, V \in L^d(\mathbb{R}^3)$ with $d > \frac{3}{2}$ and $(C^0, \Phi^0) \in \mathcal{F}_{N,K}$ be an initial data. Then, the perturbed MCTDHF system \mathcal{S}_ϵ admits solutions $(C_\epsilon(t), \Phi_\epsilon(t))$ satisfying*

- $C_\epsilon \in C^1([0, +\infty), \mathbb{C})^r$ and $\Phi_\epsilon \in C^0([0, +\infty), L^2(\mathbb{R}^3))^K$.

Moreover, for all $2 \leq q < 6$

- i) $\Phi_\epsilon(t) \in L_{loc}^{\frac{4q}{3(q-2)}}([0, +\infty), L^q(\mathbb{R}^3))^K$.

ii) The solution $(C_\epsilon(t), \Phi_\epsilon(t))$ is unique in the class

$$L^\infty([0, +\infty), \mathbb{C})^r \times L^\infty([0, +\infty), L^2(\mathbb{R}^3))^K \cap L_{loc}^{\frac{4q}{3(q-2)}}([0, +\infty), L^q(\mathbb{R}^3))^K.$$

iii) $(C_\epsilon(t), \Phi_\epsilon(t)) \in \partial\mathcal{F}_{N,K}$ for all $t > 0$.

A global H^1 theory on the system \mathcal{S}_ϵ is not possible since the total energy is not conserved, of course, since $\mathbb{I}[C] \mathbb{I}_\epsilon[C]^{-1} \neq I_K$. We mention that energy conservation can be proved using a variational principle (cf [5]) or in a direct way by working only on the equations of the flow \mathcal{S} ([26]). Moreover we do not believe that the perturbed energy

$$\left\langle \left(\left[\sum_{i=1}^N -\frac{1}{2} \Delta_{x_i} + U(x_i) \right] \mathbb{I}_\epsilon[C] + \frac{1}{2} \mathbb{W}_{C,\Phi} \right) \Phi, \Phi \right\rangle$$

is decaying during the time evolution. An alternative strategy will be to pass to the limit $\epsilon \rightarrow 0$, however this depends on whether or not the system \mathcal{S}_ϵ satisfies a uniform (in ϵ) estimate which is related to the non-decay of the perturbed energy. We hope to come back to this point in a forthcoming work.

Acknowledgements This work was supported by the Viennese Science Foundation (WWTF) via the project "TDDFT" (MA-45), the Austrian Science Foundation (FWF) via the Wissenschaftskolleg "Differential equations" (W17) and the START Project (Y-137-TEC) and the EU funded Marie Curie Early Stage Training Site DEASE (MEST-CT-2005-021122).

We thank Claude Bardos and Isabelle Catto as well as Alex Gottlieb for useful discussions and comments !!

REFERENCES

- [1] Barbec, T. Fabian, C. Kitzler, M. Milosevic, N. Scrinzi, A.: Quantum theory of single subfemtosecond extreme-ultraviolet pulse measurements. *J. Opt. Soc. Am. B*, 20:591, 2003
- [2] Barbec, T. Jungreuthmayer, Ch. Kitzler, M. Scrinzi, A. Smits, M. Zanghellini, J.: Ionization dynamics of extended multi-electron systems *Phys. Rev. A*, 70:041401(R), 2004.
- [3] Barbec, T. Kitzler, M. Scrinzi, A. M. Zanghellini, J.: Testing the multi-configuration time-dependent hartree-fock method. *J. Phys. B*, 37(4):763 - 773, 2004
- [4] Bardos, C. Catto, I. Mauser, N. Trabelsi, S.: Existence of solutions of the multiconfiguration time-dependent Hartree-Fock equations: A sufficient condition, *Applied Mathematics Letters* (2008), doi:10.1016/j.aml.2007.12.033
- [5] Bardos, C. Catto, I. Mauser, N. Trabelsi, S.: Setting and analysis of the multiconfiguration time-dependent Hartree-Fock equations. (to appear in *Archive for Rational Mechanics and Analysis*)
- [6] Bardos, C. Golse, F., Mauser, N. Gottlieb, A.: Mean-field dynamics of fermions and the time-dependent Hartree-Fock equation. *J. Math. Pures et Appl.* **82**, 665-683 (2003)
- [7] Beck, M. H., Jäckle, A., Worth, G. A. Meyer, H. -D.: The multiconfiguration time-dependent Hartree(MCTDH) method: a highly efficient algorithm for propagation wavepackets. *Phys. Rep.*, **324**, 1-105, 2000
- [8] Bowman, J.M. Carrington, T. Meyer, H. -D.: Variational Quantum Approaches for Computing Vibrational Energies of Polyatomic Molecules. *Molecular Physics* 106, 2145-2182 (2008).
- [9] Burghardt, I. Cederbaum, L.S. Köppel H. Meyer, H. -D. Worth, G.A.: Using the MCTDH wavepacket propagation method to describe multimode non-adiabatic dynamics. *International Reviews in Physical Chemistry*, Vol. 27, No. 3, (2008) 569-606.
- [10] Caillat, J., Zanghellini, J. Kitzler, M. Koch, O. Kreuzer, W., Scrinzi, A.: Correlated multielectron systems in strong laser fields - an MCTDHF approach. *Phys. Rev. A* **71**, 012712 (2005)
- [11] Castella, F.: L^2 -solutions to the Schrödinger-Poisson System: Existence, Uniqueness, Time Behaviour, and Smoothing Effects. *Math. Meth. Mod. Appl. Sci.* Vol. **7**, N. 8, pp. 1051-1083 (1997)
- [12] Cazenave, T.: An introduction to nonlinear Schrödinger equations, Second Edition, *Textos de Métodos Matemáticas* 26, Universidade Federal do Rio de Janeiro (1993).
- [13] Chadam, J.M., Glassey, R.T.: Global existence of solutions to the Cauchy problem for the time-dependent Hartree equation. *J. Math. Phys.* **16**, 1122-1230 (1975)
- [14] Friesecke, G.: The multiconfiguration equations for atoms and molecules: charge quantization and existence of solutions. *Arch. Rational Mech. Anal.* **169**, 35-71 (2003)
- [15] Gatti, F. Meyer, H. -D. Worth, G.A.: *Multidimensional Quantum Dynamics: MCTDH Theory and Applications*. Wiley-VCH, ISBN: 978-3-527-32018-9 (2009)

- [16] Ginibre, J., Velo, G.: On a class of nonlinear Schrödinger equations. I: The Cauchy problem, *J. Funct. Anal.*, 32 (1979), 1-32. with non-local interaction, *Math. Z.* **170**, 109-136 (1980)
- [17] Ginibre, J. Velo, G.: On a class of non-linear Schrödinger equations. I: Theorie de la diffusion dans l'espace d'énergie pour une classe d'équations de Schrödinger non lineaires, *C. R. Acad. Sci., Paris* 298 (1984), 137-140.
- [18] Gottlieb, A.D. and Mauser, N.J.: A new measure of correlation for electron systems, *Phys. Rev. Lett.*, **95** (12) 1230003 (2005)
- [19] Gottlieb, A.D. and Mauser, N.J.: Properties of non-freeness: an entropy measure of correlation of electrons, *Int. J. of Quantum Information*, 5(6) (2007) 10 n:33.
- [20] Koch, O., Lubich, C.: Regularity of the Multi-configuration time-dependent Hartree approximation in quantum molecular dynamics. *Math. Model. Numer. Anal.*, 41 (2007) 315-331
- [21] Le Bris, C.: A general approach for multiconfiguration methods in quantum molecular chemistry. *Ann. Inst. H. Poincaré Anal. Non Linéaire* **11**(4),441–484 (1994)
- [22] Lewin, M.: Solutions of the Multiconfiguration Equations in Quantum Chemistry. *Arch. Rational Mech. Anal.* **171**(1), 83-114 (2004)
- [23] McWeeny, R. *Methods of molecular quantum mechanics*, 2nd edition, Academic press (1992)
- [24] Strichartz, R. S.: Restrictions of Fourier transforms to quadratic surfaces and decay of solutions of wave equations, *Duke Math. J.*, 44 (1977) 705-714.
- [25] Trabelsi, S.: Solutions of the Multiconfiguration Time-Dependent Equations in Quantum Chemistry. *C. R. Acad. Sci. Paris, Ser. I* 345 (2007)
- [26] Trabelsi, S.: Analysis of the MultiConfiguration Time-Dependent Hartree-Fock equations. PhD thesis in co-tutelle of Univ. Wien and Univ. Paris 7 (2008), 46-51
- [27] Tsutsumi, Y. L^2 -Solutions for nonlinear Schrödinger Equation and Nonlinear Groups. *Funk. Ekv.*, Vol.**30**, 115-125 (1987).
- [28] Yajima, K.: Existence of Solution for Schrödinger Evolution Equations. *Commun. Math. Phys.* **110**, 415-426 (1987)
- [29] Zagatti, S. The Cauchy problem for Hartree-Fock time dependent equations. *Ann. Inst. H. Poincaré, Phys. Th.*, Vol. **56**, N. 4, 357-374 (1992).

(Norbert Mauser) WOLFGANG PAULI INST. C/O FAK. F. MATHEMATIK; UNIV. WIEN NORDBERGSTRASSE, 15, A-1090 VIENNA, AUSTRIA

(Saber Trabelsi) WOLFGANG PAULI INST. C/O FAK. F. MATH.; UNIV. WIEN, AND CEREMADE, UNIV. PARIS DAUPHINE