

A Dirac field interacting with point nuclear dynamics

Federico Cacciafesta*, Anne-Sophie de Suzzoni[†], Diego Noja[‡]

February 5, 2019

Abstract

The system describing a single Dirac electron field coupled with classically moving point nuclei is presented and studied. The model is a semi-relativistic extension of corresponding time-dependent one-body Hartree-Fock equation coupled with classical nuclear dynamics, already known and studied both in quantum chemistry and in rigorous mathematical literature. We prove local existence of solutions for data in H^σ with $\sigma \in [0, \frac{3}{2}[$. In the course of the analysis a second new result of independent interest is discussed and proved, namely the construction of the propagator for the Dirac operator with several moving Coulomb singularities.

1 Introduction

The analysis of complex atomic matter behavior starting from first principles is nowadays a well developed subject, with a rich literature both on the theoretical and computational sides. In low energy regime there is often a good or excellent agreement between theoretical description and experimental results. Things are different in presence of heavy atoms, where relativistic contributions become essential to reliable calculations of spectral and other relevant properties of the involved systems. Notwithstanding the existence

*Dipartimento di Matematica, Università degli studi di Padova, Via Trieste, 63, 35131 Padova PD - Italy. *email:* cacciafe@math.unipd.it

[†]Université Paris 13, Sorbonne Paris Cité, LAGA, CNRS (UMR 7539), 99, avenue Jean-Baptiste Clément, F-93430 Villetaneuse, France. *email:* adesuzzo@math.univ-paris13.fr

[‡]Dipartimento di Matematica e Applicazioni, Università di Milano Bicocca, via R. Cozzi, 55, 20125 Milano MI - Italy. *email:* diego.noja@unimib.it

of several partly efficient computational strategies, the understanding of the subject from a theoretical and rigorous point of view is at present rather poor. This is due to the lack of a consistent many body Dirac theory, in contrast with the many body Schrödinger theory so successful in the non relativistic regime. It is not even clear, to give a basic example, the behavior of the system composed by two Dirac particles interacting via a Coulomb potential (see [15] and the recent preprint [14]); for this elementary two particle system it is widely believed but not proved that the essential spectrum is given by the whole real line and there are no eigenvalues.

A possible and perhaps unavoidable way out of the difficulties caused by the spectral obstruction to a many body Dirac theory consists in resorting on Quantum Electrodynamics to obtain an effective theory. This suggestive program, if theoretically satisfying and promising, is however at present far from being fully developed.

In view of this incomplete and uncertain state of affairs, in this paper we want to follow a less ambitious but however non trivial goal, that is to give the local well posedness for the dynamics of a single Dirac electron field interacting with nuclear matter described, as often in Quantum Chemistry, as N moving point classical particles.

Namely, we will study the Cauchy problem

$$\begin{cases} i\frac{\partial u}{\partial t}(t, x) = (\mathcal{D} + \beta)u(t, x) - \sum_{k=1}^N \frac{Z_k}{|x - q_k(t)|} u(t, x) + \left(|u|^2 * \frac{1}{|x|} \right) (t, x) u(t, x), \\ m_k \frac{d^2 q_k}{dt^2}(t) = -\nabla_{q_k} W_q(t) \\ u(0, \cdot) = u_0, \quad q_k(0) = a_k, \quad \frac{dq_k}{dt}(0) = b_k \end{cases} \quad (1.1)$$

with $N \geq 1$, where

$$W_q(t) = - \sum_{k=1}^N Z_k \langle u, \frac{1}{|x - q_k|} u \rangle + \sum_{k \neq l} Z_k Z_l \frac{1}{|q_k - q_l|}.$$

We are considering an electron with unit mass; the units are chosen in order to have $\hbar = 1$ and $c = 1$. Here, $\mathcal{D} + \beta$ represents the massive 3D Dirac operator; we recall that \mathcal{D} is defined as $\mathcal{D} = i^{-1} \sum_{j=1}^3 \alpha_j \partial_j$ where the 4×4

Dirac matrices are given by

$$\alpha_k = \begin{pmatrix} 0 & \sigma_k \\ \sigma_k & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} I_2 & 0 \\ 0 & -I_2 \end{pmatrix}$$

and the σ_k ($k = 1, 2, 3$) are the Pauli matrices, given by

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (1.2)$$

We briefly discuss the model, referring to [28] for a comprehensive account of the subject of rigorous derivation of atomic and molecular systems, including relativistic effects and to [17] for details on variational techniques in stationary problems.

The above system contains a partial differential equation of Dirac type representing the (single) electron cloud dynamics, coupled with ordinary differential equations ruling the motion of the nuclei. The latter are described as classical point particles. The coupling shows up in two different terms in the equations: firstly the Coulomb potential evaluated at the positions of the moving nuclei appears in the Dirac equation, and then in each classical Newton equation besides the inter-particle Coulomb interaction, a further force term containing the Dirac field is present. This force term represents the Coulomb potential (at the nucleus position) due to the charge density u^*u associated to the electron field. A contribution of this kind is heuristically expected on the basis of so-called Hellman-Feynman's Theorem, and it is the analogue of a similar term in the non relativistic theory of atoms and molecules. Finally, we add to the Dirac equation a nonlinearity of Hartree type. In the Schrödinger theory the Hartree nonlinearity is an effect of a reduction from a many body theory, but we do not attempt here any theoretical justification of this term and we retain this contribution by pure analogy; we only mention that in the context of Dirac-Maxwell theory, this term appears naturally in the absence of magnetic field as a by-product of the decoupling of the equations (see [13]). For relevant rigorous results regarding well posedness of the analogous model in the Schrödinger setting we refer to [11], to the above [28] and to references therein.

We discuss briefly a last issue related to the choice of the model. In a completely relativistic model the classical nuclei should have a relativistic kinematics, and the (classical) electromagnetic potentials, including the magnetic vector potential, should solve the Maxwell equations, or the wave equation in a suitable gauge. In the semi-relativistic model presented here the dynamics of the heavy nuclei is consistent, at a first approximation, with the consideration of the instantaneous Coulomb potential only, while magnetic and retardation effects are neglected. The completely non relativistic analogous of system (1.1) has already been object of study in literature (see [11], [2], [3] and is known to be globally well posed; for a related paper on nonlinear Schrödinger equations with moving Coulomb singularities see also [33]).

We stress the fact that, in contrast with the Schrödinger case, a severe difficulty here is represented by the strong singularity produced by the moving nuclei: indeed, the Coulomb potential exhibits the same homogeneity of the (massless) Dirac operator or, in other words, it is critical with respect to the natural scaling of the operator. This is the source of several problems, especially from the point of view of dispersive dynamics: indeed, it is not known whether Strichartz estimates hold for the flow $e^{it(\mathcal{D}+m_e\beta+\frac{\mu}{|x|})}$, even in the case $m_e = 0$ (we mention the papers [10] in which a family of local smoothing estimates for such a flow is proved and [9] in which the same result is obtained in the case of Aharonov-Bohm fields), while it is interesting to notice that for the scaling critical non-relativistic counterpart, i.e. the Schrödinger equation with inverse square potential, the dispersive dynamics is now completely understood (see [6] for Strichartz, and [19] for time-decay estimates in even more general settings). Related analysis of dispersive estimates for perturbed Dirac flows with applications to nonlinear models can be found in [16], [7], [8] and references therein. Anyway, in the present paper we bypass the lack of effective dispersive estimates, adopting the strategy already working in [11], which is essentially an application of Segal Theorem [39]. The key ingredients will be the construction of a 2-parameters propagator associated to the time-dependent Hamiltonian, the fact that the non local Hartree term is Lipschitz continuous and finally a two stage fixed point argument. This allows to prove at least existence of *local* solutions for system (1.1).

As a final remark on the model, notice that a complete particle-field system should include the coupling with the electromagnetic field, and so Maxwell equations with sources. For a point particle this presumably entails serious difficulties, which in the case of the completely classical Maxwell-Lorentz system are well known and unsolved (see for example [41] for a complete discussion and [31, 32] and references therein for a rigorous treatment of a related model).

Before stating our main results, let us fix some useful notations.

Notations. With L^2 and H^σ we will denote the Lebesgue and Sobolev spaces $L^2(\mathbb{R}^3, \mathbb{C}^4)$ and $H^\sigma(\mathbb{R}^3, \mathbb{C}^4)$ respectively.

With $\mathcal{L}(X, Y)$ we will denote the space of bounded linear operators $A : X \rightarrow Y$ and we pose $\mathcal{L}(X) \equiv \mathcal{L}(X, X)$.

By the symbol $1_{N \geq 2}$ we mean the number 1 if we are in the case of several nuclei, the number 0 in the case of a single nucleus.

For the sake of brevity, when no ambiguity is possible, we will often omit the dependence $t \in [0, T]$ and $k = 1, \dots, N$ in writing expression such as $\sup_{k,t}$.

Our first result consists in showing existence of a two-parameters propagator associated to the time dependent Dirac Hamiltonian with moving Coulomb singularities

$$H(t) = \mathcal{D} + \beta + V(x, t) \quad (1.3)$$

where $V(x, t) = - \sum_{k=1}^N \frac{Z_k}{|x - q_k(t)|}$.

We will assume to be, when $N \geq 2$, in a *no-collision setting*; namely, we will require the initial positions a_k to be well-separated, together with a bound on the velocities $\dot{q}_k(t)$ (hypotheses 1.4 and first of 1.5).

Theorem 1.1. *Assume that $|Z_k| < \frac{\sqrt{3}}{2} \forall k$ and that*

$$\min\{|q_k(0) - q_l(0)| \mid k \neq l\} = 8\varepsilon_0 \quad (1.4)$$

for some $\varepsilon_0 > 0$. Then if the nuclei trajectories q_1, \dots, q_N are $W^{2,1}([0, T])$ and there exists $C_{\dot{q}}$ (independent from T) such that

$$(1 + T1_{N \geq 2}) \sup_k \|\dot{q}_k\|_{L^\infty([0, T])} \leq C_{\dot{q}}, \quad \sup_k \|\ddot{q}_k(t)\|_{L^1([0, T])} < \infty \quad (1.5)$$

for some $T > 0$, then the flow of the equation

$$i\partial_t u = H(t)u$$

is well defined and given by a family of operators $U_q(t, s)$ with

$$U_q \in \mathcal{C}([0, T]^2, \mathcal{L}(H^\sigma))$$

for any $\sigma \in [0, \frac{3}{2})$ with $H^\sigma \rightarrow H^\sigma$ norms uniformly bounded in t, s , and q ; $U_q(t, s)$ satisfies

$$U_q(t, s) \circ U_q(s, r) = U_q(t, r), \quad U_q(t, t) = \mathbb{I},$$

$$i\partial_t U_q(t, s) = H(t)U_q(t, s), \quad i\partial_s U_q(t, s) = -U_q(t, s)H(s).$$

Moreover if $q^{(1)} = (q_1^{(1)}, \dots, q_N^{(1)})$ and $q^{(2)} = (q_1^{(2)}, \dots, q_N^{(2)})$ belong to $\mathcal{C}^2([0, T])$, satisfy the above hypotheses and assuming moreover that $q^{(1)}(0) = q^{(2)}(0) = (a_1, \dots, a_N)$, then there exists C (independent from T) such that for all $t, s \in [0, T]^2$, we have

$$\|U_{q^{(1)}}(t, s) - U_{q^{(2)}}(t, s)\|_{H^\sigma \rightarrow H^{\sigma-1}} \leq C \sup_k (1 + 1_{N \geq 2} T) \|(\dot{q}_k^{(1)}) - (\dot{q}_k^{(2)})\|_{L^\infty}$$

for any $\sigma \in [1, \frac{3}{2})$.

Remark 1.1. *We recall that*

$$\mathcal{D} + \beta \pm \frac{Z}{|x|} \tag{1.6}$$

(and variants thereof) is a self-adjoint operator for $|Z| < \frac{\sqrt{3}}{2}$ on H^1 (see [38]); a distinguished self-adjoint extension can actually be built also in the wider range $|Z| \leq 1$ (see [18] and references therein; see also the recent review [20]). Similar results hold in the case of multi-centric Coulomb potentials but for atomic numbers $|Z_k| < \frac{\sqrt{3}}{2}$ (Levitán-Otelbaev theorem, [29, 27]), and we retain this condition along the paper without other comments.

Remark 1.2. *By applying a standard continuation argument, the propagator $U_q(t, s)$ defined in Theorem 1.1 can be extended to global times provided one assumes, instead of (1.5), global bounds on $|\dot{q}_k(t)|, |\ddot{q}_k(t)|$. However, in the subsequent analysis of the coupled dynamics defined by system (1.1), these two terms can be bounded only locally in time, due to the absence of positive definite conserved quantities. Therefore we will only be able to obtain a local evolution in the coupled system.*

Remark 1.3. *The proof of Theorem 1.1 borrows ideas from [26], in which the authors prove a similar result in the case of the Dirac equation perturbed by the retarded Lienard-Wiechert potentials produced by relativistically moving nuclei. The main technical tool consists there in introducing a local Lorentz transformation depending on the particle trajectories which simultaneously freezes the position of the moving singularities, in such a way to change from moving Coulomb singularities to stationary ones, and then to resort on classical theory of self-adjointness for perturbations of the Dirac operator. We stress however that the difference in the model (the Lienard-Wiechert potentials discussed in [26] are significantly more involved and require stronger assumptions) and our need of detailed estimates for subsequent analysis do not allow a reduction of the present result to the one in [26].*

Remark 1.4. *The threshold $\sigma = \frac{3}{2}$ in Theorem 1.1 seems to be structural in the following sense: in order to apply Kato's results for the construction of the propagator associated to a time-dependent Hamiltonian $H(t)$, one of the (sufficient) conditions is $H(t) \in C([0, T]; \mathcal{L}(Y, X))$. Therefore, beyond the regularity in time, which will be guaranteed by assumptions (1.5), one needs the Hamiltonian to be bounded from $H^{\sigma+1}$ into H^σ , and this fact will be true, as a consequence of generalized Hardy-Rellich inequality, only for σ up to $\frac{1}{2}$. Moreover, we stress the fact that the space $H^{\frac{3}{2}}$ appears as a natural threshold of regularity for the eigenstates of the Dirac-Coulomb operator (see the Appendix), and this seems to confirm the optimality of our result.*

Then we study local well posedness for the Cauchy problem (1.7). For the sake of simplicity, we state this result in the simplified framework of a single nucleus first. In this case, the system writes (we consider, without loss of generality, the initial condition $q(0) = 0$)

$$\begin{cases} i\frac{\partial u}{\partial t}(t, x) = (\mathcal{D} + \beta)u(t, x) - \frac{Z}{|x - q(t)|}u(t, x) + \left(|u|^2 * \frac{1}{|x|}\right)(t, x)u(t, x), \\ m\frac{d^2 q}{dt^2}(t) = \langle u(t) | \nabla \frac{Z}{|\cdot - q(t)|} | u(t) \rangle \\ u(0, \cdot) = u_0, \quad q(0) = 0, \quad \frac{dq}{dt}(0) = \dot{q}_0. \end{cases} \quad (1.7)$$

We are here using the Dirac bra-ket notation to denote

$$\langle u(t) | \nabla \frac{Z}{|x - q(t)|} | u(t) \rangle = -Z \int_{\mathbb{R}^3} \langle u(t), u(t) \rangle_{\mathbb{C}^4} \frac{x - q(t)}{|x - q(t)|^3}. \quad (1.8)$$

We get the following result.

Theorem 1.2. *Let $|Z| < \frac{\sqrt{3}}{2}$ and $\sigma \in [1, 3/2)$. There exist C_1 and C_2 depending on Z and m , such that for all $R \in \mathbb{R}_+$, all $u_0 \in H^\sigma$ such that $\|u_0\|_{H^\sigma} \leq R$, and all initial conditions q_0 such that $|\dot{q}_0| \leq C_1$, then system (1.7) admits a solution in $\mathcal{C}([0, T], H^\sigma(\mathbb{R}^3)) \times \mathcal{C}^2([0, T], \mathbb{R}^3)$, for $T = \frac{1}{C_2(1+R^2)}$;*

The analogous result in the multi-nuclear case is then the following

Theorem 1.3. *Let $N \geq 2$, $|Z_k| < \frac{\sqrt{3}}{2}$ for all $k = 1, \dots, N$ and $\sigma \in [1, 3/2)$. There exist C_1 and C_2 depending on $(Z_k)_k$ and $(m_k)_k$ and ε_0 , such that for all $R \in \mathbb{R}_+$, all $u_0 \in H^\sigma$ such that $\|u_0\|_{H^\sigma} \leq R$, and all initial conditions $(q_k(0))_k$ satisfying (1.4) and all vectors \dot{q}_0 such that $|\dot{q}_0| \leq C_1$, then system (1.7) admits a solution in $\mathcal{C}([0, T], H^\sigma(\mathbb{R}^3)) \times \mathcal{C}^2([0, T], \mathbb{R}^3)$, for $T = \frac{1}{C_2(1+R^2)}$;*

We give some remarks on these results.

Remark 1.5. *The threshold $\sigma = \frac{3}{2}$ is a consequence of Theorem 1.1, as one needs the two parameter propagator constructed before in order to prove existence of a solution. We moreover notice that this threshold appears again in the nonlinear model: indeed, in order to prove existence of solutions for equation (1.1) one needs to prove regularity properties for the nonlinear term (1.8) which, as a matter of fact, turns to be Hölder continuous for $u \in H^\sigma$ for $\sigma < \frac{3}{2}$, and would become Lipschitz continuous for $\sigma > \frac{3}{2}$. Both these facts are a consequence, again, of generalized Hardy inequality. This means that if one was able to construct some propagator on H^σ for $\sigma > \frac{3}{2}$, this would yield not only existence of solutions for system 1.1, but also local well-posedness (i.e.*

uniqueness and continuous dependence on the initial data). Unfortunately, as discussed in Remark 1.4, this threshold seems to be structural. To overcome these issues one can think to modify the setting of the problem working with weighted Sobolev spaces or to modify the model regularizing the singularity in the Coulomb potential. These developments will be the object of future work.

Remark 1.6. *If we look only at the nonlinear Dirac equation, our H^σ assumption on the regularity of the initial condition is well above the critical threshold required by the scaling (see e.g. [30], in which the authors study global well-posedness and scattering for the Dirac equation with a nonlocal nonlinear term of the form $F(u) = (|x|^\alpha * |u|^{p-1})u$ relying on Strichartz estimates). Nonetheless, our high regularity requirement seems to be unavoidable if one wants to deal with the classical Newtonian dynamics for the nuclei. Moreover, let us point out that the coupled system (1.1) does not exhibit any scaling law even in the case of massless electrons.*

Remark 1.7. *It is interesting to compare Theorem 1.2 with its non relativistic counterpart, i.e. Theorem 1 in [11]. In that case the authors prove global well posedness for the Cauchy problem (i.e. the existence of a solution for any time $t > 0$) for initial data in the space H^2 ; to do this, they first prove local well posedness and then extend the solution using energy conservation of the system. This strategy does not work for the Dirac equation (and thus in the present context), as the associated energy is not positive, and therefore cannot be used to control any H^σ norm. This is the ultimate reason why we are only able to obtain local well posedness for system (1.7).*

Remark 1.8. *All the constants in Theorem 1.3 may depend on ε_0 . In particular, the time of existence should behave like ε_0^γ for some $\gamma > 0$. The power γ that one can compute while performing the proof does not seem physically relevant, hence we did not keep track of it during the proof. This smallness on T may be replaced by a smallness assumptions on Z_k , in this case, we can have a time of existence proportional to ε_0 .*

We give a brief outline of the structure of the paper.

Section 2 will be devoted to the proof of Theorem 1.1, i.e. to the construction of the 2-parameter propagator, first in the case of a single nucleus and then with several ones. Various properties of the propagator are derived: firstly, its original definition can be extended from L^2 to H^σ for $\sigma < \frac{3}{2}$ as a consequence of Kato's theory on two-parameter propagators, secondarily a result of continuous dependence on the trajectory is given. The case of several nuclei is more involved but the results are analogous to the single nucleus case when suitable conditions on the trajectories, preventing particles are close to

collisions, are imposed.

Section 3 will be dedicated to the proofs of Theorems 1.2 and 1.3, simultaneously. We summarize the strategy as follows: the solution map is first considered as acting on the electron field u for every trajectory q , using a contraction argument in H^σ . Then a Schauder fixed point argument is performed on the (integrated) Newton equation for the nucleus trajectory, giving the final result. The properties of the solution map depend in a crucial way on the previously proved results for the non autonomous propagator.

Acknowledgments. We are grateful to prof. Éric Séré for having introduced us to the present problem and for several enlightening discussions on the topic, to Matteo Gallone for discussions and comments and to Jonas Lampart for pointing out a mistake in our original argument, that led to the present version of the paper.

2 The Dirac-Coulomb propagator with moving singularities

We will present in the next subsection the proof of Theorem 1.1 in the case of a single nucleus, that will be divided in several steps, as the strategy is clearer in this case; afterwards, in subsection 2.2, we shall present all the necessary modifications needed in order to deal with the case of several nuclei.

2.1 One nucleus

In this case, the time-dependent Hamiltonian reads

$$H(t) = \mathcal{D} + \beta - \frac{Z}{|x - q(t)|}. \quad (2.1)$$

Throughout this subsection, we will always assume that

$$|Z| < \frac{\sqrt{3}}{2} \quad (2.2)$$

which, as discussed in Remark 1.1, ensures an essentially self-adjoint (static) Dirac-Coulomb operator. Notice the following relations

$$\|f\|_{\dot{H}^1}^2 = \int_{\mathbb{R}^3} |\nabla f|^2 \cong \int_{\mathbb{R}^3} |\mathcal{D}f|^2$$

and, due to the anticommutation of the Dirac matrices,

$$\|f\|_{H^1}^2 = \int_{\mathbb{R}^3} |\nabla f|^2 + \int_{\mathbb{R}^3} |f|^2 \cong \int_{\mathbb{R}^3} |(\mathcal{D} + \beta)f|^2.$$

We split the proof into several Lemmas.

Lemma 2.1. *Let $T \in \mathbb{R}^+$, $u \in \mathcal{C}([0, T], H^\sigma) \cap \mathcal{C}^1([0, T], H^{\sigma-1})$ for $\sigma \geq 1$, $q \in \mathcal{C}^1([0, T], \mathbb{R}^3)$ and set $v(t, x) = u(t, x + q(t))$. Then u solves*

$$i\partial_t u = H(t)u \quad (2.3)$$

if and only if v solves

$$i\partial_t v = H_1(t)v \quad (2.4)$$

where $H_1(t) = \mathcal{D} + \beta - \frac{Z}{|x|} + i\dot{q}(t) \cdot \nabla$.

Proof. Straightforward computation. □

Lemma 2.2. *Let $T \in \mathbb{R}^+$. Assume (2.2) and that*

$$\sup_{t \in [0, T]} |\dot{q}(t)| \leq R_Z \quad (2.5)$$

for some suitably small constant R_Z . Then there exists a constant C such that for all $t \in [0, T]$

$$\frac{1}{C} \|f\|_{H^1} \leq \|H_1(t)f\|_{L^2} \leq C \|f\|_{H^1}. \quad (2.6)$$

In particular, for every $t \in [0, T]$, $H_1(t)$ is an isomorphism from H^1 to L^2 .

Proof. Inequality (2.6) is a consequence of general theory for Dirac-Coulomb operator. In particular, Theorem 4.4 in [43] ensures indeed that the domain of the operator $\mathcal{D} + \beta - \frac{Z}{|x|}$ (i.e. the "static" Dirac-Coulomb operator) coincides with the domain of the free Dirac operator, which is H^1 . Moreover, it is known that 0 is not in the spectrum of $\mathcal{D} + \beta - \frac{Z}{|x|}$ therefore $\mathcal{D} + \beta - \frac{Z}{|x|}$ is an isomorphism between its domain with H^1 topology and L^2 . Indeed it is a bijective linear map from the domain into L^2 , continuous for the topologies H^1 and L^2 , so by the open mapping principle its inverse $(\mathcal{D} + \beta - \frac{Z}{|x|})^{-1}$ is continuous for the L^2 and H^1 topology. As then $H_1(t) = \mathcal{D} + \beta - \frac{Z}{|x|} + i\dot{q}(t) \cdot \nabla$, under our assumption on $|\dot{q}(t)|$ the additional term can be treated as a (bounded) perturbation, and then (2.6) holds. □

Lemma 2.2 will be enough to construct, through general Kato's Theory, the two parameters propagator associated to the Hamiltonian $H_1(t)$ on the space H^1 ; anyway, we are actually able to extend this propagator to some higher Sobolev spaces, namely for any $\sigma < 3/2$; we stress the fact that we

need to go above the regularity of the domain of the Dirac-Coulomb operator, which is H^1 , and thus this step requires some additional work.

We start by providing some fundamental functional inequalities. The first one, is the following generalized Hardy inequality.

Proposition 2.3. *For any $\sigma \in [0, \frac{d}{2})$ there exists a constant C such that for any $f \in \dot{H}^\sigma(\mathbb{R}^d)$*

$$\int_{\mathbb{R}^d} \frac{|f(x)|^2}{|x|^{2\sigma}} dx \leq C \|f\|_{\dot{H}^\sigma}^2. \quad (2.7)$$

Proof. See Theorem 2.57 in [4]. □

Then, we need the following Rellich inequality ([36, 37]).

Proposition 2.4. *Let $u \in C_c^\infty(\mathbb{R}^3 \setminus \{0\})$. Then*

$$\int_{\mathbb{R}^3} \frac{|u|^2}{|x|^4} dx \leq C \int_{\mathbb{R}^3} |\Delta u|^2 dx \quad (2.8)$$

and, as a consequence,

$$\left\| \frac{u}{|x|} \right\|_{H^1} \leq C \|u\|_{H^2}. \quad (2.9)$$

Remark 2.1. *As a matter of fact the inequality was proved (in the radial case) by Rellich himself exactly in this form and with the optimal constant $C = (\frac{3}{4})^2$; the extension to the non radial case, here inspired by [12], appears probably in several other papers but we were not able to find a reference and so we include a proof for the sake of completeness. We stress the fact that the inequality is usually stated and proved on functions defined on the whole space \mathbb{R}^n but in higher dimensions n .*

Proof. We are not interested in providing optimal constant in the inequality, and so along the proof any constant appearing will be all indicated by a generic C that will be allowed to change from line to line. We use the well known spherical harmonics decomposition to write

$$u(x) = \sum_{k=0}^{\infty} u_k(r) \phi_k(\theta)$$

where $\phi_k(\theta) \in L^2(S^2)$ for $k \geq 0$ are the spherical harmonics of degree k (which might be assumed to be L^2 -normalized) which, we recall, satisfy the property $\Delta_{S^2} \phi_k = c_k \phi_k$ with $c_k = k(k+1)$. We then get, as the action of the

laplacian in spherical coordinate is given by $\Delta = \partial_{rr} + \frac{2}{r}\partial_r + \frac{1}{r^2}\Delta_{S^2}$, that we can write

$$\int_{\mathbb{R}^3} |\Delta u|^2 dx = \sum_{k=0}^{\infty} \int_0^{+\infty} \left(|\partial_{rr} u_k|^2 + \frac{c_k^2}{r^4} u_k^2 - \frac{2c_k}{r^2} u_k \partial_{rr} u_k \right) r^2 dr$$

that, after integrating by parts, becomes

$$\int_{\mathbb{R}^3} |\Delta u|^2 dx = \tag{2.10}$$

$$\sum_{k=0}^{\infty} \left(\int_0^{+\infty} |\partial_{rr} u_k|^2 r^2 dr + 2(c_k + 1) \int_0^{+\infty} |\partial_r u_k|^2 dr + c_k(c_k - 1) \int_0^{+\infty} \frac{u_k^2}{r^2} dr \right).$$

Notice that $c_k(c_k - 1) \geq 0$ for every $k \geq 0$. We now use the following estimates:

$$\int_0^{+\infty} |\partial_{rr} u_k|^2 r^2 dr \geq C \int_0^{+\infty} \frac{|\partial_r u_k|^2}{r^2} r^2 dr, \quad \forall k \geq 0$$

which is a direct application of Hardy inequality for radial functions, and

$$\int_0^{+\infty} |\partial_r u_k|^2 dr \geq C \int_0^{+\infty} \frac{|u_k|^2}{r^4} r^2 dr, \quad \forall k \geq 0,$$

which is a consequence of integration by parts and Cauchy-Schwarz. Plugging these estimates into (2.10) we thus obtain

$$\int_{\mathbb{R}^3} |\Delta u|^2 dx \geq C \sum_{k=0}^{\infty} \int_0^{+\infty} \frac{|u_k|^2}{r^4} r^2 dr$$

that is exactly (2.8).

Estimate (2.11) comes as a direct consequence of (2.8) and standard Hardy's inequality: indeed, for any $u \in C_c^\infty(\mathbb{R}^3 \setminus \{0\})$ we have

$$\left\| \frac{u}{|x|} \right\|_{H^1} \lesssim \left\| \frac{\nabla u}{|x|} \right\|_{L^2} + \left\| \frac{u}{|x|^2} \right\|_{L^2} \lesssim \|u\|_{H^2}. \tag{2.11}$$

□

The following lemma represents the key step in order to extend the propagator to higher order fractional Sobolev spaces.

Lemma 2.5. *For any $t > 0$, the Hamiltonian $H_1(t)$ is a bounded operator from H^σ into $H^{\sigma-1}$ for any $\sigma \in [1, 3/2)$.*

Proof. We need to show that the operator $\frac{1}{|x|}$ is bounded from H^σ into $H^{\sigma-1}$ for $\sigma \in [1, 3/2)$, that is inequality

$$\left\| \frac{u}{|x|} \right\|_{H^{\sigma-1}} \leq \|u\|_{H^\sigma}, \quad \sigma \in [1, \frac{3}{2}), \quad (2.12)$$

as the boundedness of the other terms is trivial. In order to prove this fact, we introduce the regularizing potential $\frac{1}{\sqrt{|x|^2 + \varepsilon^2}}$, with $\varepsilon > 0$. First, we have the following inequality, for any $u \in C_c^\infty(\mathbb{R}^3)$

$$\left\| \frac{u}{\sqrt{|x|^2 + \varepsilon^2}} \right\|_{L^2} \lesssim \|u\|_{H^1}, \quad (2.13)$$

that is a simple consequence of Hardy's inequality as $\frac{1}{\sqrt{|x|^2 + \varepsilon^2}} \leq \frac{1}{|x|}$. Then, we also have, still for any $u \in C_c^\infty(\mathbb{R}^3)$

$$\left\| \frac{u}{\sqrt{|x|^2 + \varepsilon^2}} \right\|_{H^1} \lesssim \|u\|_{H^2}. \quad (2.14)$$

In order to prove this inequality, we write

$$\left\| \frac{u}{\sqrt{|x|^2 + \varepsilon^2}} \right\|_{H^1} \lesssim \left\| \frac{\nabla u}{\sqrt{|x|^2 + \varepsilon^2}} \right\|_{L^2} + \left\| u \nabla \left(\frac{1}{\sqrt{|x|^2 + \varepsilon^2}} \right) \right\|_{L^2} = I + II.$$

For I we easily have from Hardy's inequality

$$I \leq \left\| \frac{\nabla u}{|x|} \right\|_{L^2} \leq \|u\|_{H^2}.$$

We now deal with II : first of all, notice that we have

$$\left| \nabla \left(\frac{1}{\sqrt{|x|^2 + \varepsilon^2}} \right) \right| \leq \frac{1}{|x|^2 + \varepsilon^2}.$$

Now, let us introduce two functions χ and η such that $f = f\eta + f\chi$, with $\text{supp}(\eta) \subset B(0, \tilde{\varepsilon})$, $\text{supp}(\chi) \subset B^c(0, \tilde{\varepsilon}/2)$ with $\tilde{\varepsilon}$ to be fixed later, and $\eta + \chi = 1$. We thus write

$$II^2 \leq \int \frac{|u|^2}{(|x|^2 + \varepsilon^2)^2} \leq \int \frac{|\chi u|^2}{(|x|^2 + \varepsilon^2)^2} + \int \frac{|\eta u|^2}{(|x|^2 + \varepsilon^2)^2} = II_1^2 + II_2^2.$$

The term II_1^2 gives no problem, as the support of χ allows to neglect the singularity in zero, and one simply has from (2.8)

$$II_1^2 \leq \int \frac{|u|^2}{|x|^4} \leq \|u\|_{H^2}^2.$$

On the other hand, for II_2^2 we can write

$$II_2^2 \leq \int_{B(0,\tilde{\varepsilon})} \frac{|u|^2}{\varepsilon^4} \lesssim \|u\|_{L^\infty}^2 \frac{\tilde{\varepsilon}^3}{\varepsilon^4} \leq \|u\|_{H^2}^2$$

where in the last inequality we have chosen $\tilde{\varepsilon} = \varepsilon^{4/3}$. This concludes the proof of (2.14). We can now interpolate between inequalities (2.13) and (2.14) to obtain the following family of inequalities for any $u \in C_c^\infty(\mathbb{R}^3)$: for any $\varepsilon > 0$ and any $\sigma \in [1, 2]$ we have

$$\left\| \frac{u}{\sqrt{|x|^2 + \varepsilon^2}} \right\|_{H^{\sigma-1}} \leq \|u\|_{H^\sigma}. \quad (2.15)$$

We now want to send $\varepsilon \rightarrow 0$ to retrieve our result: first, we note that

$$\left\| \left(\frac{1}{\sqrt{|x|^2 + \varepsilon^2}} - \frac{1}{|x|} \right) u \right\|_{L^2} \rightarrow 0 \quad (2.16)$$

for $\varepsilon \rightarrow 0$. More precisely, we have that

$$\left| \frac{1}{\sqrt{\varepsilon^2 + |x|^2}} - \frac{1}{|x|} \right| = \left| \frac{|x| - \sqrt{\varepsilon^2 + |x|^2}}{|x|\sqrt{\varepsilon^2 + |x|^2}} \right| = \left| \frac{\varepsilon^2}{|x|\sqrt{\varepsilon^2 + |x|^2}(|x| + \sqrt{\varepsilon^2 + |x|^2})} \right| \leq \frac{\varepsilon^2}{|x|^3}$$

and

$$\left| \frac{1}{\varepsilon + |x|} - \frac{1}{|x|} \right| \leq \frac{1}{|x|}$$

imply

$$\left| \frac{1}{\varepsilon + |x|} - \frac{1}{|x|} \right| \leq \frac{\varepsilon^s}{|x|^{3s/2}} \left(\frac{1}{|x|} \right)^{1-s/2} = \frac{\varepsilon^s}{|x|^{1+s}}$$

for $s \in (0, 1/2)$; therefore, using (2.7), we get

$$\left\| \left(\frac{1}{\sqrt{|x|^2 + \varepsilon^2}} - \frac{1}{|x|} \right) \right\|_{L^2}^2 \leq \varepsilon^{2(\sigma-1)} \int \frac{|u|^2}{|x|^\sigma} \leq \varepsilon^{2(\sigma-1)} \|u\|_{H^\sigma}^2 \quad (2.17)$$

which in particular proves (2.16).

We are now ready to prove (2.12). We use Fourier transform \mathcal{F} and then bound as follows: fix $R > 0$, then

$$\begin{aligned}
& \int_0^R \langle \xi \rangle^{\sigma-1} \left| \mathcal{F} \left(\frac{u}{|x|} \right) \right|^2 (\xi) d\xi \\
\leq & \int_0^R \langle \xi \rangle^{\sigma-1} \left| \mathcal{F} \left(\frac{u}{|x|} \right) - \mathcal{F} \left(\frac{u}{\sqrt{\varepsilon^2 + |x|^2}} \right) \right|^2 (\xi) d\xi + \int_0^R \langle \xi \rangle^{\sigma-1} \left| \mathcal{F} \left(\frac{u}{\sqrt{\varepsilon^2 + |x|^2}} \right) \right|^2 (\xi) d\xi \\
& \leq \langle R \rangle^{\sigma-1} \left\| \frac{u}{|x|} - \frac{u}{\sqrt{\varepsilon^2 + |x|^2}} \right\|_{L^2}^2 + \left\| \frac{u}{\sqrt{\varepsilon^2 + |x|^2}} \right\|_{H^\sigma}^2 \\
& \leq \|u\|_{H^\sigma}^2 (1 + \langle R \rangle^{\sigma-1} \varepsilon^{\sigma-1})^2
\end{aligned}$$

where in the last inequality we have used (2.17) and (2.15). We now take ε such that $\langle R \rangle^{\sigma-1} \varepsilon^{\sigma-1} \rightarrow 0$ to conclude

$$\int_0^R \langle \xi \rangle^{\sigma-1} \left| \mathcal{F} \left(\frac{u}{|x|} \right) \right|^2 (\xi) d\xi \leq \|u\|_{H^\sigma}^2$$

that is (2.12). □

Remark 2.2. Notice that the tempting argument of interpolating inequality (2.11) with standard Hardy's inequality to conclude the desired boundedness of the multiplication operator $\frac{1}{|x|}$ from H^σ into $H^{\sigma-1}$ does not come for free, as (2.11) is only proved for functions $u \in C_c^\infty(\mathbb{R}^3 \setminus \{0\})$ which is not dense in H^σ for $\sigma \geq \frac{1}{2}$. This fact forces our two steps interpolation procedure.

We are now in position to state the the main result of this first part, that is the existence of a two-parameter propagator associated to the time-dependent Hamiltonian $H_1(t)$.

Proposition 2.6. Suppose the hypothesis of Lemma 2.2 hold true and moreover that

$$\|\ddot{q}(t)\|_{L^1([0,T])} < \infty. \tag{2.18}$$

Then there exist

1) a family of operators $(U_1(t, s))_{t, \sigma \in [0, T]^2}$ from L^2 to L^2 strongly continuous in $(t, s) \in [0, T]$, uniformly bounded in $(t, s) \in [0, T] \times [0, T]$ and with the properties

$$\begin{aligned}
U_1(t, r) &= U_1(t, s) \circ U_1(s, r) U_1(t, r), & 0 \leq r \leq \sigma \leq t \leq T; \\
U_1(t, t) &= \mathbb{I}, & 0 \leq t \leq T; \\
i\partial_t U_1(t, s) &= H_1(t) U_1(t, s), & 0 \leq \sigma \leq t \leq T; \\
i\partial_s U_1(t, s) &= -U_1(t, s) H_1(s), & 0 \leq \sigma \leq t \leq T;
\end{aligned}$$

2) the same family of operators, again indicated with $(U_1(t, s))_{t, \sigma \in [0, T]^2}$ restrict invariantly from H^σ to H^σ for any $\sigma \in [0, \frac{3}{2})$ with the same properties as above.

Remark 2.3. The condition \dot{q} above is needed in order to ensure that $H_1(t)$ is of bounded variations (in time) as an operator from H^1 to L^2 . What is more, the operator $U_1(t, s)$ is uniformly bounded from H^1 to H^1 or from L^2 to L^2 in q in balls of $W^{2,1}$.

Proof. This result is a direct consequence of a very well known and developed theory. Indeed, Lemma 2.2 ensures that $H_1(t)$ is a bounded, continuously differentiable in time operator from H^σ to $H^{\sigma-1}$ for any $\sigma \in [1, \frac{3}{2})$. This allows to use the well known results due to Kato (see [25], [23] and, in particular, Theorem 2 in [22]; see also [40] and [42] for recent surveys) to show that $H_1(t)$ generates a two parameter propagator and a well posed dynamics. \square

Remark 2.4. The fact that the propagator is in $L^2 \rightarrow L^2$ is due to the fact that $H_1(t)$ satisfies (2.6) and that it is of bounded variations in time. Besides already quoted literature, a good reference where restriction of the evolution family to dense subset is treated is the classic treatise of Pazy, chapter V [35]. For more recent exposition, survey and clarification of some of the hypotheses in original papers, we mention [40] and [42] where by the way it is remarked that the C^1 property of the generator is the really relevant one. Also, we mention [34], in which the authors construct a propagator for a Dirac equation with a moving small potential. The meaning of the two parts of Proposition 2.6 is that equation (2.4) is well posed in both L^2 and H^σ , and hence the same holds true for the original equation (2.3), thanks to Lemma 2.1.

In order to define the propagator associated to the original equation (2.3), one only needs to re-change variables.

Proposition 2.7. Let q and Z satisfy (2.2), (2.5) and (2.18). Then the flow of the equation

$$i\partial_t u = H(t)u$$

with $H(t)$ defined by (2.1) is given by a family of operators $U(t, s) = U_q(t, s)$ satisfying

$$U_q(t, s) \circ U_q(s, r) = U_q(t, r), \quad U_q(t, t) = \mathbb{I}.$$

and

$$i\partial_t U_q(t, s) = H(t)U_q(t, s), \quad i\partial_s U_q(t, s) = -U_q(t, s)H(s)$$

with

$$U_q \in \mathcal{C}([0, T]^2, \mathcal{L}(H^\sigma))$$

for any $\sigma \in [0, \frac{3}{2})$. In particular the norms

$$\|U_q(t, s)\|_{H^\sigma \rightarrow H^\sigma}$$

are uniformly bounded in t , s , and q .

Proof. Let $I(t)$ be the smooth isometry of H^σ for any s

$$I(t)f(t, x) = f(t, x + q(t)). \quad (2.19)$$

The operators $U(t, s) = I(t)^{-1}U_1(t, s)I(s)$ satisfy the conclusions, as remarked in Lemma 2.1. \square

We now show the continuity in q of the propagator U .

Proposition 2.8. *The operator $U(t, s) = U_q(t, s)$ depends continuously on q as an operator from H^σ to $H^{\sigma-1}$, in the sense that for all $q_1, q_2 \in \mathcal{C}^1([0, T])$ satisfying the assumptions of Lemma 2.2 and all $(t, \tau) \in [0, T]^2$,*

$$\|U_{q_1}(t, \tau) - U_{q_2}(t, \tau)\|_{H^\sigma \rightarrow H^{\sigma-1}} \leq CT \|\dot{q}_1 - \dot{q}_2\|_{L^\infty([0, T])} \quad (2.20)$$

for any $\sigma \in [1, \frac{3}{2})$, with C independent from T and q (with our assumptions of boundedness on q).

Proof of Proposition 2.8. In order to prove this result, we need to give a closer look to the construction of the propagator $U_1(t, s)$. According to [22], it appears that $U_1(t, s)$ is the limit as an operator from H^1 to L^2 of

$$U_1(n, t, s) = e^{-i(t-K/n)H_1(K/n)} \prod_{k=J}^{K-1} e^{-i\frac{H_1(k/n)}{n}} e^{-i(J/n-s)H_1((J-1)/n)} \quad (2.21)$$

where $K = \lfloor nt \rfloor$ and $J = \lfloor ns \rfloor + 1$ if $t > s$ and

$$U_1(n, t, s) = U_1(n, s, t)^*$$

if $t < s$ and $U_1(n, t, t) = Id$. This means that in order to compute $U_1(t, s)$ one can cut the interval $[s, t]$ in sub-intervals of size $\frac{1}{n}$ and use the propagator $e^{i\tau H_1((J-1)/n)}$ on $[s, J/n[$, then $e^{i\tau H_1(J/n)}$ between J/n and $(J+1)/n$ and so on, and then pass to the limit for n going to ∞ . Therefore, we preliminarily prove the following

Lemma 2.9. *Let q and Z satisfy (2.2), (2.5) and (2.18). Then the sequence $U_1(n, t, s)$ defined by (2.21) is uniformly bounded in n, t, s as an operator from L^2 to itself and as an operator from H^1 to itself. More precisely,*

$$\begin{aligned} \|U_1(n, t, s)\|_{L^2 \rightarrow L^2} &\leq 1 \\ \|U_1(n, t, s)\|_{H^1 \rightarrow H^1} &\leq C_1 e^{C_1 \|\ddot{q}\|_{L^1}}. \end{aligned}$$

Remark 2.5. By standard interpolation argument, we can deduce that $U_1(n, t, s)$ is also uniformly bounded as an operator from H^σ to itself for any $\sigma \in [0, 1]$.

Proof of Lemma 2.9. Thanks to Lemma 2.2, for $m = 0, 1$

$$\|e^{itH_1(t_0)}u\|_{H^m} \leq 2\|H_1(t_0)^m e^{iH_1(t_0)t}u\|_{L^2}$$

and since $H_1(t_0)$ and $e^{itH_1(t_0)}$ commute

$$\|e^{itH_1(t_0)}u\|_{H^m} \leq 2\|e^{iH_1(t_0)t}H_1(t_0)^m u\|_{L^2}$$

and given that $H_1(t_0)$ is essentially self adjoint

$$\|e^{itH_1(t_0)}u\|_{H^m} \leq 2\|H_1(t_0)^m u\|_{L^2}.$$

Let us now prove that

$$H_1\left(\frac{K-1}{n}\right)^m \prod_{k=J}^{K-1} e^{-i\frac{H_1(k/n)}{n}} H_1\left(\frac{J}{n}\right)^{-m} \quad (2.22)$$

is bounded in $\mathcal{L}(L^2)$ uniformly in n , which would imply the result. We can rewrite (2.22) as

$$\left(\prod_{k=J+1}^{K-1} H_1(k/n)^m e^{-i\frac{H_1(k/n)}{n}} H_1\left(\frac{k}{n}\right)^{-m} H_1\left(\frac{k}{n}\right)^m H_1\left(\frac{k-1}{n}\right)^{-m} \right) H_1\left(\frac{J}{n}\right)^m e^{-i\frac{H_1(J/n)}{n}} H_1\left(\frac{J}{n}\right)^{-m}.$$

Since $H_1(k/n)$ and $e^{-i\frac{H_1(k/n)}{n}}$ commute, this is equal to

$$\left(\prod_{k=J+1}^{K-1} e^{-i\frac{H_1(k/n)}{n}} H_1\left(\frac{k}{n}\right)^m H_1\left(\frac{k-1}{n}\right)^{-m} \right) e^{-i\frac{H_1(J/n)}{n}},$$

and since H_1 is essentially self adjoint, we get $\|e^{-i\frac{H_1(k/n)}{n}}\|_{L^2 \rightarrow L^2} = 1$. Thus

$$\|H_1\left(\frac{K-1}{n}\right)^m \prod_{k=J}^{K-1} e^{-i\frac{H_1(k/n)}{n}} H_1\left(\frac{J}{n}\right)^{-m}\|_{L^2 \rightarrow L^2} \leq \prod_{k=J+1}^K \|H_1\left(\frac{k}{n}\right)^m H_1\left(\frac{k-1}{n}\right)^{-m}\|_{L^2 \rightarrow L^2}.$$

For all k ,

$$\begin{aligned} \|H_1\left(\frac{k}{n}\right)^m H_1\left(\frac{k-1}{n}\right)^{-m}\|_{L^2 \rightarrow L^2} &= \|1 + (H_1\left(\frac{k}{n}\right)^m - H_1\left(\frac{k-1}{n}\right)^m) H_1\left(\frac{k-1}{n}\right)^{-m}\|_{L^2 \rightarrow L^2} \\ &\leq 1 + C \|H_1\left(\frac{k}{n}\right) - H_1\left(\frac{k-1}{n}\right)\|_{H^1 \rightarrow L^2}. \end{aligned}$$

We get

$$\prod_{k=J+1}^K \|H_1(\frac{k}{n})^m H_1(\frac{k-1}{n})^{-m}\|_{L^2 \rightarrow L^2} \leq e^{C \sum_{k=J+1}^K \|H_1(\frac{k}{n}) - H_1(\frac{k-1}{n})\|_{H^1 \rightarrow L^2}},$$

which is uniformly bounded in n since H_1 is of bounded variations. Indeed,

$$\sum_{k=J+1}^K \|H_1(\frac{k}{n}) - H_1(\frac{k-1}{n})\|_{H^1 \rightarrow L^2} \leq \sum_{k=J+1}^K \|(\dot{q}(\frac{k}{n}) - \dot{q}(\frac{k-1}{n})) \cdot \nabla\|_{H^1 \rightarrow L^2} \leq \|\dot{q}\|_{L^1}$$

We deduce from that the result. \square

We now get back to the proof of Proposition 2.8. Writing $H_1(q, t) = H_1(t)$ and $U_1(n, q, t, s) = U_1(n, t, s)$, we have

$$\begin{aligned} & \|U_1(n, q_1, t, s) - U_1(n, q_2, t, s)\|_{H^\sigma \rightarrow H^{\sigma-1}} \\ & \leq \|e^{-i(t-\frac{K}{n})H_1(q_1, \frac{K}{n})} - e^{-i(t-\frac{K}{n})H_1(q_2, \frac{K}{n})}\|_{H^\sigma \rightarrow H^{\sigma-1}} \|U_1(n, q_1, \frac{K}{n}, s)\|_{H^\sigma \rightarrow H^\sigma} + \\ & \|e^{-i(t-\frac{K}{n})H_1(q_2, t)}\|_{H^{\sigma-1} \rightarrow H^{\sigma-1}} \|U_1(n, q_1, \frac{K}{n}, s) - U_1(n, q_2, \frac{K}{n}, s)\|_{H^\sigma \rightarrow H^{\sigma-1}}. \end{aligned}$$

Because of the boundedness from $H^{\sigma-1}$ to $H^{\sigma-1}$ of $e^{itH_1(t_0)}$ and from H^σ to H^σ of $U_1(n, q_1, \frac{K}{n}, s)$ for all t, t_0 (see Remark 2.5) and Proposition 2.7, we get that

$$\begin{aligned} & \|e^{-i(t-K/n)H_1(q_1, s+K/n)} - e^{-i(t-K/n)H_1(q_2, t)}\|_{H^\sigma \rightarrow H^{\sigma-1}} \\ & \leq 3|t - K/n| \|H_1(q_1, s + K/n) - H_1(q_2, s + K/n)\|_{H^\sigma \rightarrow H^{\sigma-1}}. \end{aligned}$$

This ensures that

$$\begin{aligned} & \|U_1(n, q_1, t, s) - U_1(n, q_2, t, s)\|_{H^\sigma \rightarrow H^{\sigma-1}} \\ & \leq C e^{C\|\dot{q}\|_{L^1}} |t - K/n| \|\dot{q}_1 - \dot{q}_2\|_{L^\infty} + \|U_1(n, q_1, K/n, s) - U_1(n, q_2, K/n, s)\|_{H^\sigma \rightarrow H^{\sigma-1}} \end{aligned}$$

which yields by induction

$$\|U_1(n, q_1, t, s) - U_1(n, q_2, t, s)\|_{H^\sigma \rightarrow H^{\sigma-1}} \leq C e^{C\|\dot{q}\|_{L^1}} |t - s| \|\dot{q}_1 - \dot{q}_2\|_{L^\infty}.$$

By letting n go to ∞ , we get

$$\|U_1(q_1, t, s) - U_1(q_2, t, s)\|_{H^\sigma \rightarrow H^{\sigma-1}} \leq C e^{C\|\dot{q}\|_{L^1}} |t - s| \|\dot{q}_1 - \dot{q}_2\|_{L^\infty}. \quad (2.23)$$

What is more, we have $U_q(t, s) = I_q(t)^{-1} U_1(q, t, s) I_q(s)$ and $I(t)$ is an isometry of H^σ , and satisfies

$$\|I_{q_1}(t) - I_{q_2}(t)\|_{H^\sigma \rightarrow H^{\sigma-1}} \lesssim |q_1(t) - q_2(t)| \leq T \|\dot{q}_1 - \dot{q}_2\|_{L^\infty}.$$

Indeed, let $u \in H^\sigma$, $v \in H^{1-\sigma}$ and define $F_q := \int \bar{v} I_q(t) u$. We have $\nabla_q F = \int \bar{v} I_q(t) \nabla u$, from which we get $|\nabla_q F| \leq \|v\|_{H^{1-\sigma}} \|u\|_{H^\sigma}$. And thus

$$|\langle v, I_{q_1}(t)u - I_{q_2}(t)u \rangle| \leq |F_{q_1} - F_{q_2}| \leq |q_1(t) - q_2(t)| \|v\|_{H^{1-\sigma}} \|u\|_{H^\sigma}.$$

We get

$$\|I_{q_1}(t) - I_{q_2}(t)\|_{H^\sigma \rightarrow H^{\sigma-1}} \lesssim |q_1(t) - q_2(t)| \leq T \|\dot{q}_1 - \dot{q}_2\|_{L^\infty}.$$

We finally get

$$\|U_{q_1}(t, s) - U_{q_2}(t, s)\|_{H^\sigma \rightarrow H^{\sigma-1}} \leq C e^{C\|\dot{q}\|_{L^1} T} \|\dot{q}_1 - \dot{q}_2\|_{L^\infty}.$$

□

Therefore, putting together Proposition 2.7 and 2.8 we obtain the proof of Theorem 1.1 in the case of a single nucleus.

2.2 Several nuclei

We now present the necessary modifications to deal with the case of several moving nuclei, i.e. when the potential V takes the form

$$V(x, t) = - \sum_{k=1}^N \frac{Z_k}{|x - q_k(t)|}, \quad q_k(0) = a_k,$$

where the a_k satisfy

$$\min\{|a_k - a_l| \mid k \neq l\} = 8\varepsilon_0 > 0.$$

To ensure that at every time $t \in [0, T]$ we have

$$\min\{|q_k(t) - q_l(t)| \mid k \neq l\} = 4\varepsilon_0 > 0,$$

we require for all k that

$$T \sup_t |\dot{q}_k(t)| \leq 2\varepsilon_0.$$

The idea is to adapt the strategy developed for a single nucleus by introducing suitable cutoffs in order to deal with each singularity simultaneously and without mutual interference. This means that instead of doing the change of variable, $x \leftarrow x + q(t)$ as in the single nucleus case, we do the change $x \leftarrow x + q_k(t) - a_k$ but only around the singularity $q_k(t)$. Since $q_k(t)$ and a_k are close (at least for small times), we can do it only around a_k .

We are inspired by a similar strategy used by Kato and Yajima in [26], who define a "local pseudo-Lorentz" transformation mapping retarded Lienard-Wiechert potentials to Coulomb potentials at fixed positions. To define this change of variable, we introduce a symmetric, real valued cut-off function $\zeta(x) = \zeta(|x|)$ (with a slight abuse of notation we will denote with ζ both the function and its radial component) having the following properties:

- $\zeta(|x|) \in C^\infty(\mathbb{R}^+)$;
- $\zeta(|x|) = 1$ for $|x| \leq 1$;
- $\zeta(|x|) = 0$ for $|x| \geq 2$;
- $\zeta(|x|) \in [0, 1]$;
- $\zeta'(|x|) \leq 3/2$.

In view of constructing our simultaneous "nuclei-freezing" transformation, we introduce for each $k = 1, \dots, N$ the functions

$$\phi^k(t, x) = x + \mathcal{T}_{q_k, \zeta}(x, t) \quad (2.24)$$

where we are denoting with

$$\mathcal{T}_{q_k, \zeta}(x, t) = \zeta\left(\frac{x - a_k}{\varepsilon_0}\right) (q_k(t) - a_k).$$

We write

$$\phi(t, x) = x + \sum_k \mathcal{T}_{q_k, \zeta}(x, t)$$

and

$$\Phi(t) : u \mapsto u(t, \phi(t, x)).$$

Note that here $\Phi(t)$ replaces the $I(t)$ defined by (2.19). We also remark that from now on, constants may not only depend on $(Z_k)_k$ but also on ε_0 but in any case, they do not depend on T .

Lemma 2.10. *There exist constants C and M_0 such that for all $t \in [0, T]$, $T \sup_k \|\dot{q}_k\|_{L^\infty} \leq M_0$ and all $u \in L^2$,*

$$\frac{1}{C} \|u\|_{L^2} \leq \|\Phi(t)u\|_{L^2} \leq C \|u\|_{L^2}.$$

Proof. By performing the change of variable $x \leftarrow \phi(t, x)$, we get

$$\|\Phi(t)u\|_{L^2} = \|\text{jac}(\phi(t))^{-1/2}u\|_{L^2},$$

where $\text{jac}(\phi(t)) = |\det \text{Jac}(\phi(t))|$ and $\text{Jac}(\phi(t))$ is the Jacobian matrix associated to ϕ .

Given that

$$\partial_j \phi(t, x) = e_j + \sum_k \zeta' \left(\left| \frac{x - a_k}{\varepsilon_0} \right| \right) \frac{x_j - a_{k,j}}{\varepsilon_0 |x - a_k|} (q_k(t) - a_k)$$

where e_j is the j -th vector of the canonical basis of \mathbb{R}^3 , and $a_{k,j}$ is the j -th coordinate of a_k , and given that the supports of $x \mapsto \zeta' \left(\left| \frac{x - a_k}{\varepsilon_0} \right| \right)$ are disjoint and away from a_k , we get that

$$|\partial_j \phi(t, x) - e_j| \leq \frac{3}{2} T \sup_k \|\dot{q}_k\|_{L^\infty} \frac{1}{\varepsilon_0}$$

and thus that

$$|\text{Jac}(\phi(t)) - I_3| \lesssim T \sup_k \|\dot{q}_k\|_{L^\infty}.$$

Therefore there exists M_0 such that for all $T \sup_k \|\dot{q}_k\|_{L^\infty} \leq M_0$, $x \mapsto \phi(t, x)$ is a bijection and such that for all $t \in [0, T]$,

$$|\text{jac}(\phi(t))^{1/2} - 1| \lesssim T \sup_k \|\dot{q}_k\|_{L^\infty} \quad \text{and} \quad |\text{jac}(\phi(t))^{-1/2} - 1| \lesssim T \sup_k \|\dot{q}_k\|_{L^\infty}$$

which ensures the lemma. \square

Lemma 2.11. *There exist M_0 and C such that for all $T \sup_k \|\dot{q}_k\|_{L^\infty} \leq M_0$ all $u \in H^1$ and all $t \in [0, T]$, the following representations and estimates hold true*

$$\begin{aligned} \nabla(\Phi(t)u) &= (\nabla u) \circ \phi(t) + P_t(u) & \text{where} & \quad \|P_t\|_{H^1 \rightarrow L^2} \lesssim T \sup_k \|\dot{q}_k\|_{L^\infty} \\ \nabla(\Phi(t)^{-1}u) &= (\nabla u) \circ \phi(t)^{-1} + Q_t(u) & \text{where} & \quad \|Q_t\|_{H^1 \rightarrow L^2} \lesssim T \sup_k \|\dot{q}_k\|_{L^\infty} \end{aligned}$$

and

$$\frac{1}{C} \|u\|_{H^1} \leq \|\Phi(t)u\|_{H^1} \leq C \|u\|_{H^1}, \quad \frac{1}{C} \|u\|_{H^2} \leq \|\Phi(t)u\|_{H^2} \leq C \|u\|_{H^2}.$$

Proof. We have

$$\nabla(\Phi(t)u) = \text{Jac}(\phi(t))(\nabla u) \circ \phi(t).$$

As $\text{Jac}(\phi(t))$ is a perturbation of the identity, we get

$$\nabla(\Phi(t)u) = (\nabla u) \circ \phi(t) + A(t, x)(\nabla u) \circ \phi(t),$$

where $A(t, x)$ is a matrix whose norm is uniformly bounded by $T \sup_k \|\dot{q}_k\|_{L^\infty}$. We have

$$\|A(t, x)(\nabla u) \circ \phi\|_{L^2} \lesssim T \sup_k \|\dot{q}_k\|_{L^\infty} \|(\nabla u) \circ \phi\|_{L^2}$$

and thanks to Lemma 2.10

$$\|A(t, x)(\nabla u) \circ \phi\|_{L^2} \lesssim T \sup_k \|\dot{q}_k\|_{L^\infty} \|u\|_{H^1}.$$

Hence,

$$P_t(u) = A(t, x)(\nabla u) \circ \phi(t) \tag{2.25}$$

satisfies the stated properties.

For the same reasons, we get

$$Q_t(u) = B(t, x)(\nabla u) \circ \phi(t)^{-1}$$

with $B(t, x) = \text{Jac}(\phi(t)^{-1}) - I_3$.

Since $\text{Jac}(\phi(t))$ is close to the identity, so is its inverse $\text{Jac}(\phi(t)^{-1})$ and thus $\|B(t, x)\| \lesssim T \sup_k \|\dot{q}_k\|_{L^\infty}$. This yields

$$\|Q_t(u)\|_{L^2} \lesssim T \sup_k \|\dot{q}_k\|_{L^\infty} \|\nabla u \circ \phi(t)^{-1}\|_{L^2}$$

and thanks to Lemma 2.10, we get that

$$\|Q_t(u)\|_{L^2} \lesssim T \sup_k \|\dot{q}_k\|_{L^\infty} \|u\|_{H^1}.$$

The equalities involving $\nabla(\Phi(t)u)$ and $\nabla(\Phi(t)^{-1}u)$ ensure the validity of inequalities for $\|\Phi(t)u\|_{H^1}$.

For H^2 , we have to compute $\Delta(\Phi(t)u)$. We have

$$\Delta(\Phi(t)u) = (\text{Jac}(\phi(t))\nabla) \cdot \nabla u \circ \phi(t) + \nabla \cdot P_t(u).$$

As $\text{Jac}(\phi(t))$ is a uniform perturbation of the identity, we have that $(\text{Jac}(\phi(t))\nabla) \cdot \nabla u \circ \phi(t)$ is a uniform perturbation of $(\Delta u) \circ \phi(t)$. Moreover, we have

$$\nabla \cdot P_t(u) = \text{Jac}(\phi(t)) \left((\nabla \cdot A(t, x)) \cdot \nabla u \circ \phi(t) + (A(t, x)\nabla) \cdot \nabla u \circ \phi(t) \right).$$

We have

$$\|(A(t, x)\nabla) \cdot \nabla u\|_{L^2} \lesssim T \sup_k \|\dot{q}_k\|_{L^\infty} \|u\|_{H^2}.$$

Besides, $\nabla \cdot A(t, x) = \Delta\phi(t)$, which gives

$$\nabla \cdot A(t, x) = \sum_k \left[\frac{2}{|x - a_k| \varepsilon_0} \zeta' \left(\frac{|x - a_k|}{\varepsilon_0} \right) + \frac{1}{\varepsilon_0^2} \zeta'' \left(\frac{|x - a_k|}{\varepsilon_0} \right) \right] (q_k(t) - a_k).$$

Assuming $\varepsilon_0 < 1$ and using that the supports of $\zeta' \left(\frac{|x-a_k|}{\varepsilon_0} \right)$ are outside a ball of center a_k and radius ε_0 , we get

$$\|(\nabla \cdot A(t, x)) \cdot \nabla u\|_{L^2} \lesssim T \sup_k \|\dot{q}_k\|_{L^\infty} \|u\|_{H^2}.$$

(We recall that the supports of $\zeta \left(\frac{|x-a_k|}{\varepsilon_0} \right)$ are disjoint.)

This ensures that

$$\|\Phi(t)u\|_{H^2} \leq C \|u\|_{H^2}$$

if $T \sup_k \|\dot{q}_k\|_{L^\infty}$ is small enough. The reverse inequality can be deduced in the same way. \square

The following result is the analogue of Lemma 2.1 in the multinuclear case.

Lemma 2.12. *If u satisfies $i\partial_t u = H(t)u$ then $v = \Phi(t)u$ satisfies $i\partial_t v = H_N(t)v$ with*

$$H_N(t)v = \mathcal{D}v + \beta v - \sum_k \frac{Z_k}{|x - a_k|} v \quad (2.26)$$

$$+ i\partial_t \phi(t, x) \cdot \left(\nabla v - P_t(\Phi(t)^{-1}v) \right) + \vec{\alpha} \cdot P_t(\Phi(t)^{-1}v) + R(t, x)v$$

where P_t is defined as in Lemma 2.11 (see also (2.25)),

$$R(t, x) = \sum_k Z_k \left(\frac{1}{|x - a_k|} - \frac{1}{|\phi(t, x) - q_k(t)|} \right).$$

and $\vec{\alpha}$ is the vector of the α_k matrices.

Proof. Straightforward computation. \square

In view of defining the two-parameter propagator and use Kato's theory as in the one nucleus case, we need the following

Proposition 2.13. *Assume that for all k , $|Z_k| < \frac{\sqrt{3}}{2}$. There exist C_1 , and C such that if the trajectories $q_k(t)$ are such that*

$$(1 + T) \sup_k \|\dot{q}_k(t)\|_{L^\infty} \leq C_1, \quad \sup_k \|\ddot{q}_k\|_{L^1([0, T])} < \infty, \quad (2.27)$$

then there exists $\delta \in \mathbb{R}_+$ such that for all $t \in [0, T]$,

$$-\delta \|u\|_{L^2}^2 + \frac{1}{C} \|u\|_{H^1}^2 \leq \|H_N(t)u\|_{L^2}^2 \leq C \|u\|_{H^1}^2$$

and

$$\|i\partial_t H_N(t)\|_{L^1([0,T], H^1 \rightarrow L^2)} \leq C \sup_k (\|\ddot{q}_k\|_{L^1} + T\|\dot{q}_k\|_{L^\infty}). \quad (2.28)$$

Moreover, for any $\sigma \in [1, \frac{3}{2})$, the operator $H_N(t)$ is bounded from H^σ into $H^{\sigma-1}$.

Proof. Thanks to the usual theory of essential self-adjointness of Dirac operators with Coulomb potentials, the proposition is already true for

$$\mathcal{D}v + \beta v - \sum_k \frac{Z_k}{|x - a_k|} v.$$

We estimate the other terms. We have

$$i\partial_t \phi(t, x) = \sum_k \zeta\left(\frac{|x - a_k|}{\varepsilon_0}\right) \dot{q}_k(t),$$

hence

$$\|i\partial_t \phi(t, x) \cdot (\nabla v - P_t(\Phi(t)^{-1}v))\|_{L^2} \lesssim \sum_k \sup_t |\dot{q}_k(t)| \|v\|_{H^1}.$$

We have

$$\|\vec{\alpha} \cdot P_t(\Phi(t)^{-1}v)\|_{L^2} \lesssim T \sup_k \|\dot{q}_k\|_{L^\infty} \|v\|_{H^1}.$$

Finally, since $\frac{1}{|x - a_k|} - \frac{1}{|\phi(t, x) - q_k(t)|}$ is supported outside the ball of center a_k and radius ε_0 , and given that outside this ball, $|\phi(t, x) - q_k(t)| \geq |x - a_k| - |q_k(t) - a_k|$ we have that for $T \sup_k \|\dot{q}_k\|_{L^\infty} \leq \frac{1}{2}$, $|\phi(t, x) - q_k(t)| \geq \frac{\varepsilon_0}{2}$. Therefore

$$\|R(t, x)\|_{L^\infty([0,T] \times \mathbb{R}^3)} \lesssim \varepsilon_0^{-1} \sum_k |Z_k|.$$

Therefore, assuming that the quantity $(1+T) \sup_k \|\dot{q}_k\|_{L^\infty}$ is small enough, we get that $H_N(t)$ satisfies

$$-\delta \|u\|_{L^2}^2 + \frac{1}{C} \|u\|_{H^1}^2 \leq \|H_N(t)u\|_{L^2}^2 \leq C \|u\|_{H^1}^2;$$

the L^2 norm appears in the term involving $R(t, x)$.

Computing the derivative of $H_N(t)$ yields

$$\partial_t H_N(t) = i\partial_t^2 \phi(t) \cdot (\nabla - P_t \circ \Phi(t)^{-1}) - i\partial_t \phi \cdot \partial_t P_t \circ \Phi(t)^{-1} + i\vec{\alpha} \cdot \partial_t P_t \circ \Phi(t) + \partial_t R(t, x).$$

We have $\|\partial_t^2 \phi\|_{L^1} \lesssim \sup_k \|\ddot{q}_k\|_{L^1}$ and $\|\nabla - P_t \circ \Phi(t)^{-1}\|_{L^\infty([0,T], H^1 \rightarrow L^2)} \leq C$ hence

$$\|i\partial_t^2 \phi(t) \cdot (\nabla - P_t \circ \Phi(t)^{-1})\|_{L^1([0,T], H^1 \rightarrow L^2)} \lesssim \sup_k \|\ddot{q}_k\|_{L^1}.$$

We have $|i\partial_t \phi| \lesssim \sup_{k,t} |\dot{q}_k(t)|$ and $P_t \circ \Phi(t)^{-1} = A(t, x) \text{Jac}(\Phi(t))^{-1} \nabla$. What is more,

$$T|\partial_t A| = T|\partial_t \text{Jac}(\phi(t))| \lesssim T \sup_k \|\dot{q}_k\|_{L^\infty}$$

and $\partial_t \text{Jac}(\Phi(t))^{-1} = -\text{Jac}(\Phi(t))^{-1} \partial_t A \text{Jac}(\Phi(t))^{-1}$, hence

$$\|\partial_t \phi\|_{L^2 \rightarrow L^2} \lesssim C_1 \text{ and } T\|\partial_t P_t \circ \Phi(t)^{-1}\|_{H^1 \rightarrow L^2} \lesssim T \sup_k \|\dot{q}_k\|_{L^\infty}.$$

This gives

$$T \sup_t \|i\partial_t \phi \cdot \partial_t P_t \circ \Phi(t)^{-1}\|_{H^1 \rightarrow L^2} \lesssim T \sup_k \|\dot{q}_k\|_{L^\infty} C_1$$

and

$$T \sup_t \|i\vec{\alpha} \cdot \partial_t P_t \circ \Phi(t)\|_{H^1 \rightarrow L^2} \lesssim T \sup_k \|\dot{q}_k\|_{L^\infty}.$$

Finally, as

$$\partial_t \left(\frac{1}{|x - a_k|} - \frac{1}{|\phi(t, x) - q_k(t)|} \right) = \frac{(\partial_t \phi - \dot{q}_k(t))(\phi - q_k)}{|\phi - q_k|^3}$$

and it is supported outside the ball of center a_k and radius ε_0 , we get

$$T \sup_t \|\partial_t R(t, x)\|_{H^1 \rightarrow L^2} \lesssim T \sup_k \|\dot{q}_k\|_{L^\infty},$$

which yields the result as $\|\cdot\|_{L^1([0,T])} \leq T\|\cdot\|_{L^\infty([0,T])}$. The last statement of the Theorem is proved when the remainders with respect to the multicenter Coulomb operator appearing in 2.26 are controlled. Multiplications by smooth decaying function are bounded operators in Sobolev spaces (see [4], in particular Thm 1.62) and moreover the term R can be bounded as in the proof of 2.10. This gives the result. \square

We are now in position of proving the main result of this subsection.

Proposition 2.14. *Let Z_k be such that $|Z_k| < \frac{\sqrt{3}}{2}$ for each k , and let $q_k(t)$ satisfy assumptions (2.27). Then the flow of the equation*

$$i\partial_t u = H(t)u$$

with $H(t)$ given by (1.3) is given by a family of operators $U(t, s) = U_q(t, s)$ satisfying

$$i\partial_t U_q(t, s) = H(t)U_q(t, s), \quad i\partial_s U_q(t, s) = -U_q(t, s)H(s)$$

and

$$U_q(t, s) \circ U_q(s, r) = U_q(t, r).$$

with

$$U_q \in \mathcal{C}([0, T]^2, \mathcal{L}(H^\sigma))$$

for any $\sigma \in [0, \frac{3}{2})$. In particular the norms

$$\|U_q(t, s)\|_{H^\sigma \rightarrow H^\sigma}$$

are uniformly bounded in t, s , and q .

Proof. As in the single nucleus case, this result is a consequence of Kato's theory and Proposition 2.13. We omit the details. \square

The following result is an ingredient needed for the continuity of the propagator U_q , that is forthcoming Proposition 2.16.

Proposition 2.15. *Let $q^{(1)} = (q_1^{(1)}, \dots, q_N^{(1)})$ and $q^{(2)} = (q_1^{(2)}, \dots, q_N^{(2)})$ be two vectors of $\mathcal{C}^2([0, T])$ satisfying assumptions (2.27). Let $H_{N,j}(t)$ (resp $\Phi_j(t)$) be the operator $H_N(t)$ (resp. $\Phi(t)$) associated to $q^{(j)}$. We assume that $q^{(1)}(0) = q^{(2)}(0) = (a_1, \dots, a_N)$. Then for all $t \in [0, T]$ and all $\sigma \in [1, \frac{3}{2})$,*

$$\|H_{N,1}(t) - H_{N,2}(t)\|_{H^\sigma \rightarrow H^{\sigma-1}} \leq C \sup_k (1+T) \|(\dot{q}_k^{(1)}) - (\dot{q}_k^{(2)})\|_{L^\infty}.$$

Proof. We have

$$\partial_j \phi_1(t, x) - \partial_j \phi_2(t, x) = \sum_k \zeta' \left(\left| \frac{x - a_k}{\varepsilon_0} \right| \right) \frac{x_j - a_{k,j}}{\varepsilon_0 |x - a_k|} (q_k^{(1)}(t) - q_k^{(2)}(t)).$$

Hence

$$|\text{Jac}(\phi_1) - \text{Jac}(\phi_2)| \leq \sup_{k,t} T |(\dot{q}_k^{(1)}) - (\dot{q}_k^{(2)})|.$$

This gives in particular

$$\|P_{t,1}(\Phi_1(t)^{-1}v) - P_{t,2}(\Phi_2(t)^{-1}v)\|_{L^2} \lesssim \sup_{k,t} T |(\dot{q}_k^{(1)}) - (\dot{q}_k^{(2)})| \|\nabla v\|_{L^2}$$

hence

$$\|P_{t,1}(\Phi_1(t)^{-1}) - P_{t,2}(\Phi_2(t)^{-1})\|_{H^\sigma \rightarrow H^{\sigma-1}} \lesssim \sup_{k,t} T |(\dot{q}_k^{(1)}) - (\dot{q}_k^{(2)})|.$$

We also have

$$|i\partial_t \phi_1 - i\partial_t \phi_2| \leq \sup_{k,t} |(\dot{q}_k^{(1)})(t) - (\dot{q}_k^{(2)})(t)|.$$

And finally,

$$R_1(t, x) - R_2(t, x) = \sum_k Z_k \left(\frac{1}{|\phi(t, x) - q_k^{(2)}(t)|} - \frac{1}{|\phi(t, x) - q_k^{(1)}(t)|} \right)$$

which yields

$$R_1(t, x) \leq C_Z \sup_{k,t} T |(\dot{q}_k^{(1)}) - (\dot{q}_k^{(2)})|.$$

This concludes the proof. \square

To conclude with, we prove the continuity of the propagator U_q with respect to q .

Proposition 2.16. *Let $q^{(1)} = (q_1^{(1)}, \dots, q_N^{(1)})$ and $q^{(2)} = (q_1^{(2)}, \dots, q_N^{(2)})$ be two vectors of $\mathcal{C}^2([0, T])$ satisfying assumptions (2.27). We assume that $q^{(1)}(0) = q^{(2)}(0) = (a_1, \dots, a_N)$. There exists C (independent from T and $q^{(1)}, q^{(2)}$) such that for all $t, s \in [0, T]^2$, we have for any $\sigma \in [1, \frac{3}{2})$,*

$$\|U_{q^{(1)}} - U_{q^{(2)}}\|_{H^\sigma \rightarrow H^{\sigma-1}} \leq C \sup_k (1 + T) \|(\dot{q}_k^{(1)}) - (\dot{q}_k^{(2)})\|_{L^\infty}$$

Proof. What we have to add with regard to the single nucleus case (i.e. Lemma 2.8), is that we also have

$$\|\Phi_1(t) - \Phi_2(t)\|_{H^\sigma \rightarrow H^{\sigma-1}} \lesssim \sup_k T \|(\dot{q}_k^{(1)}) - (\dot{q}_k^{(2)})\|_{L^\infty}.$$

such that we can bound the difference between the operators due to the different changes of variables. \square

Again, putting together Propositions 2.14 and 2.16 we obtain Theorem 1.1 in the multi-nuclei case, so its proof is concluded.

3 Local well-posedness of the electron-nuclei dynamics

This section is devoted to the proof of our main results, Theorem 1.2,1.3. In all this section, as stated in the hypotheses of the cited Theorems, we assume that the q_k satisfy the separation assumption and that $|Z_k| < \frac{\sqrt{3}}{2}$ for all k . In all the results, the constants may depend on Z_k and ε_0 .

3.1 Nonlinear estimates

In this subsection we collect some preliminary estimates that will be needed in the sequel; we will include some proofs for the sake of completeness. We start by recalling this classical version of generalized Hardy inequalities (see e.g. Theorem 2.57 in [4])

We now provide some standard estimates for the convolution term.

Lemma 3.1. *Let $u, v, w \in H^1$. Then the following estimates hold*

$$\|(uv * |x|^{-1})w\|_{L^2} \lesssim \|u\|_{L^2} \|v\|_{H^1} \|w\|_{L^2},$$

$$\|(uv * |x|^{-1})w\|_{H^1} \lesssim \|u\|_{H^1} \|v\|_{H^1} \|w\|_{H^1}.$$

Proof. The proof of the first inequality is a combination of Hölder's and Hardy's inequalities. Indeed,

$$\|(uv * |x|^{-1})w\|_{L^2} \leq \|(uv * |x|^{-1})\|_{L^\infty} \|w\|_{L^2}$$

and for all x

$$\left| \int (uv)(x-y)|y|^{-1} dy \right| \leq \|u_x\|_{L^2} \|v_x|y|^{-1}\|_{L^2}$$

where $u_x(y) = u(x-y)$. By a change of variable, $\|u_x\|_{L^2} = \|u\|_{L^2}$ and by Hardy's inequality $\|v_x|y|^{-1}\|_{L^2} \leq 4\|\nabla v_x\|_{L^2}$. Given that $\nabla v_x = -(\nabla v)_x$, we get the result.

For the second inequality, we write

$$\nabla((uv * |x|^{-1})w) = ((\nabla u)v * |x|^{-1})w + ((u\nabla v) * |x|^{-1})w + ((uv) * |x|^{-1})\nabla w.$$

By using the first inequality, we can estimate the L^2 norm of the right hand side as follows

$$\begin{aligned} \|((\nabla u)v * |x|^{-1})w\|_{L^2} &\leq \|\nabla u\|_{L^2} \|v\|_{\dot{H}^1} \|w\|_{L^2} \\ \|((u\nabla v) * |x|^{-1})w\|_{L^2} &\leq \|u\|_{\dot{H}^1} \|\nabla v\|_{L^2} \|w\|_{L^2} \\ \|((uv) * |x|^{-1})\nabla w\|_{L^2} &\leq \|u\|_{L^2} \|v\|_{\dot{H}^1} \|\nabla w\|_{L^2} \end{aligned}$$

which give the first estimate.

The estimate in the H^2 case can be obtained in the same way as above by using the Laplacian instead of the gradient. \square

In what follows we will also need the following fractional versions of the estimates above.

Lemma 3.2. *Let $s \in (0, 1/2)$ and $u, v, w \in H^{s+1}$. Then the following estimate holds*

$$\|(uv * |x|^{-1})w\|_{H^{s+1}} \leq \|u\|_{H^{s+1}} \|v\|_{H^{s+1}} \|w\|_{H^{s+1}}.$$

Remark 3.1. *As it will be clear from the proof, these estimates are not sharp, but we prefer to present them in this clear way as they will be enough for the scope of this paper.*

Proof. We start by the case $s \in (0, 1/2)$; we deal with the homogeneous Sobolev norm, as this is the problematic term. We write

$$\|(uv * |x|^{-1})w\|_{\dot{H}^{s+1}} = \|(\nabla(uv) * |x|^{-1})w\|_{\dot{H}^s} + \|(uv) * |x|^{-1} \nabla w\|_{\dot{H}^s}.$$

For $\|(uv) * |x|^{-1} \nabla w\|_{\dot{H}^s}$, we use Leibniz's inequalities to get

$$\|(uv) * |x|^{-1} \nabla w\|_{\dot{H}^s} \lesssim \|(uv) * |x|^{-1}\|_{W^{s,\infty}} \|\nabla w\|_{H^s},$$

Since $\|\nabla w\|_{H^s} \leq \|w\|_{H^{s+1}}$ and $\|(uv) * |x|^{-1}\|_{W^{s,\infty}} \leq \|(uv) * |x|^{-1}\|_{W^{1,\infty}}$ and since we have already proved

$$\|(uv) * |x|^{-1}\|_{W^{1,\infty}} \lesssim \|u\|_{H^1} \|v\|_{H^1}$$

in the previous lemma, we get

$$\|(uv) * |x|^{-1} \nabla w\|_{\dot{H}^s} \lesssim \|u\|_{H^{s+1}} \|v\|_{H^{s+1}} \|w\|_{H^{s+1}}.$$

For $\|(\nabla(uv) * |x|^{-1})w\|_{\dot{H}^s}$, we deal with one of the two terms appearing after using Leibniz rule on the gradient, the other one being analogous: we have, setting $G = (\nabla u)v * |x|^{-1}$

$$\begin{aligned} \|Gw\|_{\dot{H}^s}^2 &= \int_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{|G(x)w(x) - G(y)w(y)|^2}{|x - y|^{3+2s}} dx dy \leq \\ &\int_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{|G(x) - G(y)|^2 |w(x)|^2}{|x - y|^{3+2s}} dx dy + \int_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{|G(y)|^2 |w(x) - w(y)|^2}{|x - y|^{3+2s}} dx dy = I + II. \end{aligned}$$

The term II can be directly dealt with by estimating as

$$II \lesssim \|G\|_{L^\infty}^2 \|w\|_{\dot{H}^{s+1}}^2$$

and $\|G\|_{L^\infty}$ has been dealt with in the previous Lemma. For the term I we write instead

$$I = \int_{\mathbb{R}^3} dx \int_{|x-y| \geq 1} \frac{|G(x) - G(y)|^2 |w(x)|^2}{|x-y|^{3+2s}} dy + \int_{\mathbb{R}^3} dx \int_{|x-y| < 1} \frac{|G(x) - G(y)|^2 |w(x)|^2}{|x-y|^{3+2s}} dy = I_1 + I_2.$$

For the term I_1 we get

$$I_1 \leq \int_{\mathbb{R}^3} dx |w(x)|^2 \int_{|x-y| \geq 1} \frac{2\|G\|_{L^\infty}^2}{|x-y|^{3+2s}} \lesssim \|G\|_{L^\infty}^2 \|w\|_{L^2}^2.$$

as, since $3+2s > 3$, which is the dimension, the term $|x-y|^{-3-2s}$ is integrable in the region $|x-y| \geq 1$. For the term I_2 we write

$$I_2 = \int_{\mathbb{R}^3} dx |w(x)|^2 \int_{|x-y| < 1} \frac{dy}{|x-y|^{3+2s}} \left| \int_{\mathbb{R}^3} (\nabla u(z)) v(z) (|x-z|^{-1} - |y-z|^{-1}) dz \right|^2$$

Notice that one has the estimate, for any $s \in (0, 1/2)$,

$$(|x-z|^{-1} - |y-z|^{-1}) \lesssim \frac{|x-y|^{2s}}{|x-z|^{1+2s}} + \frac{|x-y|^{2s}}{|y-z|^{1+2s}}.$$

If $|x-z| \leq |y-z|$, this can be obtained by interpolating the obvious inequality $|(|x-z|^{-1} - |y-z|^{-1})| \leq |x-z|^{-1}$ with the inequality

$$(|x-z|^{-1} - |y-z|^{-1}) \leq \frac{|y-x|}{|x-z|^2}.$$

This is due to

$$(|x-z|^{-1} - |y-z|^{-1}) = \frac{|z-y| - |x-z|}{|x-z||x-y|} \leq \frac{|y-x|}{|x-z|^2}$$

where we have only used triangle inequality. We deal with the case $|z-y| \leq |x-z|$ in the same way

Therefore, we have

$$\begin{aligned} I_2 &\lesssim \int_{\mathbb{R}^3} dx |w(x)|^2 \int_{|x-y| < 1} \frac{dy}{|x-y|^{3-2s}} \left(\left| \int_{\mathbb{R}^3} \frac{\nabla u(z)}{|x-z|^s} \frac{v(z)}{|x-z|^{1+s}} dz \right|^2 + \left| \int_{\mathbb{R}^3} \frac{\nabla u(z)}{|y-z|^s} \frac{v(z)}{|y-z|^{s+1}} dz \right|^2 \right) \\ &\lesssim \|u\|_{H^{1+s}}^2 \|v\|_{H^{1+s}}^2 \int_{\mathbb{R}^3} dx |w(x)|^2 \int_{|x-y| < 1} \frac{dy}{|x-y|^{3-2s}} \end{aligned}$$

where we have used again (2.3) with s and $1 + s < \frac{3}{2}$. As $s > 0$, the integral in dy is finite and then we eventually get

$$I_2 \lesssim \|u\|_{H^{s+1}}^2 \|v\|_{H^{s+1}}^2 \|w\|_{L^2}^2$$

and this concludes the proof in the first case. \square

3.2 Contraction for u with fixed q

In this subsection, we assume that C_1 is the constant defined in Proposition 2.7 and in Proposition 2.13. We begin by stating a well posedness result for the nonlinear Dirac equation in H^1 .

Proposition 3.3. *Let $\sigma \in [1, 3/2)$, and $R > 0$. There exists a constant C such that for all $u_0 \in H^\sigma$, and all q that satisfies*

$$\sup_{k,t} |\dot{q}_k(t)| \leq \frac{C_1}{2}, \quad \sup_k \|\ddot{q}_k\|_{L^1([0,1])} \leq R$$

the Cauchy problem

$$\begin{cases} i\partial_t u = (\mathcal{D} + \beta)u + \sum_{k=1}^N \frac{Z_k}{|x - q_k(t)|} u + (|x|^{-1} * |u|^2)u \\ u(0, x) = u_0(x) \end{cases}$$

is well posed in $\mathcal{C}([0, T], H^\sigma)$ for $T \leq \frac{1}{C\|u_0\|_{H^\sigma}^2}, 1$ with the additional condition, if $N > 1$, that $T \sup_k \|\dot{q}_k\|_{L^\infty} \leq \frac{C_1}{2}$. Let us denote the corresponding flow by $\Psi_q(t)$. Then $\Psi_q(t)$ is continuous in the initial datum: namely, for each $u_0, v_0 \in H^1$ we have

$$\|\Psi_q(t)u_0 - \Psi_q(t)v_0\|_{\mathcal{C}([0,T], H^\sigma)} \leq C\|u_0 - v_0\|_{H^\sigma}.$$

Proof. Thanks to the assumptions on q and T in the several nuclei case ($T \sup_k \|\dot{q}_k\|_{L^\infty} \leq \frac{C_1}{2}$), the Cauchy problem admits the following Duhamel formulation for $t < T$:

$$u = U_q(t, 0)u_0 - i \int_0^t U_q(t, \tau)(|x|^{-1} * |u|^2 u) d\tau.$$

Let

$$A_q(u) = U_q(t, 0)u_0 - i \int_0^t U_q(t, \tau)(|x|^{-1} * |u|^2 u) d\tau.$$

We prove that A_q admits a fixed point by a contraction argument.

Thanks to the continuity of U_q on H^σ (see Proposition 2.14) we have

$$\|A_q(u)\|_{\mathcal{C}([0,T],H^\sigma)} \leq C\|u_0\|_{H^\sigma} + CT\|(|x|^{-1} * |u|^2)u\|_{\mathcal{C}([0,T],H^\sigma)}.$$

And thanks to the bilinear estimates of Lemma 3.2

$$\|A_q(u)\|_{\mathcal{C}([0,T],H^\sigma)} \leq C\|u_0\|_{H^\sigma} + CT\|u\|_{\mathcal{C}([0,T],H^\sigma)}^3.$$

Therefore, the ball of $\mathcal{C}([0,T],H^\sigma)$ of center 0 and radius $2C\|u_0\|_{H^\sigma}^2$ is stable under A_q for $T \leq \frac{1}{C\|u_0\|_{H^\sigma}^2}$.

What is more,

$$\|A_q(u) - A_q(v)\|_{\mathcal{C}([0,T],H^\sigma)} \leq CT\|(|x|^{-1} * |u|^2)u - (|x|^{-1} * |v|^2)v\|_{\mathcal{C}([0,T],H^\sigma)}$$

and

$$(|x|^{-1} * |u|^2)u - (|x|^{-1} * |v|^2)v = (|x|^{-1} * |u|^2)(u-v) + v|x|^{-1} * (\operatorname{Re}\langle u+v, u-v \rangle).$$

Hence, thanks to Lemma 3.1, we get that for u, v in the ball of $\mathcal{C}([0,T],H^\sigma)$ of center 0 and radius $2C\|u_0\|_{H^\sigma}^2$,

$$\|A_q(u) - A_q(v)\|_{\mathcal{C}([0,T],H^\sigma)} \leq C_2T\|u_0\|_{H^\sigma}^2\|u - v\|_{\mathcal{C}([0,T],H^\sigma)}$$

thus A_q is contracting for $T < \frac{1}{C_2\|u_0\|_{H^\sigma}^2}$, and this concludes the proof. \square

3.3 Further properties of Ψ_q

Proposition 3.4. *Let $\sigma \in [1, 3/2)$ and $R > 0$. There exists a constant C such that for all $u_0 \in H^\sigma$ and q as in the previous proposition, for $T \leq \frac{1}{C(1+\|u_0\|_{H^\sigma}^2)}$ the flow Ψ_q satisfies the following properties:*

(i)

$$\|\Psi_q(t)u_0\|_{\mathcal{C}([0,T],H^\sigma)} \leq C\|u_0\|_{H^\sigma}.$$

(ii) Ψ_q is Lipschitz-continuous in q , namely

$$\|\Psi_{q^{(1)}}(t)u_0 - \Psi_{q^{(2)}}(t)u_0\|_{\mathcal{C}([0,T],H^{\sigma-1})} \leq CT\|u_0\|_{H^\sigma} \sup_{k,t} |\dot{q}_k^{(1)}(t) - \dot{q}_k^{(2)}(t)|.$$

Proof. The property (i) is a consequence of the contraction argument made in the proof of the previous proposition.

For (ii), write $u_j = \Psi_{q^{(j)}}(t)u_0$, $j = 1, 2$. Since u_j is the fixed point of $A_{q^{(j)}}$ we get

$$u_1 - u_2 = A_{q^{(1)}}(u_1) - A_{q^{(2)}}(u_2) = I + II + III$$

with

$$\begin{aligned}
I &= U_{q^{(1)}}(t, 0)(u_0) - U_{q^{(2)}}(t, 0)(u_0) \\
II &= -i \int_0^t (U_{q^{(1)}}(t, \tau) - U_{q^{(2)}}(t, \tau)) (|x|^{-1} * |u_1(\tau)|^2) u_1(\tau) d\tau \\
III &= -i \int_0^t U_{q^{(2)}}(t, \tau) \left((|x|^{-1} * |u_1(\tau)|^2) u_1(\tau) - (|x|^{-1} * |u_2(\tau)|^2) u_2(\tau) \right) d\tau.
\end{aligned}$$

From Corollary 2.16, we have

$$\|U_{q^{(1)}}(t, \tau) - U_{q^{(2)}}(t, \tau)\|_{H^\sigma \rightarrow H^{\sigma-1}} \leq C \sup_k T \|(\dot{q}_k^{(1)}) - (\dot{q}_k^{(2)})\|_{L^\infty}.$$

Therefore, we get

$$\|I\|_{C([0, T], H^\sigma)} \leq C \sup_{k, t} T |(\dot{q}_k^{(1)}) - (\dot{q}_k^{(2)})| \|u_0\|_{H^{\sigma+1}}$$

and

$$\|II\|_{C([0, T], H^\sigma)} \leq C \sup_{k, t} T |(\dot{q}_k^{(1)}) - (\dot{q}_k^{(2)})| \|(|x|^{-1} * |u_1|^2) u_1\|_{C([0, T], H^{\sigma+1})}.$$

Since

$$T \|(|x|^{-1} * |u_1|^2) u_1\|_{C([0, T], H^{\sigma+1})} \leq C' \|u_0\|_{H^{\sigma+1}},$$

we get

$$\|II\|_{C([0, T], H^1)} \leq C \sup_{k, t} T |(\dot{q}_k^{(1)}) - (\dot{q}_k^{(2)})| \|u_0\|_{H^{\sigma+1}}.$$

We have

$$III = A_{q^{(2)}}(u_1) - A_{q^{(2)}}(u_2)$$

and since $A_{q^{(2)}}$ is contracting, this yields the result. \square

Remark 3.2. *Actually, by exploiting some refined version of estimates in Lemma 3.2, the time of existence T could be made dependent only on the H^1 norm of the initial datum u_0 . Anyway, we prefer to keep the strongest assumption with the dependence on H^σ because this simplifies significantly the proof of the Lipschitz-continuity, that is point (ii) above.*

3.4 A Schauder fixed point for q

Let $t_0 \geq 0$, $(a_k)_k \in (\mathbb{R}^3)^N$ and $(b_k)_k \in (\mathbb{R}^3)^N$.

Assuming for the moment that it is well defined, we set $P(q)$ as the vector field such that $\dot{P}(q)_k = F(q)_k$ for every k and where

$$F(q)_k = -Z_k \langle \Psi_q(u_0) | \frac{q_k - x}{|q_k - x|^3} | \Psi_q(u_0) \rangle + \sum_{l \neq k} Z_k Z_l \frac{q_k - q_l}{|q_k - q_l|^3}$$

where the following initial values are given: $P(q)_k(t = t_0)_k = a_k$, $\dot{P}(q)_k(t = t_0)_k = b_k$.

Let $R > 0$ and

$$B = \{q \in \mathcal{C}^2([t_0, t_0 + T_1], (\mathbb{R}^3)^N) | T_1 \sup_k \|\dot{q}_k\|_{L^\infty} \leq \frac{C_1}{2}, \\ \|\dot{q}_k\|_{L^\infty} \leq \frac{C_1}{2}, \sup_k \|\ddot{q}_k\|_{L^1} \leq R, q_k(t_0) = a_k, \forall k \neq l, \forall t |q_k - q_l| > 4\varepsilon_0\}$$

where M_0, C_1 are the constants fixed by Proposition 2.13.

Proposition 3.5. *Assume $u_0 \in H^1$, $\sum_k |b_k| \leq \frac{C_1}{4}$ and for all $k \neq l$, $|a_k - a_l| \geq 8\varepsilon_0$. There exists C such that if $T_1 \leq \frac{1}{C\|u_0\|_{H^1}^2}$ for $N = 1$ and $T_1 \leq \frac{1}{C(1+\|u_0\|_{H^1}^2)}$ if $N \geq 2$, then B is stable under P .*

Proof. We have

$$\|F(q)_k\|_{L^\infty} \leq C|Z_k| \|\Psi_q(t)u_0\|_{H^1}^2 + C\varepsilon_0^{-2} \sum_{k \neq l} |Z_k Z_l|.$$

Hence

$$\|F(q)_k\|_{L^1} \leq T_1 C \left(\|u_0\|_{H^1}^2 + 1_{N \geq 2} \right).$$

This yields

$$\|\dot{P}(q)_k\|_{L^\infty} \leq |b_k| + T_1 C \left(\|u_0\|_{H^1}^2 + 1_{N \geq 2} \right)$$

hence for $T_1 \leq C_2 C^{-1} \left(\|u_0\|_{H^1}^2 + 1_{N \geq 2} \right)^{-1}$ and $T_1 \leq N^{-1} \frac{C_1}{4} C^{-1} \left(\|u_0\|_{H^1}^2 + 1_{N \geq 2} \right)^{-1}$, we have

$$\|F(q)_k\|_{L^1} \leq C_2$$

and

$$\|\dot{P}(q)_k\|_{L^\infty} \leq \frac{C_1}{2}.$$

For $N \geq 2$, we have

$$T_1 \|\dot{P}(q)_k\|_{L^\infty} \leq T_1 \frac{C_1}{2}$$

hence for $T_1 \leq 1$, we have

$$T_1 \|\dot{P}(q)_k\|_{L^\infty} \leq \frac{C_1}{2}.$$

Finally, for $k \neq l$, we have

$$|q_k - q_l| \geq |a_k - a_k| - |q_k - a_k| - |q_l - a_l|$$

and since $|q_l - a_l| \leq C_1 T_1$, we get that for $T_1 \leq \frac{2\varepsilon_0}{C_1}$,

$$|q_k - q_l| \geq 4\varepsilon_0.$$

Hence B is stable under P . \square

In the next proposition, we give the key properties of the map P , that is we prove that it is Hölder continuous if $u_0 \in H^\sigma$ for $\sigma \in (1, \frac{3}{2})$. The threshold is a consequence of the threshold for the validity of Hardy inequality (2.3), that will play a key role in the proof.

Proposition 3.6. *Let $q^{(j)} \in B$ for $j = 1, 2$. Then if $\sigma \in (1, 3/2)$ there exists C and $\tilde{T} \leq T_1$ with T_1 as in Proposition 3.5 such that for all $u_0 \in H^\sigma$ we have*

$$\sup_k \|P(q^{(1)})_k - P(q^{(2)})_k\|_{C^1([t_0, t_0 + \tilde{T}])} \leq C \tilde{T}^{2s} (1_{N \geq 2} + \|u_0\|_{H^\sigma}^2) \sup_k \|\dot{q}_k^{(1)} - \dot{q}_k^{(2)}\|_{L^\infty}^{2s-2}. \quad (3.1)$$

Proof. First of all we write

$$\begin{aligned} F(q^{(1)})_k - F(q^{(2)})_k &= -Z_k \langle \Psi_{q^{(1)}}(u_0) | \frac{q_k^{(1)} - x}{|q_k^{(1)} - x|^3} | \Psi_{q^{(1)}}(u_0) \rangle \\ &\quad + Z_k \langle \Psi_{q^{(2)}}(u_0) | \frac{q_k^{(2)} - x}{|q_k^{(2)} - x|^3} | \Psi_{q^{(2)}}(u_0) \rangle \\ &\quad + 2 \sum_{k \neq l} Z_k Z_l \left(\frac{q_k^{(1)} - q_l^{(1)}}{|q_k^{(1)} - q_l^{(1)}|^3} - \frac{q_k^{(2)} - q_l^{(2)}}{|q_k^{(2)} - q_l^{(2)}|^3} \right). \end{aligned}$$

Notice that, since $|q_k^{(j)} - q_l^{(j)}| \geq 2\varepsilon_0$, we have

$$\left| \frac{q_k^{(1)} - q_l^{(1)}}{|q_k^{(1)} - q_l^{(1)}|^3} - \frac{q_k^{(2)} - q_l^{(2)}}{|q_k^{(2)} - q_l^{(2)}|^3} \right| \lesssim \varepsilon_0^{-3} (|q_k^{(1)} - q_k^{(2)}| + |q_l^{(1)} - q_l^{(2)}|),$$

so that we get

$$2 \sum_{k \neq l} Z_k Z_l \left(\frac{q_k^{(1)} - q_l^{(1)}}{|q_k^{(1)} - q_l^{(1)}|^3} - \frac{q_k^{(2)} - q_l^{(2)}}{|q_k^{(2)} - q_l^{(2)}|^3} \right) \leq C \sum_{k \neq l} |Z_k Z_l| T \varepsilon_0^{-3} \sup_k \|\dot{q}_k^{(1)} - \dot{q}_k^{(2)}\|_{L^\infty}.$$

For the other part of the difference, we have

$$\langle \Psi_{q^{(1)}}(u_0) | \frac{q_k^{(1)} - x}{|q_k^{(1)} - x|^3} | \Psi_{q^{(1)}}(u_0) \rangle - \langle \Psi_{q^{(2)}}(u_0) | \frac{q_k^{(2)} - x}{|q_k^{(2)} - x|^3} | \Psi_{q^{(2)}}(u_0) \rangle = I + II + III$$

with

$$\begin{aligned} I &= \langle \Psi_{q^{(1)}}(u_0) - \Psi_{q^{(2)}}(u_0) | \frac{q_k^{(1)} - x}{|q_k^{(1)} - x|^3} | \Psi_{q^{(1)}}(u_0) \rangle \\ II &= \langle \Psi_{q^{(2)}}(u_0) | \left(\frac{q_k^{(1)} - x}{|q_k^{(1)} - x|^3} - \frac{q_k^{(2)} - x}{|q_k^{(2)} - x|^3} \right) | \Psi_{q^{(1)}}(u_0) \rangle \\ III &= \langle \Psi_{q^{(2)}}(u_0) | \frac{q_k^{(2)} - x}{|q_k^{(2)} - x|^3} | \left(\Psi_{q^{(1)}}(u_0) - \Psi_{q^{(2)}}(u_0) \right) \rangle \end{aligned}$$

We deal with the three terms separately. For the term I (and in fact III) we can write, with $a \in (0, 1)$, and $b \in \mathbb{R}$

$$\begin{aligned} |I| &\leq \int_{\mathbb{R}^3} \frac{|\Psi_{q^{(1)}}(u_0) - \Psi_{q^{(2)}}(u_0)| |\Psi_{q^{(1)}}(u_0)|}{|q_k^{(1)} - x|^2} \\ &= \int_{\mathbb{R}^3} \frac{|\Psi_{q^{(1)}}(u_0)| |\Psi_{q^{(1)}}(u_0) - \Psi_{q^{(2)}}(u_0)|^a |\Psi_{q^{(1)}}(u_0) - \Psi_{q^{(2)}}(u_0)|^{1-a}}{|q_k^{(1)} - x|^\sigma |q_k^{(1)} - x|^b |q_k^{(1)} - x|^{2-\sigma-b}} \end{aligned}$$

and by Hölder's inequality,

$$|I| \leq C \left\| \frac{\Psi_{q^{(1)}}(u_0)}{|q_k^{(1)} - x|^\sigma} \right\|_{L^2} \left\| \frac{(\Psi_{q^{(1)}}(u_0) - \Psi_{q^{(2)}}(u_0))^a}{|q_k^{(1)} - x|^b} \right\|_{L^{2/a}} \left\| \frac{(\Psi_{q^{(1)}}(u_0) - \Psi_{q^{(2)}}(u_0))^{1-a}}{|q_k^{(1)} - x|^{2-\sigma-b}} \right\|_{L^{2/(1-a)}},$$

which identifies as

$$|I| \leq C \left\| \frac{\Psi_{q^{(1)}}(u_0)}{|q_k^{(1)} - x|^\sigma} \right\|_{L^2} \left\| \frac{(\Psi_{q^{(1)}}(u_0) - \Psi_{q^{(2)}}(u_0))}{|q_k^{(1)} - x|^{b/a}} \right\|_{L^2}^a \left\| \frac{(\Psi_{q^{(1)}}(u_0) - \Psi_{q^{(2)}}(u_0))}{|q_k^{(1)} - x|^{(2-\sigma-b)/(1-a)}} \right\|_{L^2}^{1-a}.$$

To conclude we need

$$\begin{cases} \frac{b}{a} < \sigma - 1 \\ \frac{2-\sigma-b}{1-a} \leq \sigma. \end{cases}$$

Taking the equality in the last inequalities, we get $a = 2(\sigma - 1)$, and this justifies the condition $\sigma \in (1, 3/2) \Leftrightarrow a \in (0, 1)$, and $b = 2(\sigma - 1)^2$.

Therefore one gets, again by (2.3) with s and s_1 and Proposition 3.4,

$$|I| \lesssim \|\Psi_{q^{(1)}}(u_0)\|_{H^\sigma} (\|\Psi_{q^{(1)}}(u_0)\|_{H^\sigma} + \|\Psi_{q^{(2)}}(u_0)\|_{H^\sigma})^{1-a} \|\Psi_{q^{(1)}}(u_0) - \Psi_{q^{(2)}}(u_0)\|_{H^{\sigma-1}}^a$$

which ensures

$$|I| \lesssim \|u_0\|_{H^\sigma}^2 \tilde{T}^a \sup_k \|\dot{q}_k^{(1)} - \dot{q}_k^{(2)}\|_{L^\infty}.$$

To deal with the term II we have, for $\alpha \in (0, 1)$

$$\begin{aligned} |II| &\leq \int_{\mathbb{R}^3} |\Psi_{q^{(1)}}(u_0)| |\Psi_{q^{(2)}}(u_0)| \left(\frac{|q_k^{(1)} - q_k^{(2)}|^\alpha}{|q_k^{(1)} - x|^{2+\alpha}} + \frac{|q_k^{(1)} - q_k^{(2)}|^\alpha}{|q_k^{(1)} - x|^{2+\alpha}} \right) \\ &\leq C |q_k^{(1)} - q_k^{(2)}|^\alpha \left\| \frac{\Psi_{q^{(1)}}(u_0)}{|x|^{1+\alpha/2}} \right\|_{L^2} \left\| \frac{\Psi_{q^{(2)}}(u_0)}{|x|^{1+\alpha/2}} \right\|_{L^2} \\ &\leq C |q_k^{(1)} - q_k^{(2)}|^\alpha \|\Psi_{q^{(1)}}(u_0)\|_{H^{1+\alpha/2}} \|\Psi_{q^{(2)}}(u_0)\|_{H^{1+\alpha/2}} \\ &\leq C |q_k^{(1)} - q_k^{(2)}|^\alpha \|u_0\|_{H^{1+\alpha/2}}^2. \end{aligned}$$

Taking then $\alpha = 2\sigma - 2$ and using Proposition 3.4 we get in the end

$$|II| \leq C \|u_0\|_{H^\sigma}^2 \sup_k \|q_k^{(1)} - q_k^{(2)}\|_{L^\infty}^{2s-2} \leq CT \|u_0\|_{H^\sigma}^2 \sup_k \|\dot{q}_k^{(1)} - \dot{q}_k^{(2)}\|_{L^\infty}^{2s-2};$$

note that $(2\sigma - 2) \in (0, 1)$ for $\sigma \in (1, 3/2)$, so that we obtain the Hölderianity of this term, and the proof is concluded \square

As a consequence, we are able to prove the following result.

Proposition 3.7. *Let $\sigma \in [1, 3/2)$. There exists $C = C(m)$ such that for all (a_k) and (b_k) such that for all $l \neq k$, $|a_k - a_l| \geq 8\varepsilon_0$, $(b_k)_k \leq \frac{C_1}{4}$, for all $u_0 \in H^\sigma$, the system of equations*

$$m_k \ddot{q}_k = F(q)_k$$

with initial data $q_k(t=0) = a_k$ and $\dot{q}_k(t=0) = b_k$ admits a solution in $\mathcal{C}^2([0, T])$ for $T \leq \frac{1}{C(1_{N \geq 2} + \|u_0\|_{H^\sigma}^2)}$.

Proof. This is a Schauder fixed point argument for P in

$$B(0, T) = \{q \in \mathcal{C}^2([0, T], (\mathbb{R}^3)^N) \mid T \sup_k \|\dot{q}_k\|_{L^\infty} \leq M_0,$$

$$\sum_k \|\dot{q}_k\|_{L^\infty} \leq C_1, \sup_k \|\ddot{q}_k\|_{L^1} \leq R, q_k(0) = a_k, \forall k \neq l, \forall t |q_k - q_l| > 4\varepsilon_0\}$$

for the topology of $\mathcal{C}^1([0, T])$, as a consequence of Proposition 3.5 and (3.1) in Proposition 3.6

Note that $B(0, T)$ is compact in $\mathcal{C}^1([0, T])$ because of the boundedness of the \mathcal{C}^2 norm. □

4 Appendix: a remark on regularity of the ground state of Dirac-Coulomb Hamiltonian

Let us consider the Sobolev regularity of Dirac-Coulomb eigenstates when $Z < \sqrt{3}/2$.

In particular, we are interested in the ground state. Its generic component has the form (see [5, 21])

$$f(r) = \text{const} \times e^{-ar} r^{b-1} \quad (4.1)$$

where

$$a = Z, \quad b = \sqrt{1 - (\alpha Z)^2} \equiv \sqrt{1 - \nu^2}, \quad \nu \in (0, 1) \quad (4.2)$$

The Fourier transform of the above radial function satisfies

$$\hat{f}(k) = \frac{2}{\sqrt{2\pi}} \frac{1}{k} \int_0^\infty r f(r) \sin(kr) dr$$

The above integral is the Fourier sine-transform of $r f(r) = \text{const} \times e^{-ar} r^b$.

According to the Table of Integral Transforms I, *Bateman Manuscript Project*, formula 2.4 (7) pag 72 in [1], one has

$$\hat{f}(k) = \frac{2}{\sqrt{2\pi}} \frac{1}{k} \Gamma(b+1) (a^2 + k^2)^{-\frac{1}{2}(b+1)} \sin[(b+1) \tan^{-1}(\frac{k}{a})] \quad (4.3)$$

$$= \text{const} \times \frac{1}{k} (a^2 + k^2)^{-\frac{1}{2}(b+1)} \sin[(b+1) \tan^{-1}(\frac{k}{a})] \quad (4.4)$$

This is regular at the origin while the asymptotic behavior at infinity is given by

$$\hat{f} \sim k^{-(b+2)} \quad (4.5)$$

Now $f \in H^\sigma \iff |\hat{f}|^2 (1+k^2)^s$ is integrable in \mathbb{R}^3 , from which we get the condition $f \in H^\sigma \iff k^{(-2b-4)} (1+k^2)^s k^2$ is integrable at infinity, i.e.

$$2b + 2 - 2\sigma > 1 \quad \iff \quad \sqrt{1 - \nu^2} > s - \frac{1}{2} \quad (4.6)$$

This implies that

1. $f \in H^1 \quad \forall \nu \in (0, \frac{\sqrt{3}}{2})$
2. $f \notin H^{\frac{3}{2}}$ whatever $\nu \in (0, \frac{\sqrt{3}}{2})$
3. $f \in H^\sigma \quad \sigma = \sigma(\nu) = \frac{3}{2} - \epsilon$ with $\nu^2 < 2\epsilon - \epsilon^2$

So the regularity is better and better (but lower than $H^{3/2}$) with the decreasing of the charge Z .

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