Mixed regularity of N-body Schr̈odinger evolution equation and corresponding hyperbolic cross space approximation

Long Meng

MIXED REGULARITY OF N-BODY SCHRÖDINGER EVOLUTION EQUATION AND CORRESPONDING HYPERBOLIC CROSS SPACE APPROXIMATION

LONG MENG

ABSTRACT. In this paper, we give a mathematical analysis of a time-dependent N-body electronic system in molecular dynamics. We first prove a mixed regularity of the corresponding wavefunctions. Thanks to this mixed regularity, we rigorously justify a hyperbolic cross space approximation of the N-body electronic system. The complexity of this approximation is close to that of a two-electrons problem, thus breaking the curse of dimensionality.

1. INTRODUCTION

This paper is devoted to a mathematical study of a hyperbolic cross space approximation of the following time-dependent N-body electronic system in molecular dynamics:

$$\begin{cases} i\partial_t u(t,x) = H_N(t)u(t,x), \quad t \in [0,T] =: I_T,\ x = (x_1,\cdots,x_N) \in (\mathbb{R}^3)^N \\ u(0,x) = u_0(x) \end{cases} \tag{1.1}$$

with

$$H_N(t) = \sum_{j=1}^{N} -\frac{1}{2}\Delta_j - \sum_{j=1}^{N} V(t,x_j) + \sum_{1\leqslant j<k\leqslant N} W(x_j,x_k) \tag{1.2}$$

where

$$V(t,x_j) = -\sum_{\mu=1}^{M} \frac{Z_\mu}{|x_j - a_\mu(t)|}, \qquad W(x_j,x_k) = \frac{1}{|x_j - x_k|}.$$

Here $\Delta_j := \Delta_{x_j}$ is the Laplacian operator acting on variable x_j.

In physics and quantum chemistry, Eq. (1.1) is used to describe the quantum mechanical N-body problem in which the $N \in \mathbb{N}^+$ electrons and the $M \in \mathbb{N}^+$ nuclei with total charge $Z = \sum_{\mu=1}^{M} Z_\mu$ interact by Coulomb attraction and repulsion forces. The Hamiltonian (1.2) acts on wavefunctions with variables $x_1,\cdots,x_N \in \mathbb{R}^3$, representing the coordinates of the N electrons. Each moving nucleus μ with charge $Z_\mu \in \mathbb{N}^+$ is treated in this paper as an object in classical mechanics that is positioned at $a_\mu(t) \in \mathbb{R}^3$ at any time. This model can be used to study dynamical phenomena such as chemical reactions. An analogous setting for the time-dependent Hartree–Fock model coupled with classical nuclear dynamics can be found in [2].

In mathematics, this evolution Schrödinger equation (1.1) is well studied. When $H_N(t) = H_N(0)$ is independent of t, the Stone theorem guarantees the existence and uniqueness of the unitary group $U_0(t,s) = \exp(-i(t-s)H_N(0))$ such that for every $t,s \in \mathbb{R}$, we have $U_0(t,s)\big(H^2((\mathbb{R}^3)^N)\big) \subset H^2((\mathbb{R}^3)^N)$. When $H_N(t)$ is dependent on t, the problem (1.1) becomes much more delicate: By using the Duhamel formula and Strichartz' estimates, local-in-time existence and uniqueness of solutions in $C^0(I_T, H^2((\mathbb{R}^3)^N))$ has been proved in [12] for the one-body problem and in [13] for the N-body problem (with $T \lesssim (ZN+N^2)^{-2-}$).

In numerical analysis, this electronic configuration space $(\mathbb{R}^3)^N$ is typically high-dimensional for large $N \in \mathbb{N}^+$. Conventional discretizations of partial differential equations by finite differences or finite element methods scale exponentially with respect to the dimension of the configuration space. This is known as the *curse of dimensionality*. To overcome this problem, models such as the time-dependent Hartree–Fock model and the multiconfiguration Hartree–Fock model are used (see e.g., [3] and [1] for the mathematical study of these two models).

In this paper, we attack directly the N-body problem (1.1) by using hyperbolic cross space approximation. The complexity of our hyperbolic cross space approximation is close to that of a two-electron problem (see Remark 1.6), thus breaking the curse of dimensionality of (1.1). Our method is based on the study of a mixed regularity of solutions to (1.1) provided u_0 is regular enough and satisfies some antisymmetric property (due to Pauli's principle).

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1.1. **Mixed regularity and hyperbolic cross space approximation for eigenvalue problem.** For the eigenvalue problem associated with the time-independent operator $H_N(0)$:

$$H_N(0)u_* = \lambda u_* \qquad \text{with} \qquad \lambda < 0, \tag{1.3}$$

the curse of dimensionality can be overcome by using spare grid methods or the hyperbolic cross space approximation (see, e.g., [5] for its numerical implementation and [7, 9, 14–16] for its mathematical foundation). These results are based on the observation that the antisymmetry of the wavefunction u_* can improve its regularity. According to Pauli's principle, the antisymmetry of the wavefunction u_* is a natural physical property for fermions. In this paper, the antisymmetry is defined as in our previous work [9].

Definition 1.1 (Generalized antisymmetric function)**.** *Let $I \subset \{1, \cdots, N\}$. When $|I| > 1$, a wavefunction u is antisymmetric with respect to I if and only if, for any $j, k \in I$,*

$$u(P_{j,k}x) = -u(x),$$

where

$$P_{j,k}(\cdots, x_j, \cdots, x_k, \cdots) := (\cdots, x_k, \cdots, x_j, \cdots).$$

When $|I| = 1$ or $I = \varnothing$, every wavefunction u is antisymmetric with respect to I.

Due to Pauli's principle, the electronic wavefunction (with spin $\{\pm\frac{1}{2}\}$) satisfies the following property (see, e.g., [14, Section 1] for more details).

Proposition 1.2 (Antisymmetry of the electronic wavefunction)**.** *For any electronic wavefunction u and for any fixed spin state, we can find two sets I_1 and I_2 satisfying $I_1 \bigcap I_2 = \varnothing$ and $I_1 \bigcup I_2 = \{1, \cdots, N\}$ such that u is antisymmetric w.r.t. I_1 and I_2.*

In this paper, we assume the following.

Assumption 1.3. *The initial datum u_0 is antisymmetric w.r.t. I_1 and I_2, with I_1 and I_2 being given as in Proposition 1.2.*

Let $I \subset \{1, \cdots, N\}$. The mixed regularity is associated with the following fractional Laplacian operator:

$$\mathcal{L}_I = \prod_{j \in I} (1 - \Delta_j)^{1/2} \tag{1.4}$$

that is defined wit the help of Fourier transform (see Section 2.1). In particular, if $I = \varnothing$, we have $\mathcal{L}_I = \mathbb{1}$.

Relying on the antisymmetry of the wavefunction u_*, it is shown in [14, 15] that, any eigenfunction u_* antisymmetric w.r.t. I_1 and I_2 of problem (1.3) satisfies

$$\sum_{\ell=1,2} \|\mathcal{L}_{I_\ell} u_*\|^2_{H^1((\mathbb{R}^3)^N)} < +\infty. \tag{1.5}$$

The proof is based on Hardy-type inequalities for Coulomb systems (see (1.8) below with $I = I_\ell$, $\alpha_{I_\ell} = 1$ and $\beta_{I_\ell} = 0$ for $\ell = 1, 2$). Thanks to these Hardy-type inequalities, a hyperbolic cross space approximation of any eigenfunction of (1.3) and its convergence have been studied in [15].

Later, by using $r12$-methods and interpolation of Sobolev spaces, Kreusler and Yserentant [7] show that any eigenfunction u_* of problem (1.3) satisfies

$$\|\mathcal{L}^{\alpha}_{\{1,\cdots,N\}} u_*\|_{H^s((\mathbb{R}^3)^N)} < +\infty, \tag{1.6}$$

for $s = 0$ and $\alpha = 1$ or $s = 1$ and $\alpha < 3/4$. This regularity is independent of the antisymmetry of u_*, and the bound $3/4$ is the best possible: It can neither be reached nor surpassed except for the totally antisymmetric eigenfunctions (i.e., antisymmetric w.r.t. $\{1, \cdots, N\}$). However, lacking Hardy-type inequalities associated with this mixed regularity, they could not prove the convergence of the corresponding hyperbolic cross space approximation of eigenfunctions.

Recently, we proved a more general mixed regularity of (1.3) for u_* antisymmetric w.r.t. I_1 and I_2 (see [9]):

$$\sum_{\ell=1,2} \|\mathcal{L}^{\alpha_{I_\ell}}_{I_\ell} \mathcal{L}^{\beta_{I_\ell}}_{I^c_\ell} u_*\|^2_{H^1((\mathbb{R}^3)^N)} < +\infty. \tag{1.7}$$

Here $I^c = \{1, \cdots, N\} \backslash I$, $\alpha_I \in [0, 5/4), \beta_I \in [0, 3/4)$ and $\alpha_I + \beta_I < 3/2$. One can easily recover (1.5) by setting $\alpha_I = 1$ and $\beta = 0$, and (1.6) by setting $\alpha_I = \beta_I < \frac{3}{4}$. Compared with [14], our proof is based on a more delicate study of the relationship between the fractional Laplacian operator and Coulomb-type potentials: For $\alpha_I \in [0, 5/4)$, $\beta_I \in [0, 3/4)$ and $\alpha_I + \beta_I < 3/2$,

$$\left\| \mathcal{L}^{\alpha_I}_I \mathcal{L}^{\beta_I}_{I^c} \left[\sum_{j=1}^N V(0, x_j) + \sum_{1 \leqslant j < k \leqslant N} W(x_j, x_k) \right] u_* \right\|_{H^{-1}((\mathbb{R}^3)^N)} \leqslant \|\mathcal{L}^{\alpha_I}_I \mathcal{L}^{\beta_I}_{I^c} u_*\|_{L^2((\mathbb{R}^3)^N)}. \tag{1.8}$$

Based on the above inequality, new hyperbolic cross space approximations of eigenfunctions have been studied in [9]. Let

$$(\mathcal{P}_{\alpha,\beta}^{R,\Omega,\mathrm{eigen}}u)(x) := \int_{(\mathbb{R}^3)^N} \mathbb{1}_{\alpha,\beta}^{R,\Omega,\mathrm{eigen}}(\xi)\widehat{u}(\xi)e^{2\pi i\xi\cdot x}d\xi \tag{1.9}$$

where $\mathbb{1}_{\alpha,\beta}^{R,\Omega,\mathrm{eigen}}$ is the characteristic function of the hyperbolic cross space $\mathcal{D}_{\alpha,\beta}^{\mathrm{eigen}}(R,\Omega)$

$$\mathcal{D}_{\alpha,\beta}^{\mathrm{eigen}}(R,\Omega) := \left\{(\omega_1,\cdots,\omega_N)\in(\mathbb{R}^3)^N;\ \sum_{\ell=1,2}\prod_{i\in I_\ell}\left(1+\left|\frac{\omega_i}{\Omega}\right|^2\right)^{\alpha}\prod_{j\in I^c}\left(1+\left|\frac{\omega_j}{\Omega}\right|^2\right)^{\beta}\leqslant R^2\right\}. \tag{1.10}$$

Then there exists a constant C_{mix} independent of Z and N such that

- for any $\Omega \geqslant C_{\mathrm{mix}}\sqrt{N}\max\{Z,N\}$,
- for any $\alpha\in[0,5/4), \beta\in[0,3/4)$ and $\alpha+\beta<3/2$,

we have

$$\|u_* - \mathcal{P}_{\alpha,\beta}^{R,\Omega,\mathrm{eigen}}u_*\|_{L^2((\mathbb{R}^3)^N)} \leqslant \frac{2\sqrt{2}\pi e^{5/8}}{R}\|u_*\|_{L^2((\mathbb{R}^3)^N)} \tag{1.11}$$

(see [9, Theorem 2.5]). In particular, whenever we take any $\alpha=\beta<\frac{3}{4}$, this new hyperbolic cross space approximation does not rely on the antisymmetry of the wavefunction. Therefore, it also works for the bosonic N-body system where the wavefunction is no longer (partially) antisymmetric. In addition according to [16, Chp. 8], $|\mathcal{D}_{1,1}^{\mathrm{eigen}}(2^L,1)|\lesssim(2^L)^{1+}$. Then $|\mathcal{D}_{\alpha,\beta}^{\mathrm{eigen}}(2^L,1)|\lesssim(2^L)^{\frac{1+}{\min\{\alpha,\beta\}}}$. This implies that the rate of convergence in (1.11) for the case $\alpha_I=\beta_I\approx\frac{3}{4}$ does not deteriorate at all with the number of electrons: It behaves almost the same as with the expansion of a one-electron wavefunction.

1.2. **Mixed regularity and hyperbolic cross space approximation of** (1.1)**.** We first study a mixed regularity for the time-dependent problem (1.1) analogous to (1.5). Then, we consider a hyperbolic cross space approximation of (1.1). Here we justify the approximation of Eq. (1.1) rather than only the approximation of solutions as in (1.11).

1.2.1. *Mixed regularity.* As for (1.6), our mixed regularity is also associated with the operator $\mathcal{L}_I$. Our main result on mixed regularity (i.e., Theorem 2.6) states that under Assumption 1.3, for $p=3-$ and $T\lesssim(ZN+N^2)^{-2-}$ (see Remark 2.3), we have

$$\sum_{\ell=1,2}\|\mathcal{L}_{I_\ell}u\|_{L^\infty([0,T],L^2((\mathbb{R}^3)^N))}\leqslant\sum_{\ell=1,2}\|\mathcal{L}_{I_\ell}u\|_{X_{p,T}}\lesssim_p\sum_{\ell=1,2}\|\mathcal{L}_{I_\ell}u_0\|_{L^2((\mathbb{R}^3)^N)} \tag{1.12}$$

where $X_{p,T}$, defined in Section 2.2, is our functional space for the evolution problem (1.1).

Remark 1.4 (Regularity of the initial datum u_0)**.** *Under Assumption 1.3, the regularity $\mathcal{L}_{I_\ell}u_0\in L^2((\mathbb{R}^3)^N)$, $\ell=1,2$ is reasonable. For simplicity, we assume that u_0 is totally antisymmetric (i.e., antisymmetric w.r.t. $\{1,\cdots,N\}$). For models such as Hartree–Fock, the initial datum u_0 can be written as a Slater determinant $u(x)=\bigwedge_{j=1}^N\phi_j$ with $\phi_j\in H^1(\mathbb{R}^3)$. Then it is not difficult to see that for the Hartree–Fock initial datum, we have $\mathcal{L}_{\{1,\cdots,N\}}u_0\in L^2((\mathbb{R}^3)^N)$.*

Remark 1.5. *For the evolution problem* (1.1)*, we can not consider the fractional Laplacian operator $\mathcal{L}_I^{\alpha_I}\mathcal{L}_{I^c}^{\beta_I}$ as in* (1.7)*. In the proof of* (1.7)*, Eq.* (1.8) *is used, and the $H^{-1}((\mathbb{R}^3)^N)$ norm in the left-hand side plays an important role to balance the operator $\mathcal{L}_I^{\alpha_I}\mathcal{L}_{I^c}^{\beta_I}$. Here we rather show that for some $\theta>0$ and $2<p<6$,*

$$\|\mathcal{L}_IQu\|_{X_{p,T}}\leqslant CT^\theta\|\mathcal{L}_Iu\|_{X_{p,T}}$$

where Q is defined by (2.11) *(see the proof of Theorem 2.6 or Section 2.4.2 below).*

1.2.2. *Hyperbolic cross space approximation of* (1.1). With our mixed regularity in hand, we can now study the corresponding hyperbolic cross space approximation of (1.1) under Assumption 1.3.

Define by $\mathcal{D}_R$ the following hyperbolic cross space

$$\mathcal{D}_R=\left\{(\omega_1,\cdots,\omega_N)\in(\mathbb{R}^3)^N\ ;\ \sum_{\ell=1,2}\prod_{j\in\mathcal{I}_\ell}(1+|2\pi\omega_j|^2)^{1/2}\leqslant R\right\}. \tag{1.13}$$

Let $\chi_R:(\mathbb{R}^3)^N\to[0,1]$ be a function with values $\chi_R(\omega)=1$ for $\omega\in\mathcal{D}_R$. Then, we can define the following operator:

$$(P_{\chi_R}u)(x)=\left(\frac{1}{\sqrt{2\pi}}\right)^{3N}\int_{(\mathbb{R}^3)^N}\chi_R(\xi)\mathcal{F}_{x_1,\cdots,x_N}(u)(\xi)\exp(i2\pi\xi\cdot x)\,d\xi.$$

Here $\mathcal{F}_{x_1,\cdots,x_N}(u)$ is the Fourier transform for N electrons defined in Section 2.1.

In [15] and [9], only the error bound between the eigenfunctions to (1.3) and the hyperbolic cross space approximation of these eigenfunctions (i.e., (1.11)) has been considered. Compared with the result (1.11) for the eigenvalue problem (1.3), we can justify the following hyperbolic cross space approximation of (1.1):

$$\begin{cases} i\partial_t u_R = H_{N,R}(u_R), \quad t \in I_T, \\ u_R(0,x) = P_{\chi_R}(u_0)(x) \end{cases} \tag{1.14}$$

with

$$H_{N,R}(u) = \sum_{j=1}^{N} -\frac{1}{2}\triangle_j u - \sum_{j=1}^{N}\sum_{\mu=1}^{M} P_{\chi_R}(V(t,x_j)u) + \sum_{1\leqslant j<k\leqslant N} P_{\chi_R}(W(x_j,x_k)u).$$

Then our main result on the hyperbolic cross space approximation (i.e., Theorem 2.8) states that under Assumption 1.3, a solution u_R to (1.14) exists in $X_{p,\infty}$. Furthermore, for $p = 3-$ and $T \lesssim (ZN+N^2)^{-2-}$,

$$\|u-u_R\|_{L^\infty([0,T],L^2((\mathbb{R}^3)^N))} \leqslant \|u-u_R\|_{X_{p,T}} \lesssim_p \frac{1}{R}\sum_{\ell=1,2}\|\mathcal{L}_{I_\ell}u_0\|_{L^2((\mathbb{R}^3)^N)}. \tag{1.15}$$

Remark 1.6 (Complexity of (1.14))**.** *Notice that* $|\mathcal{D}_R| \lesssim |\mathcal{D}_{1,0}^{\text{eigen}}(R,1)|$. *Then according to [16], the complexity of our hyperbolic cross space approximation is close to that of a two-electron problem.*

Remark 1.7 (N-dependence of the initial datum u_0)**.** *In above estimate* (1.15)*, the error bound depends on* $\|\mathcal{L}_{I_\ell}u_0\|_{L^2((\mathbb{R}^3)^N)}$ *which is also an N-dependent quantity. In molecular dynamics, in many cases, we can assume that before the nuclei move (i.e., at $t=0$), the electrons are in a stable state (in the ground state). This means that u_0 is the first eigenfunction of* (1.3)*. According to [15, Theorem 9], with the scaling $x \to \frac{x}{|\Omega|}$ with Ω given as in* (1.11)*, we know that there exists $C>0$ such that for any $N \geqslant 1$,*

$$\sum_{\ell=1,2}\left\|\tau_\Omega^{-1}\mathcal{L}_{I_\ell}\tau_\Omega u_0\right\|_{L^2((\mathbb{R}^3)^N)} \leqslant C\|u_0\|_{L^2((\mathbb{R}^3)^N)},$$

where $\tau_\Omega u(\cdot) = |\Omega|^{\frac{3N}{2}}u(\frac{\cdot}{|\Omega|})$. *Thus the N-dependence of u_0 can be overcome if we replace the operator P_{χ_R} by $\tau_\Omega^{-1}P_{\chi_R}\tau_\Omega$. We refer to [5] for its numerical implementation.*

Remark 1.8 (Constraints on T)**.** *We shall point out that the constraint $T \lesssim (ZN+N^2)^{-2-}$ is due to mathematical techniques. This constraint is not relative to our mixed regularity: We have this constraint even for quantitative estimates of the existence of solutions (i.e.,* (2.7)*). Indeed, as the Hamiltonian* (1.2) *is not homogeneous, it is possible to overcome the constraint of T by using scaling.*

Remark 1.9 (Explanation of the construction of P_{χ_R}.)**.** *The operator P_{χ_R} can be regarded as a generalization of the projector $P_{\mathbb{1}_{\mathcal{D}_R}}$ where $\mathbb{1}_{\mathcal{D}_R}$ is the characteristic function of $\mathcal{D}_R$. For the eigenvalue problem* (1.3)*, it is easy to see that*

$$\|(1-P_{\chi_R})u_*\|_{L^2((\mathbb{R}^3)^N)} \leqslant \|(1-P_{\mathbb{1}_{\mathcal{D}_R}})u_*\|_{L^2((\mathbb{R}^3)^N)}.$$

However, concerning the evolution problem (1.1)*, there is no reason to assume that similar inequality holds true on our functional space $X_{p,T}$: for some $p, T > 0$,*

$$\|(1-P_{\chi_R})u\|_{X_{p,T}} \lesssim \|(1-P_{\mathbb{1}_{\mathcal{D}_R}})u\|_{X_{p,T}}.$$

As a result, if we use directly $P_{\mathbb{1}_{\mathcal{D}_R}}$, there is no reason to show that the numerical discretization such as wavelet basis discretization [5] can be considered. To avoid this issue, we have to consider a more general operator P_{χ_R} such that we can consider as many as possible numerical discretizations in this paper.

Organisation of this paper. This paper is organised as follows.

In Section 2, we first introduce our functional spaces, and then state our main results. To better understand our methods, we point out the main difficulties of the proofs and our strategies to handle them in Section 2.4.

Then in Section 3, we introduce the Strichartz estimates and some Sobolev inequalities on our functional spaces. Section 4 is devoted to the proof of the existence and mixed regularity of (1.1) (i.e., Theorems 2.5-2.6). Then in Section 5, we rigorously justify our approximation (1.14) (i.e., the proof of Theorem 2.8).

Finally in Appendix A, we adapt the Calderón-Zygmund inequality and the Mikhlin multiplier theorem to our functional spaces. This is the basis of the proof of our Sobolev inequalities.

2. Set-up and main results

In this section, we first introduce our notations and functional spaces. Then we state the main results. To better understand this paper and our method, we end this section by explaining the main difficulties and our strategies to handle them.

2.1. **Some notations.** To avoid ambiguity, we first clarify notations used in this paper.

We say $a \lesssim b$, it means that there exists a constant C independent of N and Z such that $a \leqslant Cb$. We say $a \lesssim_p b$, it means that there exists a constant $C(p)$ only dependent on p such that $a \leqslant C(p)b$. We shall point out that whenever we use $a \lesssim b$ (resp. $a \lesssim_p b$), the constant C (resp. $C(p)$) is always independent of N and Z.

Then we define our convention for the Fourier transform. Let $f \in L^2(\mathbb{R}^3)$ and $g \in L^2((\mathbb{R}^3)^N)$, then the Fourier transforms of f and g are respectively

$$\mathcal{F}_y(f)(\xi_y) := \int_{\mathbb{R}^3} f(y) e^{-2\pi i \xi_y \cdot y} dy,$$

and

$$\mathcal{F}_{x_1,\cdots,x_N}(g)(\xi) := \mathcal{F}_{x_N} \circ \cdots \circ \mathcal{F}_{x_1}(g)(\xi), \quad \xi := (\xi_1, \cdots, \xi_N) \text{ with } \xi_k \in \mathbb{R}^3,\ k = 1, \cdots, N.$$

The subscript y or x_j is used to indicate on which variable the Fourier transform acts.

For any $I \subset \{1, \cdots, N\}$, we define the operator

$$\mathcal{L}_I = \prod_{j \in I} (1 - \Delta_j)^{1/2}. \tag{2.1}$$

This operator is defined in the Fourier transform sense:

$$\mathcal{F}_{x_1,\cdots,x_N}(\mathcal{L}_I g)(\xi) := \prod_{j \in I} (1 + |2\pi \xi_i|^2)^{1/2} \mathcal{F}_{x_1,\cdots,x_N}(g)(\xi).$$

Finally, we also need to clarify some notations used in Strichartz estimates: for any $2 \leqslant p \leqslant 6$,

(1) p' is defined as follows

$$\frac{1}{p'} + \frac{1}{p} = 1; \tag{2.2}$$

(2) θ_p is define by

$$\frac{2}{\theta_p} = 3\left(\frac{1}{2} - \frac{1}{p}\right). \tag{2.3}$$

The pair (p, θ_p) is called Schrödinger admissible on $\mathbb{R}^3$. In particular, $(6, 2)$ is the endpoint Schrödinger admissible pair on $\mathbb{R}^3$. The notation θ_p' is also defined by (2.2).

2.2. **Functional spaces.** For the N-body problem (1.1), one of the main difficulties is the complexity of the functional space due to the singularity of the Coulomb potentials.

First of all, let $\mathcal{H} = L^2((\mathbb{R}^3)^N)$. For every set $I \subset \{1, \cdots, N\}$, we define the Hilbert space $\mathcal{H}_I := L^2_I((\mathbb{R}^3)^N)$ of the wavefunctions antisymmetric with respect to I by

$$\mathcal{H}_I := \{g \in \mathcal{H};\ u \text{ is antisymmetric with respect to } I\}. \tag{2.4}$$

Concerning mixed regularity, we also define

$$H^1_{I,\mathrm{mix}} := \{g \in \mathcal{H}_I;\ \mathcal{L}_I g \in \mathcal{H}\}$$

endowed with the norm

$$\|g\|_{H^1_{I,\mathrm{mix}}} := \|\mathcal{L}_I g\|_{\mathcal{H}}.$$

For two functional space A and B, we also need the functional space for bounded operators from A to B which is defined by the norm:

$$\|T\|_{\mathcal{B}(A,B)} := \sup_{\|u\|_A = 1} \|Tu\|_B.$$

If $B = A$, then we use the shorthand $\mathcal{B}(A) = \mathcal{B}(A, A)$.

Now we introduce our functional space for the evolution problem (1.1). Concerning the potential between electrons and nuclei $V(\cdot, x_j)$, we need the following functional space: For $1 < p < \infty$,

$$L^{p,2}_{x_j} = L^p(\mathbb{R}^3_{x_j}, L^2((\mathbb{R}^3)^{N-1}))$$

with the norm

$$\|g\|^p_{L^{p,2}_{x_j}} = \int_{\mathbb{R}^3_{x_j}} \left(\int_{(\mathbb{R}^3)^{N-1}} |g|^2 \, dx_1 \cdots \widehat{dx_j} \cdots dx_N \right)^{p/2} dx_j.$$

The notation $\widehat{dx_j}$ means that the integration over the j-th coordinate is omitted. We also use the shorthand $L^{p,2}_j$ for $L^{p,2}_{x_j}$.

Concerning the potential between electrons and electrons $W(x_j, x_k)$, to deal with the potential $W(x_j, x_k)$, we need first to change the variable: Let

$$r_{j,k} := \frac{1}{2}(x_j - x_k),\ R_{j,k} := \frac{1}{2}(x_j + x_k),$$

and let $\mathcal{R}_{j,k}$ be a unitary operator defined as follows

$$\begin{aligned}&\mathcal{R}_{j,k} g(r_{j,k}, R_{j,k}, x_1, \cdots, x_{j-1}, x_{j+1}, \cdots, x_{k-1}, x_{k+1}, \cdots, x_N)\\ &\quad = g(\cdots, x_{j-1}, (r_{j,k} + R_{j,k}), x_{j+1}, \cdots, x_{k-1}, (R_{j,k} - r_{j,k}), x_{k+1}, \cdots).\end{aligned} \tag{2.5}$$

Then, the functional space for $W(x_j, x_k)$ is defined by

$$L^{p,2}_{j,k} = L^p(\mathbb{R}^3_{r_{j,k}}, L^2((\mathbb{R}^3)^{N-1}))$$

with the norm

$$\|g\|^p_{L^{p,2}_{j,k}} = \int_{\mathbb{R}^3_{r_{j,k}}} \left(\int_{(\mathbb{R}^3)^{N-1}} |\mathcal{R}_{j,k} g|^2 \, dR_{j,k} dx_1 \cdots \widehat{dx_i} \cdots \widehat{dx_j} \cdots dx_N \right)^{p/2} dr_{j,k}.$$

Obviously,

$$\|g\|_{L^{p,2}_{j,k}} = \|\mathcal{R}_{j.k} g\|_{L^{p,2}_{r_{j,k}}}. \tag{2.6}$$

For future convenience, we will use the notation $L^{p,2}_D$ with $D \subset \{1, \cdots, N\}$ and $1 \leqslant |D| \leqslant 2$ to above functional space. More precisely, if $D = \{j\} \subset \{1, \cdots, N\}$, we have

$$L^{p,2}_D = L^{p,2}_j;$$

if $D = \{j, k\} \subset \{1, \cdots, N\}$, we have

$$L^{p,2}_D = L^{p,2}_{j,k}.$$

For the time-dependent problem (1.1), the full functional space that we use is the following: for some $p > 2$,

$$X_{p,T} = L^\infty_t(I_T, \mathcal{H}) \bigcap_{\substack{D \subset \{1, \cdots, N\}\\ 1 \leqslant |D| \leqslant 2}} L^{\theta_p}_t(I_T, L^{p,2}_D)$$

with the norm

$$\|u\|_{X_{p,T}} = \max \left\{ \|u\|_{L^\infty_t(I_T, \mathcal{H})}, \max_{\substack{D \subset \{1, \cdots, N\}\\ 1 \leqslant |D| \leqslant 2}} \|u\|_{L^{\theta_p}_t(I_T, L^{p,2}_D)} \right\}.$$

Remark 2.1 (Dual space)**.** *It is easy to see that for any $D \subset \{1, \cdots, N\}$ and $1 \leqslant |D| \leqslant 2$, the dual space of $L^{\theta_p}_t(I_T, L^{p,2}_D)$ is $L^{\theta'_p}_t(I_T, L^{p',2}_D)$.*

Concerning mixed regularity for the time-dependent problem (1.1), we also need the following functional space

$$X^1_{I,p,T} = \{u \in X_{p,T} \bigcap L^\infty_t(I_T, \mathcal{H}_I);\ \mathcal{L}_I u \in X_{p,T}\}$$

with the norm

$$\|u\|_{X^1_{I,p,T}} = \|\mathcal{L}_I u\|_{X_{p,T}}.$$

2.3. **Main results.** Now we can state our main results. Before going further, we need the following assumption.

Assumption 2.2. *Let α, $p > 0$ and $T > 0$ be chosen such that*

(1) $\frac{6}{3-2\alpha} < p < 6$ and $0 < \alpha < \frac{1}{2}$;
(2) $1/\theta_p < 1/\theta'_{\widetilde{p}}$ for some $\frac{6}{1+2\alpha} < \widetilde{p} < 6$;
(3) $C_{T,1}(Z+N)NT^{1/\theta'_{\widetilde{p}} - 1/\theta_p} < \frac{1}{2}$ with $C_T := \max\{C_{T,1}, C_{T,2}, C_{T,3}\} \geqslant 1$. Here $C_{T,1}$, $C_{T,2}$ and $C_{T,3}$ are constants only dependent on $\alpha, p, \widetilde{p}$ given by (4.12), (4.31) and (5.7) respectively.

Remark 2.3 (Nonemptiness of Assumption 2.2 and estimate on T)**.** *In Assumption 2.2, we can take $\alpha = \frac{1}{2}-$, $p = 3-$ and $\widetilde{p} = 3+$. Under this choice, $1/\theta'_{\widetilde{p}} - 1/\theta_p = \frac{1}{2}-$. Thus Assumption 2.2 is not empty and $T \lesssim (ZN + N^2)^{-2-}$.*

Remark 2.4 (Endpoint Schrödinger admissible)**.** *For Theorem 2.5 and Theorem 2.6 below, the condition* (1) *and* (2) *in Assumption 2.2 on $p, \widetilde{p}$ can be relaxed: One can reach $p = 6$ or $\widetilde{p} = 6$ for these two results. However, due to Corollary 3.5, $p = 6$ and $\widetilde{p} = 6$ is excluded for Theorem 2.8.*

Concerning the existence of solutions to (1.1), we have

Theorem 2.5 (Existence of solutions). *Let $a_\mu \in \mathcal{H}$. For every $u_0 \in \mathcal{H}$, the problem* (1.1) *has a unique global-in-time solution $u \in X_{p,\infty}$.*

Furthermore, under Assumption 2.2 on p and T, we have

$$\|u\|_{X_{p,T}} \lesssim_p \|u_0\|_{\mathcal{H}}. \tag{2.7}$$

Indeed, this result can be found in [13] in a more complicated setting. Here we modify the proof to make it compatible with Theorem 2.6 and Theorem 2.8 below. The details of its proof can be found in Section 4.1.

Concerning the mixed regularity of solutions to (1.1), we have

Theorem 2.6 (Mixed regularity). *Let $I \subset \{1, \cdots, N\}$. For every $u_0 \in H^1_{I,\mathrm{mix}}$, under Assumption 2.2, the problem* (1.1) *has a unique solution $u \in X^1_{I,p,T}$ and*

$$\|u\|_{X^1_{I,p,T}} \lesssim_p \|u_0\|_{H^1_{I,\mathrm{mix}}}. \tag{2.8}$$

The proof of Theorem 2.5 is provided in Section 4.2.

Remark 2.7. *Compared with Theorem 2.5, we do not know if $u \in X^1_{I,p,\infty}$. This is because that u satisfies the conservation law (i.e., $\|u(t)\|_{\mathcal{H}} = \|u_0\|_{\mathcal{H}}$ for any $t \in \mathbb{R}$) while $\mathcal{L}_I u$ does not.*

Finally, concerning the justification of the hyperbolic cross space approximation (1.14), we have

Theorem 2.8 (Justification of hyperbolic cross space approximation). *Let $a_\mu \in L^\infty(\mathbb{R})$, and I_1, I_2 be the set given as in Proposition 1.2. For every $u_0 \in H^1_{I_1,\mathrm{mix}} \bigcap H^1_{I_2,\mathrm{mix}}$, the problem* (1.14) *has a unique global-in-time solution $u_R \in X_{p,\infty}$*

Furthermore, under Assumption 2.2, we have

$$\|u - u_R\|_{X_{p,T}} \lesssim_p \frac{1}{R} \sum_{\ell=1,2} \|u_0\|_{H^1_{I_\ell,\mathrm{mix}}}. \tag{2.9}$$

This proof is provided in Section 5.

2.4. **Main difficulties and strategies.** Before giving the proof, to better understand this paper and our method, we shall explain the main difficulties and our strategies to handle them.

2.4.1. *Basic idea of the proof of Theorem 2.5.* We recall the free propagator $U_0(t) = \exp\{\frac{1}{2} it \sum_{j=1}^N \triangle\}$, and denote the integral operator S and Q respectively by

$$Su(t) := \int_0^t U_0(t-\tau)u(\tau)\, d\tau \tag{2.10}$$

and

$$Qu(t) := \sum_{j=1}^N S\Big(V(\cdot, x_j)u(\cdot, x)\Big)(t) + \sum_{1\leqslant j<k\leqslant N} S\Big(W(x_j, x_k)u(\cdot, x)\Big)(t). \tag{2.11}$$

By Duhamel's formula, solutions u to (1.1) satisfy

$$u(t) = U_0(t)u_0 - iQu(t). \tag{2.12}$$

As in [13], the basic idea for Theorem 2.5 is to show the invertibility of $1 + iQ$ on $X_{p,T}$ for T small enough. This follows from the fact that for some $\theta > 0$, $2 < p \leqslant 6$ and $0 < T < 1$,

$$\|Qu\|_{X_{p,T}} \leqslant CT^\theta \|u\|_{X_{p,T}}.$$

Then for $CT^\theta \leqslant \frac{1}{2}$, we have $\|Qu\|_{X_{p,T}} \leqslant \frac{1}{2}\|u\|_{X_{p,T}}$. Thus it is easy to see that $1 + iQ$ is invertible on $X_{p,T}$. Finally from (2.12), we infer that

$$u(t) = (1 + iQ)^{-1}U_0 u_0 \in X_{p,T}.$$

2.4.2. *Main difficulties and strategies for the proof of Theorem 2.6.* Concerning mixed regularity of the evolution equation (1.1), we use the same strategy as explained in Section 2.4.1: We are going to show that $1+iQ$ is invertible on $X^1_{I,p,T}$. The main difficulty of this paper is to show that

$$\|Qu\|_{X^1_{I,p,T}} \leqslant CT^\theta \|u\|_{X^1_{I,p,T}}.$$

Its proof is much more delicate than the one for the existence (i.e., Theorem 2.5).

Let

$$\mathcal{L}_{I,j} = \prod_{m\in I\setminus\{j\}} (1 - \Delta_j)^{1/2}, \qquad \mathcal{L}_{I,j,k} = \prod_{m\in I\setminus\{j,k\}} (1 - \Delta_j)^{1/2}. \tag{2.13}$$

In particular, if $j \notin I$, we have $I\backslash\{j\} = I$. Before going further, we first give a glimpse into $\mathcal{L}_I Qu$:

$$\begin{aligned}\mathcal{L}_I Qu = &\sum_{j=1}^{N} S\Big((1-\Delta_j)^{\gamma_j}\big[V(\cdot,x_j)\mathcal{L}_{I,j}u\big]\Big)(t)\\ &+\sum_{1\leqslant j<k\leqslant N} S\Big((1-\Delta_j)^{\gamma_j}(1-\Delta_k)^{\gamma_j}\big[W(x_j,x_k)\mathcal{L}_{I,j,k}u\big]\Big)(t),\end{aligned} \tag{2.14}$$

where $\gamma_j = 1/2$ if $j \in I$, otherwise $\gamma_j = 0$. It is not difficult to see that we have two main difficulties: The fractional Laplacian operator $(1-\Delta_j)^{1/2}$ on the functional space $L_D^{p,2}$, and the singularity of Coulomb-type potentials.

Operator $\mathcal{L}_I$ on $L_D^{p,2}$. For the eigenvalue problem (1.3), there is no problem: Thanks to the Plancherel theorem on Hilbert space $\mathcal{H}$, we have

$$\|\mathcal{L}_I v\|_{\mathcal{H}}^2 = \sum_{J\subset I}\Big\|\bigotimes_{j\in J}\nabla_j\, v\Big\|_{\mathcal{H}}^2.$$

For each ∇_j, we can use directly the Leibniz rule: $\nabla_y(f_1(y)f_2(y)) = f_2(y)\nabla_y f_1(y) + f_1(y)\nabla_y f_2(y)$. However, due to our functional space $L_D^{p,2}$, this identity no longer holds in our problem.

To overcome this problem, we use the fact that

$$(1-\Delta_j)^{1/2} = \frac{1}{(1-\Delta_j)^{1/2}} - \frac{\nabla_j}{(1-\Delta_j)^{1/2}}\cdot(\nabla_j). \tag{2.15}$$

It remains to study the operators $\frac{1}{(1-\Delta_j)^{1/2}}$ and $\frac{\nabla_j}{(1-\Delta_j)^{1/2}}$ on the functional space $L_D^{p,2}$ for some $p>0$, especially on $L_j^{p,2}$ and $L_{j,k}^{p,2}$. This can be studied by using the Calderón-Zygmund inequality and Mikhlin's multiplier theorem (see Appendix A). Theorem 3.6 shows that for any $1<p<\infty$,

$$\frac{1}{(1-\Delta_j)^{1/2}},\ \frac{\nabla_j}{(1-\Delta_j)^{1/2}} \in \mathcal{B}(L_D^{p,2}) \tag{2.16}$$

with $j \in D \subset \{1,\cdots,N\}$ and $1 \leqslant |D| \leqslant 2$.

Singularity of Coulomb-type potentials. With Eq. (2.16) in hand, in order to prove (2.14), it suffices to study the terms such as

$$S\Big(\nabla_j[V(\cdot,x_j)\mathcal{L}_{I,j}u]\Big)$$

and

$$S\Big(\nabla_j\otimes\nabla_k[W(x_j,x_k)\mathcal{L}_{I,j,k}u]\Big).$$

In particular,

$$\begin{aligned}\nabla_j\otimes\nabla_k[W(x_j,x_k)\mathcal{L}_{I,j}u] = &[\nabla_j\otimes\nabla_k|x_j-x_k|^{-1}]u + [\nabla_j|x_j-x_k|^{-1}]\otimes\nabla_k u\\ &+\nabla_j u\otimes[\nabla_k|x_j-x_k|^{-1}] + |x_j-x_k|^{-1}[\nabla_j\otimes\nabla_k u].\end{aligned}$$

Terms like $\nabla_j\otimes\nabla_k|x_j-x_k|^{-1} \sim |x_j-x_k|^{-3}$ have very high singularities at $x_j = x_k$.

To overcome this problem, as the study of the eigenvalue problem (1.3) in [9, 14], we would like to use the property that $u_0 \in H^1_{I,\mathrm{mix}}$ is antisymmetric w.r.t. I. This implies that $u \in \mathcal{H}_I$ (see (4.14)). From [9, Lemma 3.7 and Corollary 3.8], we have

Lemma 2.9. *[9, Lemma 3.7] Let $a \in \mathbb{R}^3$. Denote the functional space $Y_s(\mathbb{R}^3)$ by*

$$Y_s(\mathbb{R}^3) := \{f(y) \in L^2(\mathbb{R}^3); |y-a|^{2s-2}\nabla_y f \in L^2(\mathbb{R}^3)\}.$$

Then for $s \in [0,3/2)$ and $f \in Y_{s,\mathrm{anti}}(\mathbb{R}^3\times\mathbb{R}^3)$, we have

$$\left\|\frac{f}{|\cdot-a|^s}\right\|_{L^2(\mathbb{R}^3)} \leqslant \frac{2}{|2s-3|}\left\|\frac{\nabla_y f}{|\cdot-a|^{s-1}}\right\|_{L^2(\mathbb{R}^3)}.$$

and

Lemma 2.10. *[9, Corollary 3.8] Denote the functional space $Y_{anti,s}(\mathbb{R}^3\times\mathbb{R}^3)$ by*

$$Y_{s,\mathrm{anti}}(\mathbb{R}^3\times\mathbb{R}^3) := \{f \in L^2(\mathbb{R}^3\times\mathbb{R}^3); f(y,z) = -f(z,y), |y-z|^{s-2}\nabla_y\otimes\nabla_z f \in L^2(\mathbb{R}^3\times\mathbb{R}^3)\}.$$

Then for $s \in [2,5/2)$ and $f \in Y_{s,\mathrm{anti}}(\mathbb{R}^3\times\mathbb{R}^3)$, we have

$$\left\|\frac{f}{|y-z|^s}\right\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)} \leqslant \frac{4}{|2s-5||2s-3|}\left\|\frac{\nabla_y\otimes\nabla_z f}{|y-z|^{s-2}}\right\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)}.$$

However, similar property can not be used if we calculate directly the terms like $S(|x_j-x_k|^{-3}\mathcal{L}_{I,j,k}u)$ as for the standard dispersive problem (see e.g., [12, 13]): Applying Strichartz estimates for N-body problem (i.e., Lemma 3.2) as the standard dispersive problem, we will have

$$\|S(|x_j-x_k|^{-3}\mathcal{L}_{I,j,k}u)\|_{X_{p,T}} \lesssim \||x_j-x_k|^{-3}\mathbb{1}_{|x_j-x_k|\leqslant 1}\mathcal{L}_{I,j,k}u\|_{L^{\theta'_{\widetilde{p}}}(I_T,L^{\widetilde{p}',2}_{j,k})} + \||x_j-x_k|^{-3}\mathbb{1}_{|x_j-x_k|>1}\mathcal{L}_{I,j,k}u\|_{L^1(I_T,\mathcal{H})}$$

for some $2\leqslant p,\widetilde{p}\leqslant 6$ and $\frac{1}{p'}+\frac{1}{p}=1$. Here to deal with terms associated with the potential $W(x_j,x_k)$, we have to consider the functional space $L^{\widetilde{p}',2}_{j,k}$. Notice that

$$\||x_j-x_k|^{-3}\mathbb{1}_{|x_j-x_k|\leqslant 1}\mathcal{L}_{I,j,k}u(t,\cdot)\|^{\widetilde{p}'}_{L^{\widetilde{p}',2}_{j,k}} = \int_{\mathbb{R}^3_{r_{j,k}}} \frac{\|\mathcal{R}_{j,k}\mathcal{L}_{I,j,k}u(t,r_{j,k},\cdot)\|^{\widetilde{p}'}_{L^2((\mathbb{R}^3)^{N-1})}}{|r_{j,k}|^{3\widetilde{p}'}}\mathbb{1}_{|r_{j,k}|\leqslant 2}dr_{j,k},$$

Notice that for any $2\leqslant\widetilde{p}\leqslant 6$, $|r_{j,k}|^{-3\widetilde{p}'}\notin L^1_{\mathrm{loc}}(\mathbb{R}^3_{r_{j,k}})$ since $3\widetilde{p}'\geqslant\frac{18}{5}>3$. Thus we may obtain

$$\||x_j-x_k|^{-3}\mathbb{1}_{|r_{j,k}|\leqslant 2}\mathcal{L}_{I,j,k}u(t,\cdot)\|^{\widetilde{p}'}_{L^{\widetilde{p}',2}_{j,k}}=\infty$$

even for functions $u(t,\cdot)\in C_0^\infty((\mathbb{R}^3)^N)$. This is the reason why we can not calculate directly terms like $S(|x_j-x_k|^{-3}\mathcal{L}_{I,j,k}u)$.

Nevertheless, we can study $\mathcal{L}_IQu$ in scalar product: For any $D\subset\{1,\cdots,N\}$ and $1\leqslant|D|\leqslant 2$, and for any $u(t,x)\in X_{p,T}$ and $v(t,x)\in L_t^{\theta'_p}(I_T,L_D^{p',2})$ or $v(t,x)\in L_t^\infty(I_T,\mathcal{H})$, we are going to prove

$$\left|\int_0^T\langle S(|x_j-x_k|^{-3}\mathcal{L}_{I,j,k}u)(t),v(t)\rangle\,dt\right| \lesssim T^\theta\|u\|_{X^1_{I,p,T}}\min\{\|v\|_{L_t^{\theta'_p}(I_T,L_D^{p',2})},\|v\|_{L_t^\infty(I_T,\mathcal{H})}\} \tag{2.17}$$

for some $\theta>0$. The advantage of this method is that the above problem can be studied on $\mathcal{H}$:

$$\begin{aligned}&\left|\int_0^T\langle S(|x_j-x_k|^{-3}\mathcal{L}_{I,j,k}u)(t),v(t)\rangle\,dt\right|\\ &\quad=\left|\int_0^T\langle|x_j-x_k|^{-2-\alpha}\mathcal{L}_{I,j,k}u(s),|x_j-x_k|^{\alpha-1}S^*v(s)\rangle\,ds\right|\\ &\quad\leqslant\int_0^T\||x_j-x_k|^{-2-\alpha}\mathcal{L}_{I,j,k}u(s)\|_{\mathcal{H}}\||x_j-x_k|^{\alpha-1}S^*v(s)\|_{\mathcal{H}}\,ds.\end{aligned}$$

When $0\leqslant\alpha<\frac{1}{2}$, we can use Lemma 2.10. However, $\alpha=0$ shall be excluded: In the proof, we will use the following inequality

$$\||x_j-x_k|^{\alpha-1}S^*v(s)\|_{\mathcal{H}}\leqslant\||\cdot|^{\alpha-1}\mathbb{1}_{|\cdot|\leqslant 1}\|_{L^r(\mathbb{R}^3)}\|S^*v(s)\|_{L^{p,2}_{j,k}}+\|S^*v(s)\|_{\mathcal{H}}. \tag{2.18}$$

Here $2\leqslant p\leqslant 6$ and $\frac{1}{r}+\frac{1}{p}=\frac{1}{2}$. This implies that $r\geqslant 3$. However when $\alpha=0$, we have $\||\cdot|^{-1}\mathbb{1}_{|\cdot|\leqslant 1}\|_{L^r(\mathbb{R}^3)}=\infty$ for any $r\geqslant 3$. Thus $\alpha=0$ shall be excluded.

2.4.3. *Basic idea of the proof of Theorem 2.8.* Concerning the hyperbolic cross space approximation, our main difficulty comes from the operator P_{χ_R} on $X_{p,T}$. For general function $g\in X_{p,T}$, we even do not know if there exists a functional space $\widetilde{X}$ such that

$$\|P_{\chi_R}g\|_{X_{p,T}}\lesssim\|g\|_{\widetilde{X}}.$$

However, we mainly study $P_{\chi_R}Qu$ or $(1-P_{\chi_R})Qu$: The $\mathcal{H}$-bounded operator P_{χ_R} can be absorbed by operator S (defined by (2.10)). This is the purpose of Proposition 3.3 and Corollary 3.5.

Let u and u_R be the unique solution to the evolution equation (1.1) and its hyperbolic cross space approximation (1.14) respectively. Concerning the study of the error bound between u and u_R, we split $u-u_R$ into two parts: $u-P_{\chi_R}u$ and $P_{\chi_R}u-u_R$. We will see in the proof of Theorem 2.8 that for T small enough

$$\|u-u_R\|_{X_{p,T}}\leqslant\|u-P_{\chi_R}u\|_{X_{p,T}}+\|P_{\chi_R}u-u_R\|_{X_{p,T}}\leqslant\|u-P_{\chi_R}u\|_{X_{p,T}}+\frac{1}{2}\|u-u_R\|_{X_{p,T}}.$$

On the other hand, Lemma 5.1 shows that $\|u-P_{\chi_R}u\|_{X_{p,T}}\lesssim\frac{1}{R}\sum_{\ell=1,2}\|u_0\|^1_{H_{I_\ell,\mathrm{mix}}}$. As a result,

$$\|u-u_R\|_{X_{p,T}}\lesssim\frac{1}{R}\sum_{\ell=1,2}\|u_0\|^1_{H_{I_\ell,\mathrm{mix}}}.$$

3. Preliminary

We start with introducing some fundamental tools used in this paper.

3.1. **Strichartz estimates.** In this subsection, we introduce the Strichartz estimates used for the study of the N-body problem in [13] on the functional space $X_{p,T}$.

The following two lemmas (i.e., Lemma 3.1 and Lemma 3.2) about the dispersive estimates and standard Strichartz estimates can be found in [13, Lemma 2.2 and Lemma 2.3]. However, compared with [13], our Lemma 3.1 and Lemma 3.2 are global-in-time. This is because in [13], an additional time-dependent magnetic potential $A(t,x)$ is added, which complicates the arguments.

Lemma 3.1 (Dispersive estimate)**.** *Let $D \subset \{1, \cdots, N\}$, $1 \leqslant |D| \leqslant 2$, then*

$$\|U_0(t)g\|_{L_D^{\infty,2}} \lesssim_p |t|^{-3/2}\|g\|_{L_D^{1,2}}.$$

Proof. For the reader's convenience, we provide the detail of the proof.

For the case $D = \{j\}$ (i.e., $|D| = 1$), it is just the normal dispersive estimate inequality (see, e.g., [11, Eq. (2.22)]):

$$\|U_0(t)g\|_{L_D^{\infty,2}} = \|e^{\frac{1}{2}it\Delta_j}g\|_{L_D^{\infty,2}} \lesssim_p |t|^{-3/2}\|g\|_{L_D^{1,2}}.$$

For the other case, let $D = \{j,k\}$ (i.e., $|D| = 2$). Note that

$$R_{j,k}\nabla_j = \frac{1}{2}(\nabla_{r_{j,k}} + \nabla_{R_{j,k}})\mathcal{R}_{j,k}, \qquad R_{j,k}\nabla_k = \frac{1}{2}(\nabla_{R_{j,k}} - \nabla_{r_{j,k}})\mathcal{R}_{j,k} \tag{3.1}$$

and

$$-\mathcal{R}_{j,k}\triangle_x - \mathcal{R}_{j,k}\triangle_y = -\triangle_{r_{j,k}}\mathcal{R}_{j,k} - \triangle_{R_{j,k}}\mathcal{R}_{j,k}. \tag{3.2}$$

Then, we know

$$\mathcal{R}_{j,k}U_0(t)u = \widetilde{U}_0(t)\mathcal{R}_{j,k}u.$$

with $\widetilde{U}_0(t) = \exp\left(\frac{1}{2}i(\sum_{m\neq j,k}\triangle_m + \triangle_{r_{j,k}} + \triangle_{R_{j,k}})\right)$.

Therefore,

$$\begin{aligned}\|U_0(t)g\|_{L_{j,k}^{\infty,2}} &= \|\mathcal{R}_{j,k}U_0(t)g\|_{L_{r_{j,k}}^{\infty,2}} = \|\widetilde{U}_0(t)\mathcal{R}_{j,k}g\|_{L_{r_{i,j}}^{\infty,2}} \\ &\lesssim_p |t|^{-3/2}\|\mathcal{R}_{j,k}g\|_{L_{r_{j,k}}^{1,2}} \lesssim_p |t|^{-3/2}\|g\|_{L_{j,k}^{1,2}}.\end{aligned}$$

Hence the lemma. □

Then, using the above dispersive estimates, we have the following Strichartz estimates:

Lemma 3.2 (Strichartz estimate)**.** *For $D, D' \subset \{1, \cdots, N\}, 1 \leqslant |D|, |D'| \leqslant 2$ and $2 \leqslant p, \widetilde{p} \leqslant 6$, we have*

$$\|U_0(t)g\|_{L_t^{\theta_p}(\mathbb{R},L_D^{p,2})} \lesssim_p \|g\|_{\mathcal{H}}, \tag{3.3a}$$

$$\left\|\int_{\mathbb{R}} U(s)^*u(s)ds\right\|_{\mathcal{H}} \lesssim_{\widetilde{p}} \|u\|_{L_t^{\theta'_{\widetilde{p}}}(\mathbb{R},L_{D'}^{p',2})}, \tag{3.3b}$$

$$\|Su\|_{L_t^{\theta_p}(\mathbb{R},L_D^{p,2})} \lesssim_{p,\widetilde{p}} \|u\|_{L_t^{\theta'_{\widetilde{p}}}(\mathbb{R},L_{D'}^{\widetilde{p}',2})}. \tag{3.3c}$$

Here $\frac{2}{\theta_p} = 3(\frac{1}{2} - \frac{1}{p})$.

This is the standard Strichartz estimate. One can easily obtain these estimates by using [6].

Normally, operators bounded on $\mathcal{H}$ can not be bounded on $L_D^{p,2}$. However, the following tells us that after adding the operator S, the bounded operator P on $\mathcal{H}$ is also bounded on $L_D^{p,2}$ if $[P, U_0] = 0$. This is an essential ingredient for the study of our hyperbolic cross space approximation.

Proposition 3.3. *If $2 \leqslant p, \widetilde{p} < 6$, for any operator P acting on $\mathcal{H}$, if $[P, U_0] = 0$ and $\|Pf_0\|_{L^2} \leqslant \|f\|_{\mathcal{H}}$, then*

$$\|PSu(\cdot,x)\|_{L_t^{\theta_p}(\mathbb{R},L_D^{p,2})} \lesssim_{p,\widetilde{p}} \|u\|_{L_t^{\theta'_{\widetilde{p}}}(\mathbb{R},L_{D'}^{\widetilde{p}',2})}.$$

Remark 3.4. *Let $P = P_{\chi_R}$. As P_{χ_R} is a Fourier multiplier, it is possible to reach the endpoint acse $p, \widetilde{p} = 6$ in Proposition 3.3 by repeating the arguments in [6].*

Proof. We are going to use the Christ-Kiselev lemma [4] to prove this lemma.

Since P and U_0 commute, we have

$$\left\|P\int_{\mathbb{R}} U_0(t-s)u(s,x)ds\right\|_{L_t^{\theta_p}(\mathbb{R},L_D^{p,2})} = \left\|U_0(t)P\int_{\mathbb{R}} U_0(s)^*u(s,x)ds\right\|_{L_t^{\theta_p}(\mathbb{R},L_D^{p,2})}.$$

By (3.3a) and $[P, U_0] = 0$, we have

$$\left\|P\int_{\mathbb{R}} U_0(t-s)u(s,x)ds\right\|_{L_t^{\theta_p}(\mathbb{R},L_D^{p,2})} \lesssim_p \left\|P\int_{\mathbb{R}} U_0(s)^*u(s,x)ds\right\|_{\mathcal{H}}.$$

Then, by $\|Pu_0\|_{\mathcal{H}} \leqslant \|u\|_{\mathcal{H}}$ and (3.3b), we have

$$\left\| P\int_{\mathbb{R}} U_0(t-s)u(s,x)ds \right\|_{L_t^{\theta_p}(\mathbb{R},L_D^{p,2})} \lesssim_p \left\| \int_{\mathbb{R}} U_0(s)^* u(s,x)ds \right\|_{\mathcal{H}} \lesssim_{p,\widetilde{p}} \|u\|_{L_t^{\theta'_{\widetilde{p}}}(\mathbb{R},L_{D'}^{\widetilde{p}',2})}.$$

Then by Christ-Kiselev lemma, for any $2 \leqslant p, \widetilde{p} < 6$ we have

$$\left\| P\int_{\mathbb{R}} U_0(t-s)u(s,x)ds \right\|_{L_t^{\theta_p}(\mathbb{R},L_D^{p,2})} \lesssim_{p,\widetilde{p}} \|u\|_{L_t^{\theta'_{\widetilde{p}}}(\mathbb{R},L_{D'}^{\widetilde{p}',2})}.$$

□

Corollary 3.5. *For $D, D' \subset \{1,\cdots,N\}, 1 \leqslant |D|, |D'| \leqslant 2$ and $2 \leqslant p, \widetilde{p} < 6$, we have*

$$\|P_{\chi_R} Su\|_{L_t^{\theta_p}(\mathbb{R},L_D^{p,2})} \lesssim_{p,\widetilde{p}} \|u\|_{L_t^{\theta'_{\widetilde{p}}}(\mathbb{R},L_{D'}^{\widetilde{p}',2})}, \tag{3.4a}$$

$$\left\| \left(\sum_{1\leqslant \ell\leqslant 2} \mathcal{L}_{I_\ell} \right)^{-1} (1-P_{\chi_R})Su \right\|_{L_t^{\theta_p}(\mathbb{R},L_D^{p,2})} \lesssim_{p,\widetilde{p}} \frac{1}{R} \|u\|_{L_t^{\theta'_{\widetilde{p}}}(\mathbb{R},L_{D'}^{\widetilde{p}',2})}. \tag{3.4b}$$

Proof. By the definition of P_{χ_R}, we have

$$[P_{\chi_R}, U_0] = 0$$

and

$$\|P_{\chi_R} u\|_{\mathcal{H}} \leqslant \|u\|_{\mathcal{H}}.$$

Let $P = P_{\chi_R}$, then we get (3.4a).

Concerning (3.4b), we have

$$\|(1-P_{\chi_R})u\|_{\mathcal{H}} \leqslant \|\mathbb{1}_{\mathcal{D}_R^c} \mathcal{F}_{x_1,\cdots,x_N}(u)\|_{\mathcal{H}}$$

For all wave vector ω outside the domain $\mathcal{D}_R$, we have

$$1 \leqslant \frac{1}{R} \sum_{1\leqslant \ell\leqslant 2} \prod_{i\in\mathcal{I}_l} (1+|2\pi\omega_i|^2)^{1/2}.$$

By definition of χ_R, we know

$$R\left\| \left(\sum_{1\leqslant \ell\leqslant 2} \mathcal{L}_{I_\ell} \right)^{-1} (1-P_{\chi_R})u \right\|_{\mathcal{H}} \leqslant R\left\| \left(\sum_{1\leqslant \ell\leqslant 2} \mathcal{L}_{I_\ell} \right)^{-1} (1-P_{\mathbb{1}_{\mathcal{D}_R}})u \right\|_{\mathcal{H}} \leqslant \|u\|_{\mathcal{H}}. \tag{3.5}$$

Given $[\mathcal{L}_{I_\ell}, U_0] = 0$, then take $P = R(1-P_{\chi_R})\left(\sum_{\ell=1,2} \mathcal{L}_{I_\ell}\right)^{-1}$, we get conclusion. □

3.2. **Sobolev inequalities.** For the study of mixed regularity, we need some Sobolev inequalities on functional space $L_D^{p,2}$. To do so, we study the Calderón-Zygmund inequality and Mikhlin multiplier theorem to our functional space $L_j^{p,2}$ in Section A. Then we generalize these results to the functional space $L_{j,k}^{p,2}$.

Theorem 3.6. *For $1 < p < \infty$, and $D \subset \{1,\cdots,N\}$ with $1 \leqslant |D| \leqslant 2$, we have*

$$\|\nabla_j g\|_{L_D^{p,2}} \lesssim_p \|(1-\triangle_j)^{1/2} g\|_{L_D^{p,2}}, \tag{3.6a}$$

$$\|g\|_{L_D^{p,2}} \lesssim_p \|(1-\triangle_j)^{1/2} g\|_{L_D^{p,2}}. \tag{3.6b}$$

Proof. We first consider the case $j \notin D$. By the Plancherel theorem on variable x_j, it is easy to see that (3.6a)-(3.6b) hold.

Now we assume that $j \in D$. If $|D| = 1$, then $D = \{j\}$. In this case, we use Theorem A.2. For the first inequality, we only need to study equivalently the following inequality

$$\|\nabla_j (1-\triangle_j)^{-1/2} g\|_{L_j^{p,2}} \lesssim_p \|g\|_{L_j^{p,2}}. \tag{3.7}$$

Then Theorem A.2 with $n = 3$ and

$$a(\xi) = \frac{\xi}{(1+|\xi|^2)^{1/2}} \quad \text{for } \xi \in \mathbb{R}^3.$$

implies (3.7). The second and third estimates can be treated in the same manner.

Finally, we assume that $j \in D$ and $|D| = 2$. We can assume that $D = \{j, k\}$ with $k \in \{1, \cdots, N\} \backslash \{j\}$. We study first (3.6a). By the Plancherel theorem on variable $R_{j,k}$, (2.6), (3.1) and (3.7),

$$\begin{aligned}
\|\nabla_j g\|_{L^{p,2}_{j,k}} &= \frac{1}{2}\|(\nabla_{r_{j,k}} - \nabla_{R_{j,k}})\mathcal{R}_{j,k} g\|_{L^{p,2}_{r_{j,k}}} \\
&= \frac{1}{2}\|(\nabla_{r_{j,k}} - i2\pi\xi_{R_{j,k}})\mathcal{F}_{R_{j,k}}\mathcal{R}_{j,k} g\|_{L^{p,2}_{r_{j,k}}} \\
&= \frac{1}{2}\|\nabla_{r_{j,k}} \exp(-i2\pi r_{j,k}\cdot\xi_{R_{j,k}})\mathcal{F}_{R_{j,k}}\mathcal{R}_{j,k} g\|_{L^{p,2}_{r_{j,k}}} \\
&\lesssim_p \|(1 - \frac{1}{4}\triangle_{r_{j,k}})^{1/2} \exp(-i2\pi r_{j,k}\cdot\xi_{R_{j,k}})\mathcal{F}_{R_{j,k}}\mathcal{R}_{j,k} g\|_{L^{p,2}_{r_{j,k}}} \\
&= \|(1 - \frac{1}{4}|\nabla_{r_{j,k}} - i2\pi\xi_{R_{j,k}}|)^{1/2}\mathcal{F}_{R_{j,k}}\mathcal{R}_{j,k} g\|_{L^{p,2}_{r_{j,k}}} \\
&= \|(1 - \frac{1}{4}|\nabla_{r_{j,k}} + \nabla_{R_{j,k}}|^2)^{1/2}\mathcal{R}_{j,k} g\|_{L^{p,2}_{r_{j,k}}} = \|(1-\Delta_j)^{1/2} g\|_{L^{p,2}_{j,k}}.
\end{aligned}$$

Here we have the fact that for any function $f(y)$ with $y \in \mathbb{R}^3$, we have

$$\begin{aligned}
&(1 - \frac{1}{4}\triangle_y)^{1/2}\exp(-i2\pi a\cdot\xi_y) f(y) \\
&= \mathcal{F}_y^{-1}\Big[(1 - \pi^2|\xi_y|^2)^{1/2}\mathcal{F}_y\big(\exp(-i2\pi a\cdot\xi_y) f\big)(\xi_y)\Big](y) \\
&= \mathcal{F}_y^{-1}\Big[(1 - \pi^2|\xi_y|^2)^{1/2}\mathcal{F}_y\big(f\big)(\xi_y + a)\Big](y) = (1 - \frac{1}{4}|\nabla_y - i2\pi a|^2)^{1/2} f(y);
\end{aligned}$$

and in the last identity, we use (3.2). This gives (3.6a) for $|D| = 2$ and $j \in D$. Eq. (3.6b) can be studied analogously. Now the proof is completed. □

4. Existence and mixed regularity of solutions

In this section, we are going to study the existence and mixed regularity of solutions to (1.1). We shall point out that the proof of the existence and uniqueness of solution can be regarded as an adjustment of [13] under our setting, and we mainly focus on our mixed regularity of the solution.

4.1. **Existence of solutions.** In this subsection, we are going to study the existence of solutions to (1.1) in $X_{p,T}$. As mentioned above, the study of mixed regularity of solutions is our main object rather than existence. So we prove the existence of solutions by using the same method as for mixed regularity. It will help us to understand the proof of mixed regularity. In addition, we shall point out that this method is not the best way for the proof of the existence of solutions, but as explained in Section 2.4.2, it is necessary for our study of mixed regularity.

Proof of Theorem 2.5. As explained in Section 2.4.1, we are going to show that $\|Qu\|_{X_{p,T}} \leqslant CT^\theta\|u\|_{X_{p,T}}$ for some $\theta > 0$, $2 < p \leqslant 6$ and $T > 0$. Here we use the method for mixed regularity and consider this problem in the scalar product: For any $D \subset \{1, \cdots, N\}$ and $1 \leqslant |D| \leqslant 2$, and for any $u(t,x) \in X_{p,T}$ and $v(t,x) \in L_t^{\theta_p'}(I_T, L_D^{p',2})$ or $v(t,x) \in L_t^1(I_T, \mathcal{H})$, we are going to prove

$$\left|\int_0^T \langle (Qu)(t), v(t)\rangle\, dt\right| \lesssim T^\theta\|u\|_{X_{p,T}} \min\{\|v\|_{L_t^{\theta_p'}(I_T, L_D^{p',2})}, \|v\|_{L_0^\infty(I_T,\mathcal{H})}\}$$

for some $\theta > 0$.

To do so, we split the study into the case of potentials between electrons and nuclei, and the case of potentials between electrons and electrons.

Step 1. Study of the potentials electrons and nuclei. For any $0 < \alpha < \frac{1}{2}$, we have

$$\begin{aligned}
&\left|\int_0^T \Big\langle S\Big(\frac{1}{|x_j - a_\mu(\cdot)|}u(\cdot,x)\Big)(t), v(t,x)\Big\rangle\, dt\right| \\
&\quad= \left|\int_0^T \Big\langle \frac{1}{|x_j - a_\mu(s)|^\alpha}u(s,x), \frac{1}{|x_j - a_\mu(s)|^{1-\alpha}}S^*\big(v(\cdot,x)\big)(s)\Big\rangle\, ds\right| \\
&\quad\leqslant \int_0^T \left\|\frac{1}{|x_j - a_\mu(s)|^\alpha}u(s,x)\right\|_{\mathcal{H}} \left\|\frac{1}{|x_j - a_\mu(s)|^{1-\alpha}}S^*\big(v(\cdot,x)\big)(s)\right\|_{\mathcal{H}} ds. \qquad (4.1)
\end{aligned}$$

According to the Hölder inequality, for any $2 \leqslant r < \frac{3}{\alpha}$ and $\frac{1}{r} + \frac{1}{p_1} = \frac{1}{2}$,

$$\begin{aligned}\Big\| \frac{1}{|x_j - a_\mu(s)|^\alpha} u(s,x) \Big\|_{\mathcal{H}} &= \Big\| \frac{1}{|x_j - a_\mu(s)|^\alpha} \|u(s,x_j,\cdot)\|_{L^2((\mathbb{R}^3)^{N-1})} \Big\|_{L^2_j(\mathbb{R}^3)} \\ &\leqslant \|u(s)\|_{\mathcal{H}} + \Big\| \frac{1}{|x_j - a_\mu(s)|^\alpha} \mathbb{1}_{|x_j - a_\mu(s)| \leqslant 1} \Big\|_{L^r_{\mathbb{R}^3}} \|u(s)\|_{L^{p_1,2}_j} \\ &\lesssim_{\alpha,p_1} \|u(s)\|_{\mathcal{H}} + \|u(s)\|_{L^{p_1,2}_j},\end{aligned} \tag{4.2}$$

and for any $2 \leqslant \widetilde{r} < \frac{3}{1-\alpha}$ and $\frac{1}{\widetilde{r}} + \frac{1}{\widetilde{p}} = \frac{1}{2}$,

$$\Big\| \frac{1}{|x_j - a_\mu(s)|^{1-\alpha}} (S^*v)(s) \Big\|_{\mathcal{H}} \lesssim_{\alpha,\widetilde{p}} \|(S^*v)(s)\|_{\mathcal{H}} + \|(S^*v)(s)\|_{L^{\widetilde{p},2}_j}. \tag{4.3}$$

Now we are going to apply the dual form of the Strichartz estimate (3.3c) to S^*v. Before going further, we have to add the restriction $2 \leqslant \widetilde{p} \leqslant 6$ to use the Strichartz estimates. Then gathering together $2 \leqslant \widetilde{r} < \frac{3}{1-\alpha}$ and $\frac{1}{\widetilde{r}} + \frac{1}{\widetilde{p}} = \frac{1}{2}$, we have

$$\frac{6}{1+2\alpha} < \widetilde{p} \leqslant 6. \tag{4.4}$$

Then for any $D \subset \{1, \cdots, N\}$ and $0 \leqslant |D| \leqslant 2$ and for any $\widetilde{p}$ satisfying (4.4) and p satisfying $2 < p \leqslant 6$,

$$\|(S^*v)(s)\|_{L^\infty_t(I_T,\mathcal{H})} \lesssim_{p,\widetilde{p}} \min\{\|v\|_{L^{\theta'_p}_t(I_T, L^{p',2}_D)}, \|v\|_{L^1_t(I_T,\mathcal{H})}\} \tag{4.5}$$

and

$$\|(S^*v)(s)\|_{L^{\theta_{\widetilde{p}}}_t(I_T, L^{\widetilde{p},2}_j)} \lesssim_{p,\widetilde{p}} \min\{\|v\|_{L^{\theta'_p}_t(I_T, L^{p',2}_D)}, \|v\|_{L^1_t(I_T,\mathcal{H})}\}. \tag{4.6}$$

To make the mapping Q from $X_{p,T}$ to itself, we need to set $p_1 = p$. Thus, $2 \leqslant p_1 = p \leqslant 6$. This and $2 \leqslant r < \frac{3}{\alpha}$, $\frac{1}{r} + \frac{1}{p_1} = \frac{1}{2}$ imply that

$$\frac{6}{3-2\alpha} < p \leqslant 6. \tag{4.7}$$

As a result, from (4.1)-(4.3) and (4.5)-(4.6) we infer that, under condition (1)-(2) in Assumption 2.2 on $\alpha, p, \widetilde{p}$, for any $0 < T < 1$ and any $D \subset \{1, \cdots, N\}$ with $1 \leqslant |D| \leqslant 2$,

$$\begin{aligned}&\Big| \int_0^T \Big\langle S\Big(\frac{1}{|x_j - a_\mu(\cdot)|} u(\cdot,x) \Big)(t), v(t,x) \Big\rangle \, dt \Big| \\ &\leqslant \int_0^T \Big\| \frac{1}{|x_j - a_\mu(s)|^\alpha} u(s,x) \Big\|_{\mathcal{H}} \Big\| \frac{1}{|x_j - a_\mu(s)|^{1-\alpha}} S^*\big(v(\cdot,x)\big)(s) \Big\|_{\mathcal{H}} \, ds \\ &\lesssim_{\alpha,p,\widetilde{p}} \Big(\|u\|_{L^1_t(I_T,\mathcal{H})} + \|u(s)\|_{L^1_t(I_T, L^{p,2}_j)} \Big) \|S^*v\|_{L^\infty(I_T,\mathcal{H})} \\ &\quad + \Big(\|u\|_{L^{\theta'_{\widetilde{p}}}_t(I_T,\mathcal{H})} + \|u\|_{L^{\theta'_{\widetilde{p}}}_t(I_T, L^{p,2}_j)} \Big) \|S^*v\|_{L^{\theta_{\widetilde{p}}}_t(I_T, L^{\widetilde{p},2}_j)} \\ &\lesssim_{\alpha,p,\widetilde{p}} T^{1/\theta'_{\widetilde{p}} - 1/\theta_p} \Big(\|u\|_{L^\infty_t(I_T,\mathcal{H})} + \|u\|_{L^{\theta_p}_t(I_T, L^{p,2}_j)} \Big) \min\{\|v\|_{L^{\theta'_p}_t(I_T, L^{p',2}_D)}, \|v\|_{L^1_t(I_T,\mathcal{H})}\}.\end{aligned} \tag{4.8}$$

Here we also use the assumption that $1/\theta'_{\widetilde{p}} - 1/\theta_p > 0$. As $u \in X_{p,T}$, by duality, for any $0 < T < 1$ and any $D \subset \{1, \cdots, N\}$ with $1 \leqslant |D| \leqslant 2$,

$$\max\left\{ \Big\| S\Big(\frac{1}{|x_j - a_\mu(\cdot)|} u(\cdot,x) \Big) \Big\|_{L^\infty_t(I_T,\mathcal{H})}, \Big\| S\Big(\frac{1}{|x_j - a_\mu(\cdot)|} u(\cdot,x) \Big) \Big\|_{L^{\theta_p}_t(I_T, L^{p,2}_D)} \right\} \lesssim_{\alpha,p,\widetilde{p}} T^{\theta'_{\widetilde{p}} - \theta_{\widetilde{p}}} \|u\|_{X_{p,T}}.$$

As a result, we infer that under under condition (1)-(2) in Assumption 2.2 on $\alpha, p, \widetilde{p}$ and $0 < T < 1$,

$$\|S(V(\cdot,x_j)u)\|_{X_{p,T}} \lesssim_{\alpha,p,\widetilde{p}} Z T^{1/\theta'_{\widetilde{p}} - 1/\theta_p} \|u\|_{X_{p,T}} \tag{4.9}$$

Step 2. Study of the potentials between electrons and electrons. The proof of Step 2 is essentially the same as for Step 1. So we just point out the difference.

For $\frac{1}{|x_j - x_k|}$, the estimates (4.2) and (4.3) become: For any $2 \leqslant r < \frac{3}{\alpha}$ and $\frac{1}{r} + \frac{1}{p_1} = \frac{1}{2}$,

$$\Big\| \frac{1}{|x_j - x_k|^\alpha} u(s) \Big\|_{\mathcal{H}} \lesssim_{\alpha,p} \|u(s)\|_{\mathcal{H}} + \|u(s)\|_{L^{p,2}_{j,k}},$$

and for any $2 \leqslant \widetilde{r} < \frac{3}{1-\alpha}$ and $\frac{1}{\widetilde{r}} + \frac{1}{\widetilde{p}} = \frac{1}{2}$,

$$\left\| \frac{1}{|x_j - x_k|^{1-\alpha}} (S^* v)(s) \right\|_{\mathcal{H}} \lesssim_{\alpha,\widetilde{p}} \|(S^* v)(s)\|_{\mathcal{H}} + \|(S^* v)(s)\|_{L^{\widetilde{p},2}_{j,k}}.$$

Then arguing as for Step 1, we need to set $p_1 = p$, and p satisfies (4.7). Then under condition (1)-(2) in Assumption 2.2 on $\alpha, p, \widetilde{p}$, for any $0 < T < 1$ and any $D \subset \{1, \cdots, N\}$ with $1 \leqslant |D| \leqslant 2$,

$$\begin{aligned}
&\left| \int_0^T \Big\langle S\Big(\frac{1}{|x_j - x_k|} u(\cdot, x) \Big)(t), v(t,x) \Big\rangle dt \right| \\
&\leqslant \int_0^T \left\| \frac{1}{|x_j - x_k|^{\alpha}} u(s,x) \right\|_{\mathcal{H}} \left\| \frac{1}{|x_j - x_k|^{1-\alpha}} (S^* v(\cdot, x))(s) \right\|_{\mathcal{H}} ds \\
&\lesssim_{\alpha,p,\widetilde{p}} T^{1/\theta'_{\widetilde{p}} - 1/\theta_p} \Big(\|u\|_{L^\infty_t(I_T,\mathcal{H})} + \|u\|_{L^{\theta_p}_t(I_T, L^{p,2}_{j,k})} \Big) \min\{\|v\|_{L^{\theta'_p}_t(I_T, L^{p',2}_D)}, \|v\|_{L^1_t(I_T,\mathcal{H})}\}. \qquad (4.10)
\end{aligned}$$

As a result under condition (1)-(2) in Assumption 2.2 on $\alpha, p, \widetilde{p}$ and $0 < T < 1$,

$$\|S(W(x_j, x_k)u)\|_{X_{p,T}} \lesssim_{\alpha,p,\widetilde{p}} T^{1/\theta'_{\widetilde{p}} - 1/\theta_p} \|u\|_{X_{p,T}}. \qquad (4.11)$$

Step 3. Conclusion. From (4.1) and (4.11), we infer that under condition (1)-(2) in Assumption 2.2 on $\alpha, p, \widetilde{p}$ and $0 < T < 1$, there exists a constant $C_{T,1} := C_{T,1}(\alpha, p, \widetilde{p}) \geqslant 1$ such that

$$\|Qu\|_{X_{p,T}} \leqslant C_{T,1}(Z + N) N T^{1/\theta'_{\widetilde{p}} - 1/\theta_p} \|u\|_{X_{p,T}}. \qquad (4.12)$$

Now let $C_{T,1}(Z + N) N T^{1/\theta'_{\widetilde{p}} - 1/\theta_p} \leqslant \frac{1}{2}$, we get

$$\|Qu\|_{X_{p,T}} \leqslant \frac{1}{2} \|u\|_{X_{p,T}}.$$

Note that $T < 1$ under the condition $C_{T,1}(Z + N) N T^{1/\theta'_{\widetilde{p}} - 1/\theta_p} \leqslant \frac{1}{2}$. Thus under Assumption 2.2 on p, T, we know $1 + iQ$ is invertible on $X_{p,T}$. As a result,

$$u = (1 + iQ)^{-1}(U_0(\cdot) u_0) \qquad (4.13)$$

and

$$\|u\|_{X_{p,T}} = \|(1 + iQ)^{-1}(U_0(\cdot) u_0)\|_{X_{p,T}} \leqslant 2\|U_0(\cdot) u_0\|_{X_{p,T}} \lesssim_p \|u_0\|_{\mathcal{H}}.$$

This gives (2.7) and shows the uniqueness of the solution $u \in X_{p,T}$. Besides, it is easy to see that $\|u\|_{L^\infty_t(\mathbb{R},\mathcal{H})} = \|u_0\|_{\mathcal{H}}$. The standard continuation procedure for the solutions to (1.1) yields a unique global-in-time solution $u \in X_{p,\infty}$. This completes the proof of Theorem 2.5. □

4.2. **Mixed regularity.** Now we can study the mixed regularity of the unique solution.

Proof of Theorem 2.6. Before going further, we first show that $u(t,x)$ is antisymmetric w.r.t. I for any $t \in I_T$ with under condition (3) in Assumption 2.2 on T. Let $j, k \in I$, then we know that $u_0 = -P_{j,k} u_0$. Under Assumption 2.2, from (4.13) we infer

$$u = -(1 + iQ)^{-1}(U_0(\cdot) P_{j,k} u_0) = -P_{j,k}(1 + iQ)^{-1}(U_0(\cdot) u_0) = -P_{j,k} u.$$

Here we use the fact that $U_0(\cdot) P_{j,k} = P_{j,k} U_0$ and $Q P_{j,k} = P_{j,k} Q$. As a result, we infer that under Assumption 2.2 on p, T,

$$u = -P_{j,k} u \qquad \text{in} \quad X_{p,T}. \qquad (4.14)$$

Hence u is antisymmetric w.r.t. I for any $t \in I_T$.

As explained in Section 2.4.2, we are going to show: For any $D \subset \{1, \cdots, N\}$ and $1 \leqslant |D| \leqslant 2$, and for any $u(t,x) \in X^1_{I,p,T}$ and $v(t,x) \in L^{\theta'_p}_t(I_T, L^{p',2}_D)$ or $v(t,x) \in L^\infty_t(I_T, \mathcal{H})$, we are going to prove

$$\left| \int_0^T \langle (\mathcal{L}_I Q u)(t), v(t) \rangle \, dt \right| \lesssim T^\theta \|u\|_{X^1_{I,p,T}} \min\{\|v\|_{L^{\theta'_p}_t(I_T, L^{p',2}_D)}, \|v\|_{L^\infty_0(I_T,\mathcal{H})}\}$$

for some $\theta > 0$ and $2 < p \leqslant 6$. We also split the study into the case of potentials between electrons and nuclei, and the case of potentials between electrons and electrons.

Step 1. Study of the potentials electrons and nuclei. First of all, we assume $j \notin I$. Then we have

$$\mathcal{L}_I \frac{1}{|x_j - a_\mu(t)|} u = \frac{1}{|x_j - a_\mu(t)|} \mathcal{L}_I u.$$

According to (4.9), we infer that under condition (1)-(2) in Assumption 2.2 and for any $0 < T < 1$,

$$\|S \mathcal{L}_I (V(\cdot, x_j) u)\|_{X^1_{I,p,T}} = \|S(V(\cdot, x_j) \mathcal{L}_I u)\|_{X^1_{I,p,T}} \lesssim_{\alpha,p,\widetilde{p}} Z T^{1/\theta'_{\widetilde{p}} - 1/\theta_p} \|u\|_{X^1_{I,p,T}}. \qquad (4.15)$$

Now we consider the case $j \in I$. By (2.15) we have

$$\begin{aligned}\mathcal{L}_I \frac{1}{|x_j - a_\mu(t)|} u &= (1-\Delta_j)^{1/2} \frac{1}{|x_j - a_\mu(t)|} \mathcal{L}_{I,j} u \\ &= (1-\Delta_j)^{-1/2} \left[\frac{1}{|x_j - a_\mu(t)|} \mathcal{L}_{I,j} u \right] - \left[(1-\Delta_j)^{-1/2} \nabla_j\right] \cdot \nabla_j \left[\frac{1}{|x_j - a_\mu(t)|} \mathcal{L}_{I,j} u \right] \end{aligned} \tag{4.16}$$

where $\mathcal{L}_{I,j}$ is defined by (2.13). For the first term on the right-hand side of (4.16), from (4.8), we infer that under condition (1)-(2) in Assumption 2.2 and for any $0 < T < 1$ and any $D \subset \{1, \cdots, N\}$ with $1 \leqslant |D| \leqslant 2$

$$\begin{aligned}&\left| \int_0^T \left\langle S(1-\Delta_j)^{-1/2} \Big(\frac{1}{|x_j - a_\mu(\cdot)|} \mathcal{L}_{I,j} u(\cdot, x), v(t,x) \right\rangle dt \right| \\ &= \left| \int_0^T \left\langle S \Big(\frac{1}{|x_j - a_\mu(\cdot)|} \mathcal{L}_{I,j} u(\cdot, x), (1-\Delta_j)^{-1/2} v(t,x) \right\rangle dt \right| \\ &\lesssim_{\alpha,p,\tilde{p}} T^{1/\theta'_{\tilde{p}} - 1/\theta_p} \left(\|u\|_{L_t^\infty(I_T, \mathcal{H})} + \|u\|_{L_t^{\theta_p}(I_T, L_j^{p,2})} \right) \\ &\quad \times \min\{ \|(1-\Delta_j)^{-1/2} v\|_{L_t^{\theta'_p}(I_T, L_D^{p',2})}, \|(1-\Delta_j)^{-1/2} v\|_{L_0^\infty(I_T, \mathcal{H})} \} \\ &\lesssim_{\alpha,p,\tilde{p}} T^{1/\theta'_{\tilde{p}} - 1/\theta_p} \left(\|u\|_{L_t^\infty(I_T, \mathcal{H})} + \|u\|_{L_t^{\theta_p}(I_T, L_j^{p,2})} \right) \min\{ \|v\|_{L_t^{\theta'_p}(I_T, L_D^{p',2})}, \|v\|_{L_0^\infty(I_T, \mathcal{H})} \}. \end{aligned} \tag{4.17}$$

Here we use the fact that $[S, (1-\Delta_j)^{1/2}] = 0$ in the first equation and Theorem 3.6 in the last inequality.

For the second term on the right-hand side of (4.16), notice that

$$\nabla_j \Big[\frac{1}{|x_j - a_\mu(\cdot)|} \mathcal{L}_{I,j} u(\cdot, x) \Big] = \frac{1}{|x_j - a_\mu(\cdot)|} \mathcal{L}_{I,j} \nabla_j u(\cdot, x) + \Big[\nabla_j \frac{1}{|x_j - a_\mu(\cdot)|} \Big] \mathcal{L}_{I,j} u(\cdot, x),$$

and by Lemma 2.9,

$$\begin{aligned}&\left\| |x_j - a_\mu(\cdot)|^{1-\alpha} \Big[\nabla_j \frac{1}{|x_j - a_\mu(\cdot)|} \Big] \mathcal{L}_{I,j} u(\cdot, x) \right\|_{\mathcal{H}} \\ &\quad \lesssim \left\| \frac{1}{|x_j - a_\mu(\cdot)|^{1+\alpha}} \mathcal{L}_{I,j} u(\cdot, x) \right\|_{\mathcal{H}} \lesssim_\alpha \left\| \frac{1}{|x_j - a_\mu(\cdot)|^{\alpha}} \mathcal{L}_{I,j} \nabla_j u(\cdot, x) \right\|_{\mathcal{H}}. \end{aligned}$$

Thus,

$$\left\| |x_j - a_\mu(\cdot)|^{1-\alpha} \nabla_j \Big[\frac{1}{|x_j - a_\mu(\cdot)|} \mathcal{L}_{I,j} u(\cdot, x) \Big] \right\|_{\mathcal{H}} \lesssim_\alpha \left\| \frac{1}{|x_j - a_\mu(\cdot)|^{\alpha}} \mathcal{L}_{I,j} \nabla_j u \right\|_{\mathcal{H}}. \tag{4.18}$$

Then we have

$$\begin{aligned}&\left| \int_0^T \left\langle S[(1-\Delta_j)^{-1/2} \nabla_j] \cdot \left(\nabla_j \Big[\frac{1}{|x_j - a_\mu(\cdot)|} \mathcal{L}_{I,j} u(\cdot, x) \Big] \right), v(t,x) \right\rangle dt \right| \\ &\lesssim_\alpha \int_0^T \left\| \Big[\frac{1}{|x_j - a_\mu(s)|^\alpha} \mathcal{L}_{I,j} \nabla_j u(s, x) \Big] \right\|_{\mathcal{H}} \left\| \frac{1}{|x_j - a_\mu(s)|^{1-\alpha}} S^* \big((1-\Delta_j)^{-1/2} \nabla_j v(\cdot, x) \big)(s) \right\|_{\mathcal{H}} ds. \end{aligned} \tag{4.19}$$

Proceeding as for (4.8) and (4.17), we infer that for under condition (1)-(2) in Assumption 2.2,for any $0 < T < 1$ and any $D \subset \{1, \cdots, N\}$ with $1 \leqslant |D| \leqslant 2$,

$$\begin{aligned}&\left| \int_0^T \left\langle S[(1-\Delta_j)^{-1/2} \nabla_j] \cdot \left(\nabla_j \Big[\frac{1}{|x_j - a_\mu(\cdot)|} \mathcal{L}_{I,j} u(\cdot, x) \Big] \right), v(t,x) \right\rangle dt \right| \\ &\lesssim_{\alpha,p,\tilde{p}} T^{1/\theta'_{\tilde{p}} - 1/\theta_p} \left(\|\nabla_j \mathcal{L}_{I,j} u\|_{L_t^\infty(I_T, \mathcal{H})} + \|\nabla_j \mathcal{L}_{I,j} u\|_{L_t^{\theta_p}(I_T, L_j^{p,2})} \right) \\ &\quad \times \min\left\{ \|(1-\Delta_j)^{-1/2} \nabla_j v\|_{L_t^{\theta'_p}(I_T, L_D^{p',2})}, \|(1-\Delta_j)^{-1/2} \nabla_j v\|_{L_t^1(I_T, \mathcal{H})} \right\} \\ &\lesssim_{\alpha,p,\tilde{p}} T^{1/\theta'_{\tilde{p}} - 1/\theta_p} \left(\|\mathcal{L}_I u\|_{L_t^\infty(I_T, \mathcal{H})} + \|\mathcal{L}_I u\|_{L_t^{\theta_p}(I_T, L_j^{p,2})} \right) \min\{ \|v\|_{L_t^{\theta'_p}(I_T, L_D^{p',2})}, \|v\|_{L_t^1(I_T, \mathcal{H})} \}. \end{aligned} \tag{4.20}$$

Here in the last inequality, we use Theorem 3.6 again. As a result, (4.16), (4.17) and (4.20) show that under condition (1)-(2) in Assumption 2.2 and for any $0 < T < 1$ and $j \in I$,

$$\|\mathcal{L}_I S(V(\cdot, x_j) u)\|_{X^1_{I,p,T}} \lesssim_{\alpha,p,\tilde{p}} Z T^{1/\theta'_{\tilde{p}} - 1/\theta_p} \|u\|_{X^1_{I,p,T}}.$$

Finally, this and (4.15) imply that for under condition (1)-(2) in Assumption 2.2 and for any $0 < T < 1$,

$$\|\mathcal{L}_I S(V(\cdot, x_j) u)\|_{X^1_{I,p,T}} \lesssim_{\alpha,p,\tilde{p}} Z T^{1/\theta'_{\tilde{p}} - 1/\theta_p} \|u\|_{X^1_{I,p,T}}. \tag{4.21}$$

Step 2. Study of the potentials between electrons and electrons. Now we consider the potentials such as $W(x_j, x_k)$. We have to split the study into three cases: $\{j,k\}\bigcap I = \varnothing$, $|\{j,k\}\bigcap I| = 1$ or $\{j,k\}\bigcap I = \{j,k\}$.

Case 1. When $\{j,k\}\bigcap I = \varnothing$, it means that

$$\mathcal{L}_I \frac{1}{|x_j - x_k|} u = \frac{1}{|x_j - x_k|} \mathcal{L}_I u.$$

From (4.11), we infer that under under condition (1)-(2) in Assumption 2.2 and $0 < T < 1$,

$$\left\| S\mathcal{L}_I(|x_j - x_k|^{-1}u)\right\|_{X_{p,T}} = \left\| S(|x_j - x_k|^{-1}\mathcal{L}_I u)\right\|_{X_{p,T}} \lesssim_{\alpha,p,\widetilde{p}} T^{1/\theta'_{\widetilde{p}} - 1/\theta_p} \|u\|_{X^1_{I,p,T}} \tag{4.22}$$

Case 2. For the case $|\{j,k\}\bigcap I| = 1$, we can assume that $j \in I$ but $k \notin I$. The case $j \notin I$ but $k \in I$ can be treated in the same manner. For $j \in I$ and $k \notin I$, we have

$$\mathcal{L}_I \frac{1}{|x_j - x_k|} u = (1 - \Delta_j)^{1/2} \frac{1}{|x_j - x_k|} \mathcal{L}_{I,j} u.$$

Indeed, this proof is essentially the same as for Step 1. in this proof: By replacing $a_\mu(t)$ by x_k, from (4.19) we will have

$$\begin{aligned}
&\left| \int_0^T \left\langle S[(1-\Delta_j)^{-1/2}\nabla_j] \cdot \left(\nabla_j \Big[\frac{1}{|x_j - x_k|} \mathcal{L}_{I,j} u(\cdot, x)\Big]\right), v(t,x) \right\rangle dt \right| \\
&\quad \lesssim_\alpha \int_0^T \left\| \Big[\frac{1}{|x_j - x_k|^\alpha} \mathcal{L}_{I,j} \nabla_j u(s,x)\Big]\right\|_{\mathcal{H}} \left\| \frac{1}{|x_j - x_k|^{1-\alpha}} S^*\big((1-\Delta_j)^{-1/2}\nabla_j v(\cdot,x)\big)(s)\right\|_{\mathcal{H}} ds.
\end{aligned}$$

Then proceeding as for (4.10), we infer that that under under condition (1)-(2) in Assumption 2.2 and $0 < T < 1$,

$$\left\| S\mathcal{L}_I(|x_j - x_k|^{-1}u)\right\|_{X_{p,T}} \lesssim_{\alpha,p,\widetilde{p}} T^{1/\theta'_{\widetilde{p}} - 1/\theta_p} \|u\|_{X^1_{I,p,T}} \tag{4.23}$$

Case 3. Finally, we consider the case $\{j,k\} \subset I$. In this case, we have

$$\mathcal{L}_I \frac{1}{|x_j - x_k|} u = (1 - \Delta_j)^{1/2}(1 - \Delta_k)^{1/2} \frac{1}{|x_j - x_k|} \mathcal{L}_{I,j,k} u.$$

According to (2.15), we have

$$\begin{aligned}
\mathcal{L}_I \frac{1}{|x_j - x_k|} u = & \frac{1}{(1-\Delta_j)^{1/2}} \frac{1}{(1-\Delta_k)^{1/2}} \frac{1}{|x_j - x_k|} \mathcal{L}_{I,j,k} u \\
& + \frac{\nabla_j}{(1-\Delta_j)^{1/2}} \frac{1}{(1-\Delta_k)^{1/2}} \cdot \nabla_j \Big[\frac{1}{|x_j - x_k|} \mathcal{L}_{I,j,k} u\Big] \\
& + \frac{1}{(1-\Delta_j)^{1/2}} \frac{\nabla_k}{(1-\Delta_k)^{1/2}} \cdot \nabla_k \Big[\frac{1}{|x_j - x_k|} \mathcal{L}_{I,j,k} u\Big] \\
& + \Big[\frac{\nabla_j}{(1-\Delta_j)^{1/2}} \otimes \frac{\nabla_k}{(1-\Delta_k)^{1/2}}\Big] \cdot \left(\nabla_j \otimes \nabla_k \Big[\frac{1}{|x_j - x_k|} \mathcal{L}_{I,j,k} u\Big]\right).
\end{aligned} \tag{4.24}$$

Now the study of $S\mathcal{L}_I(|x_j - x_k|^{-1}u)$ is split into the study of the above four terms on the right-hand side of (4.24).

Concerning the first term, from (4.11), we infer that, under condition (1)-(2) in Assumption 2.2 and for any $0 < T < 1$ and any $D \subset \{1, \cdots, N\}$ with $1 \leqslant |D| \leqslant 2$,

$$\begin{aligned}
\left\| S \frac{1}{(1-\Delta_j)^{1/2}} \frac{1}{(1-\Delta_k)^{1/2}} \Big(\frac{1}{|x_j - x_k|} \mathcal{L}_{I,j,k} u\Big)\right\|_{X_{p,T}} &\lesssim_p \left\| S\Big(\frac{1}{|x_j - x_k|} u\Big)\right\|_{X_{p,T}} \\
&\lesssim_{\alpha,p,\widetilde{p}} T^{1/\theta'_{\widetilde{p}} - 1/\theta_p} \|\mathcal{L}_{I,j,k} u\|_{X_{p,T}} \lesssim_{\alpha,p,\widetilde{p}} T^{1/\theta'_{\widetilde{p}} - 1/\theta_p} \|\mathcal{L}_I u\|_{X_{p,T}}.
\end{aligned} \tag{4.25}$$

Here in the first inequality and the last inequality, we use (3.6b).

The second term on the right-hand side of (4.24) can be studied as for (4.18) by replacing a_μ by x_j:

$$\left\| |x_j - x_k|^{1-\alpha} \nabla_j \Big[\frac{1}{|x_j - x_k|}\Big] \mathcal{L}_{I,j,k} u(\cdot, x)\right\|_{\mathcal{H}} \lesssim \left\| \frac{1}{|x_j - x_k|^\alpha} \mathcal{L}_{I,j,k} \nabla_j u\right\|_{\mathcal{H}}.$$

Then proceeding as for (4.10) and using Theorem 3.6, we infer that under condition (1)-(2) in Assumption 2.2 and for any $0<T<1$ and any $D\subset\{1,\cdots,N\}$ with $1\leqslant|D|\leqslant 2$,

$$\begin{aligned}
&\Big|\int_0^T\Big\langle S\frac{\nabla_j}{(1-\Delta_j)^{1/2}}\frac{1}{(1-\Delta_j)^{1/2}}\cdot\Big(\nabla_j\Big[\frac{1}{|x_j-x_k|}\mathcal{L}_{I,j}u(\cdot,x)\Big]\Big),v(t,x)\Big\rangle\,dt\Big|\\
&\quad\lesssim_\alpha\int_0^T\Big\|\Big[\frac{1}{|x_j-x_k|^\alpha}\mathcal{L}_{I,j,k}\nabla_j u(s,x)\Big]\Big\|_{\mathcal{H}}\\
&\qquad\times\Big\|\frac{1}{|x_j-x_k|^{1-\alpha}}S^*\Big(\frac{\nabla_j}{(1-\Delta_j)^{1/2}}\frac{1}{(1-\Delta_j)^{1/2}}v(\cdot,x)\Big)(s)\Big\|_{\mathcal{H}}\,ds\\
&\quad\lesssim_{\alpha,p,\tilde p}T^{1/\theta'_{\tilde p}-1/\theta_p}\Big(\|\mathcal{L}_I u\|_{L_t^\infty(I_T,\mathcal{H})}+\|\mathcal{L}_I u\|_{L_t^{\theta_p}(I_T,L^{p,2}_{j,k})}\Big)\min\{\|v\|_{L_t^{\theta'_p}(I_T,L_D^{p',2})},\|v\|_{L_t^1(I_T,\mathcal{H})}\}.
\end{aligned}$$

Hence, under condition (1)-(2) in Assumption 2.2 and for any $0<T<1$ and any $D\subset\{1,\cdots,N\}$ with $1\leqslant|D|\leqslant 2$,

$$\Big\|S\frac{\nabla_j}{(1-\Delta_j)^{1/2}}\frac{1}{(1-\Delta_k)^{1/2}}\Big(\frac{1}{|x_j-x_k|}\mathcal{L}_{I,j,k}u\Big)\Big\|_{X_{p,T}}\lesssim_{\alpha,p,\tilde p}T^{1/\theta'_{\tilde p}-1/\theta_p}\|\mathcal{L}_I u\|_{X_{p,T}}. \tag{4.26}$$

Analogously, for the third term on the right-hand side of (4.24), we have that under condition (1)-(2) in Assumption 2.2 and for any $0<T<1$ and any $D\subset\{1,\cdots,N\}$ with $1\leqslant|D|\leqslant 2$,

$$\Big\|S\frac{1}{(1-\Delta_j)^{1/2}}\frac{\nabla_k}{(1-\Delta_k)^{1/2}}\Big(\frac{1}{|x_j-x_k|}\mathcal{L}_{I,j,k}u\Big)\Big\|_{X_{p,T}}\lesssim_{\alpha,p,\tilde p}T^{1/\theta'_{\tilde p}-1/\theta_p}\|\mathcal{L}_I u\|_{X_{p,T}}. \tag{4.27}$$

It remains to study the last term on the right-hand side of (4.24) where we will use Lemma 2.10 and (4.14) (i.e., u is antisymmetric w.r.t. $\{j,k\}$). We have

$$\begin{aligned}
\nabla_j\otimes\nabla_k\Big[\frac{1}{|x_j-x_k|}\mathcal{L}_{I,j,k}u\Big]&=\frac{1}{|x_j-x_k|}\nabla_j\otimes\nabla_k\mathcal{L}_{I,j,k}u+\big[\nabla_j\frac{1}{|x_j-x_k|}\big]\otimes\nabla_k\mathcal{L}_{I,j,k}u\\
&\quad+\big[\nabla_k\frac{1}{|x_j-x_k|}\big]\otimes\nabla_j\mathcal{L}_{I,j,k}u+\big[\nabla_j\otimes\nabla_k\mathcal{L}_{I,j,k}\frac{1}{|x_j-x_k|}\big]u.
\end{aligned}$$

Thus, from Lemma 2.9, Lemma 2.10 and (4.14),

$$\begin{aligned}
&\Big\||x_j-x_k|^{1-\alpha}\nabla_j\Big[\frac{1}{|x_j-x_k|}\Big]\mathcal{L}_{I,j,k}u(\cdot,x)\Big\|_{\mathcal{H}}\\
&\quad\lesssim\Big\|\frac{1}{|x_j-x_k|^\alpha}\mathcal{L}_{I,j,k}\nabla_j\otimes\nabla_k u\Big\|_{\mathcal{H}}+\Big\|\frac{1}{|x_j-x_k|^{1+\alpha}}\mathcal{L}_{I,j,k}\nabla_j u\Big\|_{\mathcal{H}}\\
&\qquad+\Big\|\frac{1}{|x_j-x_k|^{1+\alpha}}\mathcal{L}_{I,j,k}\nabla_k u\Big\|_{\mathcal{H}}+\Big\|\frac{1}{|x_j-x_k|^{2+\alpha}}\mathcal{L}_{I,j,k}u\Big\|_{\mathcal{H}}\\
&\quad\lesssim\Big\|\frac{1}{|x_j-x_k|^\alpha}\mathcal{L}_{I,j,k}\nabla_j\otimes\nabla_k u\Big\|_{\mathcal{H}}.
\end{aligned}$$

Now proceeding as for (4.10) and using Theorem 3.6, we infer that under condition (1)-(2) in Assumption 2.2 and for any $0<T<1$ and any $D\subset\{1,\cdots,N\}$ with $1\leqslant|D|\leqslant 2$,

$$\begin{aligned}
&\Big|\int_0^T\Big\langle S\Big[\frac{\nabla_j}{(1-\Delta_j)^{1/2}}\otimes\frac{\nabla_k}{(1-\Delta_j)^{1/2}}\Big]\cdot\Big(\nabla_j\otimes\nabla_k\Big[\frac{1}{|x_j-x_k|}\mathcal{L}_{I,j}u(\cdot,x)\Big]\Big),v(t,x)\Big\rangle\,dt\Big|\\
&\quad\lesssim_\alpha\int_0^T\Big\|\frac{1}{|x_j-x_k|^\alpha}\mathcal{L}_{I,j,k}\nabla_j\otimes\nabla_k u(s,x)\Big\|_{\mathcal{H}}\\
&\qquad\times\Big\|\frac{1}{|x_j-x_k|^{1-\alpha}}S^*\Big(\frac{\nabla_j}{(1-\Delta_j)^{1/2}}\otimes\frac{\nabla_k}{(1-\Delta_j)^{1/2}}v(\cdot,x)\Big)(s)\Big\|_{\mathcal{H}}\,ds\\
&\quad\lesssim_{\alpha,p,\tilde p}T^{1/\theta'_{\tilde p}-1/\theta_p}\Big(\|\mathcal{L}_I u\|_{L_t^\infty(I_T,\mathcal{H})}+\|\mathcal{L}_I u\|_{L_t^{\theta_p}(I_T,L^{p,2}_{j,k})}\Big)\min\{\|v\|_{L_t^{\theta'_p}(I_T,L_D^{p',2})},\|v\|_{L_t^1(I_T,\mathcal{H})}\}.
\end{aligned}$$

As a result, under condition (1)-(2) in Assumption 2.2 and for any $0<T<1$ and any $D\subset\{1,\cdots,N\}$ with $1\leqslant|D|\leqslant 2$,

$$\Big\|S\Big[\frac{\nabla_j}{(1-\Delta_j)^{1/2}}\otimes\frac{\nabla_k}{(1-\Delta_j)^{1/2}}\Big]\cdot\Big(\nabla_j\otimes\nabla_k\Big[\frac{1}{|x_j-x_k|}\mathcal{L}_{I,j}u(\cdot,x)\Big]\Big)\Big\|_{X_{p,T}}\lesssim_{\alpha,p,\tilde p}T^{1/\theta'_{\tilde p}-1/\theta_p}\|\mathcal{L}_I u\|_{X_{p,T}}. \tag{4.28}$$

Now we conclude from (4.25)-(4.28) that under condition (1)-(2) in Assumption 2.2 and for any $0<T<1$,

$$\Big\|S\Big(\frac{1}{|x_j-x_k|}u(\cdot,x)\Big)\Big\|_{X^1_{I,p,T}}\lesssim_{\alpha,p,\tilde p}T^{1/\theta'_{\tilde p}-1/\theta_p}\|u\|_{X^1_{I,p,T}}. \tag{4.29}$$

Conclusion for all cases. Finally we can conclude from (4.22), (4.23) and (4.29) that under condition (1)-(2) in Assumption 2.2 and for any $0 < T < 1$,

$$\Big\| S\Big(\frac{1}{|x_j - x_k|} u(\cdot, x)\Big)\Big\|_{X^1_{I,p,T}} \lesssim_{\alpha,p,\widetilde{p}} ZT^{1/\theta'_{\widetilde{p}} - 1/\theta_p} \|u\|_{X^1_{I,p,T}}. \tag{4.30}$$

Step 3. Conclusion. From (4.21) and (4.30), we infer that for any $0 < T < 1$, p satisfying (4.7) and $\widetilde{p}$ satisfying (4.4), there exists a constant $C_{T,2} := C_{T,2}(\alpha, p, \widetilde{p}) \geqslant 1$ such that

$$\|Qu\|_{X^1_{I,p,T}} \leqslant C_{T,2}(Z+N)NT^{1/\theta'_{\widetilde{p}} - 1/\theta_p} \|u\|_{X^1_{I,p,T}}. \tag{4.31}$$

Now let $C_{T,2}(Z+N)NT^{1/\theta'_{\widetilde{p}} - 1/\theta_p} \leqslant \frac{1}{2}$, we get

$$\|Qu\|_{X^1_{I,p,T}} \leqslant \frac{1}{2}\|u\|_{X^1_{I,p,T}}.$$

Thus under Assumption 2.2, we have that $1 + iQ$ is invertible on $X^1_{I,p,T}$. As a result,

$$\|u\|_{X^1_{I,p,T}} = \|(1+iQ)^{-1}(U_0(\cdot)u_0)\|_{X^1_{I,p,T}} \leqslant 2\|U_0(\cdot)u_0\|_{X^1_{I,p,T}} \lesssim_q \|u_0\|_{H^1_{I,\mathrm{mix}}}.$$

This gives (2.8) and shows the uniqueness of the solution u in $X^1_{I,p,T}$. Hence the theorem. □

5. Justification of the hyperbolic cross space approximation (1.14)

Now we are going to prove Theorem 2.8, in particular (2.9). Before going further, we need the following result which can be regarded as an evolution version of (1.11).

Lemma 5.1. *Let $u_0 \in H^1_{I_1,\mathrm{mix}} \bigcap H^1_{I_2,\mathrm{mix}}$. Under Assumption 2.2 we have*

$$\|(1 - P_{\chi_R})u\|_{X_{p,T}} \lesssim_p \frac{1}{R} \sum_{\ell=1,2} \|u_0\|_{H^1_{I_\ell,\mathrm{mix}}}. \tag{5.1}$$

Proof. By Duhamel formula (2.12), we know

$$(1 - P_{\chi_R})u(t) = (1 - P_{\chi_R})U_0(t)u_0 + i(1 - P_{\chi_R})Qu(t).$$

Thus, by (3.3a),

$$\begin{aligned}\|(1 - P_{\chi_R})u\|_{X_{p,T}} &\leqslant \|U_0(t)(1 - P_{\chi_R})u_0\|_{X_{p,T}} + \|(1 - P_{\chi_R})Qu(t)\|_{X_{p,T}} \\ &\lesssim_p \|(1 - P_{\chi_R})u_0\|_{\mathcal{H}} + \|(1 - P_{\chi_R})Qu(t)\|_{X_{p,T}}.\end{aligned}$$

According to (3.5), we have

$$\|(1 - P_{\chi_R})u_0\|_{\mathcal{H}} \leqslant \frac{1}{R}\Big\| \sum_{\ell=1,2} \mathcal{L}_{I_\ell} u_0\Big\|_{\mathcal{H}} \leqslant \frac{1}{R} \sum_{\ell=1,2} \|u\|_{H^1_{I_\ell,\mathrm{mix}}}. \tag{5.2}$$

Thus,

$$\begin{aligned}\|(1 - P_{\chi_R})u\|_{X_{p,T}} &\leqslant \|U_0(t)(1 - P_{\chi_R})u_0\|_{X_{p,T}} + \|(1 - P_{\chi_R})Qu(t)\|_{X_{p,T}} \\ &\lesssim_p \frac{1}{R} \sum_{\ell=1,2} \|u_0\|_{H^1_{I_\ell,\mathrm{mix}}} + \|(1 - P_{\chi_R})Qu(t)\|_{X_{p,T}}.\end{aligned} \tag{5.3}$$

It remains to show that $\|(1 - P_{\chi_R})Qu(t)\|_{X_{p,T}} \lesssim_p \frac{1}{R}\sum_{\ell=1,2} \|u_0\|_{H^1_{I_\ell,\mathrm{mix}}}$. To do so, here we are going to prove

$$\|(1 - P_{\chi_R})Qu(t)\|_{X_{p,T}} \lesssim_p \frac{1}{R} \sum_{\ell=1,2} \|u(t)\|_{X^1_{I_\ell,p,T}}. \tag{5.4}$$

Then by (2.8), under Assumption 2.2 we have

$$\|(1 - P_{\chi_R})Qu(t)\|_{X_{p,T}} \lesssim_p \frac{1}{R} \sum_{\ell=1,2} \|u_0\|_{H^1_{I_\ell,\mathrm{mix}}}.$$

This and (5.3) give (5.1). Hence this lemma.

Now to end the proof, we prove (5.4) by using Corollary 3.5. As for the mixed regularity, we consider this problem in the scalar product: For any $D \subset \{1, \cdots, N\}$ and $1 \leqslant |D| \leqslant 2$, and for any $u(t,x) \in X^1_{I,p,T}$ and $v(t,x) \in L^{\theta'_p}_t(I_T, L^{p',2}_D)$ or $v(t,x) \in L^\infty_t(I_T, \mathcal{H})$, we are going to prove

$$\Big| \int_0^T \langle (1 - P_{\chi_R})Qu)(t), v(t)\rangle \, dt \Big| \lesssim T^\theta \sum_{\ell=1,2} \|u\|_{X^1_{I_\ell,p,T}} \min\{\|v\|_{L^{\theta'_p}_t(I_T, L^{p',2}_D)}, \|v\|_{L^\infty_y(I_T,\mathcal{H})}\}$$

for some $\theta > 0$ and $p > 2$.

Indeed, we have

$$\begin{aligned}&\left|\int_0^T \langle (1-P_{\chi_R})Qu)(t), v(t)\rangle\, dt\right| \\ &\quad \leqslant \sum_{\ell=1,2}\sum_{j=1}^{N}\left|\int_0^T \left\langle \mathcal{L}_{I_\ell} V(s,x_j)u(s), S^*\Big[\Big(\sum_{\ell=1,2}\mathcal{L}_{I_\ell}\Big)^{-1}(1-P_{\chi_R})v\Big](s)\right\rangle ds\right| \\ &\quad + \sum_{\ell=1,2}\sum_{1\leqslant j<k\leqslant N}\left|\int_0^T \left\langle \mathcal{L}_{I_\ell} W(x_j,x_k)u(s), S^*\Big[\Big(\sum_{\ell=1,2}\mathcal{L}_{I_\ell}\Big)^{-1}(1-P_{\chi_R})v\Big](s)\right\rangle ds\right|. \end{aligned} \tag{5.5}$$

The proof of the terms on the right-hand side of (5.5) is essentially the same as Step 1. and Step 2. of the proof of Theorem 2.6: We only need to replace the Strichartz estimate (3.3c) used in the proof of Theorem 2.6 by Strichartz estimate (3.4b). Then under Assumption 2.2, we obtain (5.4). □

Proof of Theorem 2.8. We first consider the existence of solutions to (1.14). The proof is essentially the same as for Theorem 2.5, but we need the following modification: replace the Strichartz estimate (3.3c) used in the proof of Theorem 2.6 by Strichartz estimate (3.4a) as for Lemma 5.1. Then we know that for every $u_0 \in \mathcal{H}$, the problem (1.14) has a unique global-in-time solution $u_R \in X_{p,\infty}$.

Now we consider (2.9). Indeed, we have

$$\|u-u_R\|_{X_{p,T}} \leqslant \|u-P_{\chi_R}u\|_{X_{p,T}} + \|P_{\chi_R}u-u_R\|_{X_{p,T}}. \tag{5.6}$$

Now we are going to study $P_{\chi_R}u-u_R$. By the Duhamel formula (2.12), we have

$$P_{\chi_R}u-u_R = -iP_{\chi_R}Q(u-u_R).$$

Replacing Strichartz estimate (3.3c) by (3.4a) and proceeding as for Step 1. and Step 2. in the proof of Theorem 2.5, we infer that under condition (1)-(2) in Assumption 2.2 and $0<T<1$, there exists a constant $C_{T,3} := C_{T,3}(\alpha,p,\widetilde{p}) \geqslant 1$ such that

$$\|P_{\chi_R}Q(u-u_R)\|_{X_{p,T}} \leqslant C_{T,3}(Z+N)NT^{1/\theta'_{\widetilde{p}}-1/\theta_p}\|u-u_R\|_{X_{p,T}}. \tag{5.7}$$

Then under Assumption 2.2,

$$\|P_{\chi_R}u-u_R\|_{X_{p,T}} \leqslant \|P_{\chi_R}Q(u-u_R)\|_{X_{p,T}} \leqslant \frac{1}{2}\|u-u_R\|_{X_{p,T}}$$

Inserting this into (5.6), we infer that under Assumption 2.2,

$$\|u-u_R\|_{X_{p,T}} \leqslant \|u-P_{\chi_R}u\|_{X_{p,T}} + \frac{1}{2}\|u-u_R\|_{X_{p,T}}.$$

Thus, from Lemma 5.1 under Assumption 2.2,

$$\|u-u_R\|_{X_{p,T}} \leqslant 2\|u-P_{\chi_R}u\|_{X_{p,T}} \lesssim_p \sum_{\ell=1,2}\frac{1}{R}\|u_0\|_{H^1_{I_\ell,\mathrm{mix}}}.$$

This ends the proof. □

Appendix A. Calderón-Zygmund inequality

This appendix is devoted to the study of the Calderón-Zygmund inequality and Mikhlin multiplier theorem on our functional space $L^{p,2}_j$. Indeed, this is a special case of the Calderón-Zygmund inequality for operator-valued kernels:

Theorem A.1. *[8, Theorem 2.1.9] Let A and B be two reflexive Banach spaces. Let T is a bounded operator from $L^2(\mathbb{R}^n, A)$ to $L^2(\mathbb{R}^n, B)$ defined by*

$$Tf(x) = \int_{\mathbb{R}^n} K(x-y)f(y)dy$$

with K being a $\mathcal{B}(A,B)$-valued function defined on $\mathbb{R}^n\backslash\{0\}$ and satisfying

$$\int_{|x|\geqslant 2|y|}\|K(x-y)-K(x)\|_{\mathcal{B}(A,B)}dx \leqslant C.$$

Then T is bounded from $L^p(A)$ to $L^p(B)$ with $1<p<\infty$.

To apply this Calderón-Zygmund inequality to our problem for the fractional Laplacian operator, we have to use the Mikhlin multiplier theorem.

If $a : \mathbb{R}^n \to \mathbb{C}$ is a bounded measurable function, it determines a bounded linear operator

$$T_a : L^2(\mathbb{R}^n, \mathbb{C}) \to L^2(\mathbb{R}^n, \mathbb{C})$$

given by

$$T_a u := \widecheck{a\widehat{u}}$$

for $u \in L^2(\mathbb{R}^n \times \mathbb{R}^m, \mathbb{C})$. Here $\widehat{u}(\xi_x, y) := \int_{\mathbb{R}^n} e^{-2\pi i x\cdot\xi_x} u(x,y)dx$ is the Fourier transform and $\check{u}(x,y)$ is the corresponding inverse Fourier transform.

Theorem A.2 (Mikhlin multiplier). *Let $m, n \in \mathbb{N}_0$. Let $a : \mathbb{R}^n\backslash\{0\} \to \mathbb{C}$ be a C^{n+2} function that satisfies the inequality*

$$|\partial^\alpha a(\xi)| \leqslant \frac{C}{|\xi|^\alpha}$$

for every $\xi \in \mathbb{R}^n\backslash\{0\}$ and every multi-index $\alpha = (\alpha_1, \cdots, \alpha_n) \in \mathbb{N}_0^n$ with $|\alpha| \leqslant n+2$. Then for any $1 < p < \infty$,

$$\|T_a f\|_{L^p(\mathbb{R}^n, L^2(\mathbb{R}^m))} \lesssim_n \|f\|_{L^p(\mathbb{R}^n, L^2(\mathbb{R}^m))}.$$

The proof of Theorem A.2 is exactly the same as the standard Mikhlin multiplier theorem (see, e.g., [10, Theorem 8.2]). The only difference is that we use Theorem A.1 with $A = B = L^2(\mathbb{R}^m)$ instead of the normal Calderón-Zygmund inequality.

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Long Meng: CERMICS, École des ponts ParisTech, 6 and 8 av. Pascal, 77455 Marne-la-Vallée, France
Email address: long.meng@enpc.fr