On the mixed regularity of N-body Coulombic wavefunctions

Long Meng

A note about the mixed regularity of Schrödinger Coulomb system

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Abstract

In this note, we proved some inequalities for Coulomb-type potential by extending the Herbst's inequality. Based on these inequalities, we can prove the optimal mixed regularity of Schrödinger Coulomb system directly even in consideration of Paulli exclusion principle. And we provided a hyperbolic cross space approximation, and deduced the estimates for L^2-norm and H^1-semi-norm of the errors.

1 Introduction and results

For most applications of molecular simulation, the matter is described by an assembly of nuclei equipped with electrons. And in the quantum world, the state of electrons is modelled by the N-body Hamiltonian operator:

$$H = -\frac{1}{2}\sum_{i=1}^{N} \triangle_i - V_{ne} + V_{ee} \tag{1}$$

with

$$V_{ne} := \sum_{i=1}^{N}\sum_{\nu=1}^{M} \frac{Z_\nu}{|x_i - a_\nu|},$$

and

$$V_{ee} := \frac{1}{2}\sum_{i,j=1, i\neq j}^{N} \frac{1}{|x_i - x_j|},$$

where $a_1 \cdots, a_M$ are the positions of nuclei endowed with the charge $Z_1, \cdots, Z_M$ respectively, and $x_1, \cdots, x_N$ are the coordinates of given N electrons. And the right hand-side terms respectively model the kinetic energy, the attraction between nuclei and electrons V_{ne}, the repulsion between electrons V_{ee}.

Mathematically, the electronic ground state or excited state problem can be expressed by the Euler-Lagrange equation which is indeed the eigenvalue problem of the operator (1):

$$Hu = \lambda u. \tag{2}$$

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In quantum mechanics, in addition to the spatial coordinates, a particle such as the electron may have internal degrees of freedom, the most important of which is spin. For example, the electrons have two kinds of spin $\sigma = \pm 1/2$ (here $\sigma = 1$ or $\sigma = 2$ for convenience). But here, we consider a more general kinds of particles equipped with q spin states. And we label them by the integer

$$\sigma \in \{1, \cdots, q\}.$$

And a wave function of N particles with q spin states can be written as

$$u : (\mathbb{R}^3)^N \times \{1, \cdots, q\}^N \to \quad \mathbb{C} : (x, \sigma) \to u(x, \sigma).$$

For fixed spin state σ, we can rewrite the wavefunction $u(x, \sigma)$ by $u(x)$ and

$$u : (\mathbb{R}^3)^N \to \mathbb{C} : x \to u(x, \sigma).$$

There are two kinds of particles: fermions and bosons. For fermions, the particles satisfy the Pauli exclusion principle. Mathematically speaking, let $P_{i,j}$ be a permutation which exchange the space coordinates x_i and x_j and the spins σ_i and σ_j simultaneously, then

$$u(P_{i,j}(x, \sigma)) = -u(x, \sigma).$$

In particular, the identical fermions are totally anti-symmetric. And for bosons, they satisfy the Bose–Einstein statistics which means the particles occupy the symmetric quantum states. Particularly for the identical bosons, they are totally symmetric.

Problem (2) is well-explored mathematically (see for example [HS00], and about the regularity properties of the eigenfunction of problem (2) [Kat57, HOHOS94, FHOHOS02, HOHOS01, FHOHOS05, HOHOLT08, FHOHOS09]). However,the advantage of this model vanishes when it comes to performing real calculation because of its large dimensionality. Thus models such as Hartree-Fock and Kohn-Sham are proposed, see for example [LBL05]. However they are no true, unbiased discretizations of the Schrödinger equation in the sense of numerical analysis.

Decades ago, H. Yserentant [Yse04, Yse07, Yse11, KY12] proposed a mixed regularity about the eigenfunctions of problem (2), and this result can help to break the complexity barriers in computational quantum mechanics. For fixed spin state σ, the particles are categorized into q subsets in terms of the spin states

$$\mathcal{I}_l := \{i; \sigma_i = l\}, \qquad s = 1, \cdots, q.$$

If $\exists l \in \{1, \cdots, q\}$ such that $i, j \in \mathcal{I}_l$, then

$$u(P_{i,j}x, \sigma) = -u(x, \sigma). \tag{3}$$

herein $P_{i,j}$ is a permutation which only exchanges the space coordinate x_i and x_j. If $x_i = x_j$, $u(x) = 0$. Thus the wavefunctions can counterbalance the singularity of the interaction potential between electrons. Based on this observation, H. Yserentant proved in [Yse04, Yse07] that the wavefunction u of problem (2) under spin state σ satisfies

$$\int \left(1 + \sum_{i=1}^{N} |2\pi\xi_i|^2\right) \left(\sum_{l=1}^{q} \prod_{k \in \mathcal{I}_l} (1 + |2\pi\xi_k|^2)\right) |\mathcal{F}(u)|^2 \, \mathrm{d}\xi < \infty$$

where $\mathcal{F}(u) := \int_{\mathbb{R}^d} u(x)e^{-2\pi i\xi\cdot x}dx$ is the Fourier transform of u.

Later, by using $r12$-methods and interpolation of Sobolev space, H.C. Kreusler and H. Yserentant [KY12] proved that the wavefunction u of problem (2) without regard to the spin state satisfies

$$\int \left(1+\sum_{i=1}^{N}|2\pi\xi_i|^2\right)^s \left(\prod_{k=1}^{N}(1+|2\pi\xi_k|^2)\right)^t |\mathcal{F}(u)|^2\, d\xi < 0,$$

for $s = 0, t = 1$ or $s = 1, t < 3/4$. And the bound $3/4$ is the best possible and can neither be reached nor surpassed.

But what is the best mixed regularities in consideration of the spin states? And is there an error estimate for it? In this note, we are trying to answer these questions.

The spin states of fermions can be divided into three cases which will provide different regularities:

(A) Any two particles have different spin states: for any $l \in \{1,\cdots,q\}$, $|\mathcal{I}_l| \leqslant 1$. In brief, $q = N$.

(B) Some particles have the same spin states while the others do not: there exists a $l \in \{1,\cdots,q\}$, such that $1 < |\mathcal{I}_l| < N$. In brief, $1 < q < N$.

(C) The particles are identical: there exists a $l \in \{1,\ldots,q\}$, such that $\mathcal{I}_l = \{1,\cdots,N\}$ and if $k \neq l$, $\mathcal{I}_k = \varnothing$. In brief, $q = 1$.

Indeed, the case (A) means that the wavefunction u is totally non-anti-symmetric (for any $i,j \in \{1,\cdots,N\}$, the equation (3) does not hold); and the case (B) means the wavefunction u has some kind of anti-symmetric property (for some $l \in \{1,\cdots,q\}$ and any $i,j \in \mathcal{I}_l$, the equation (3) holds); and the case (C) means that the wavefunction u is totally anti-symmetric (for any $i,j \in \{1,\cdots,N\}$, the equation (3) holds).

In particular, the bosons can be viewed as a exception of case (A), since they are non-anti-symmetric either.

Similar to [Yse04], we consider the test functions in $\mathcal{D}_{\mathcal{I}}$ which is the space of the infinite differentiable functions

$$u : (\mathbb{R}^3)^N \to \mathbb{C} : \quad (x_1,\cdots,x_N) \to u(x_1,\cdots,x_N)$$

having a bounded support with spin states taken into account. And its completion in $L^2((\mathbb{R}^3)^N), H^1((\mathbb{R}^3)^N)$ is denoted by $L^2_{\mathcal{I}}((\mathbb{R}^3)^N), H^1_{\mathcal{I}}((\mathbb{R}^3)^N)$ respectively.

For the case (B), define the operator $\mathcal{L}_{\mathcal{I},\alpha,\beta}$ by

$$\mathcal{L}_{\mathcal{I},\alpha,\beta} := \left(\sum_{l=1}^{q}\left(\prod_{j\in\mathcal{I}_l}(1+|\nabla_j|^2)^{\alpha}\right)\left(\prod_{i\in\mathcal{I}\setminus\mathcal{I}_l}(1+|\nabla_i|^2)^{\beta}\right)\right)^{1/2}.$$

where ∇_i is the gradient for the coordinate x_i. This operator is defined by the Fourier transform, for details see Section 2.

Specially for the case (A) or case (C), we define another operator $\mathcal{L}_{\alpha}$ by

$$\mathcal{L}_{\mathcal{I},\alpha} := \prod_{i=1}^{N}(1+|\nabla_i|^2)^{\alpha/2}.$$

It can be considered as a special case of operator $\mathcal{L}_{\mathcal{I},\alpha,\beta}$: $q=1$, $\mathcal{I}_l=\varnothing$ for case (A); and for the case (C), $q=1$, $\mathcal{I}_l=\{1,\cdots,N\}$.

Based on these operators, we introduce the following functional space $X_{\mathcal{I},\alpha,\beta}$ and $X_{\mathcal{I},\alpha}$ which is defined by

$$X_{\mathcal{I},\alpha,\beta}((\mathbb{R}^3)^N):=\{u,\mathcal{L}_{\mathcal{I},\alpha,\beta}u\in H^1_{\mathcal{I}}((\mathbb{R}^3)^N)\},$$

and

$$X_{\mathcal{I},\alpha}((\mathbb{R}^3)^N):=\{u,\mathcal{L}_{\mathcal{I},\alpha}u\in H^1_{\mathcal{I}}((\mathbb{R}^3)^N)\},$$

endowed with the norm

$$\|u\|_{\mathcal{I},\alpha,\beta}:=\|\mathcal{L}_{\mathcal{I},\alpha,\beta}u\|_{H^1_{\mathcal{I}}((\mathbb{R}^3)^N)},$$

and

$$\|u\|_{\mathcal{I},\alpha}:=\|\mathcal{L}_{\mathcal{I},\alpha}u\|_{H^1_{\mathcal{I}}((\mathbb{R}^3)^N)}.$$

Theorem 1.1. *Let u be the solution of the eigenvalue problems of operator 2 under the fixed spin state σ, then we have the following results:*

- *For the case (A),*
$$u\in\bigcap_{0\leqslant\beta<0.75}X_{\mathcal{I},\beta}.$$
- *For the case (B),*
$$u\in\bigcap_{0\leqslant\alpha,\beta<0.75}\ \bigcap_{\substack{1\leqslant\alpha<1.25,\\ \alpha+\beta<1.5,\\ 0<\beta}}X_{\mathcal{I},\alpha,\beta}.$$
- *For the case (C),*
$$u\in\bigcap_{0\leqslant\alpha<0.75}\ \bigcap_{1\leqslant\alpha<1.25}X_{\mathcal{I},\alpha}.$$

By Sobolev's interpolation, we can get the following corollary:

Corollary 1.2. *Under the assumption of Theorem 1.1:*

- *For the case (B),*
$$u\in\bigcap_{\substack{0\leqslant\alpha<1.25,\\ 0<\beta<0.75,\\ \alpha+\beta<1.5}}X_{\mathcal{I},\alpha,\beta}.$$
- *For the case (C),*
$$u\in\bigcap_{0\leqslant\alpha<1.25}X_{\mathcal{I},\alpha}.$$

Remark 1.3. *The optimality can be gotten from Lemma 3.8.*

Let

$$\mathcal{H}(R)=\left\{(\omega_1,\cdots,\omega_N)\in(\mathbb{R}^3)^N\,|\,\sum_{l=1}^{N}\left(\prod_{i\in\mathcal{I}_l}\left(1+\left|\frac{\omega_i}{\Omega}\right|^2\right)^{\alpha}\right)\left(\prod_{j\in\mathcal{I}\setminus\mathcal{I}_l}\left(1+\left|\frac{\omega_i}{\Omega}\right|^2\right)^{\beta}\right)\leqslant R^2\right\}$$

and we define the projector

$$(P_R u)(x) = \int \chi_R(\xi)\widehat{u}(\xi)\exp(2\pi i\xi\cdot x)\,\mathrm{d}\xi$$

with χ_R the characteristic function of the domain $\mathcal{H}(R)$.

Then we have the following norm convergence rate:

Theorem 1.4. *Under the conditions of α, β in Theorem 1.1, for all eigenfunctions $u \in H^1(\lambda)$ with fixed spin state σ and λ non-positive, and for Ω large enough, we have*

$$\|u - P_R u\|_{L^2((\mathbb{R}^3)^N)} \leqslant \frac{\sqrt{2q}}{R} e^{0.625}\|u\|_{L^2((\mathbb{R}^3)^N)},$$

and

$$\|\nabla(u - P_R u)\|_{L^2((\mathbb{R}^3)^N)} \leqslant \frac{\sqrt{2q}}{R} e^{0.625}\Omega\|u\|_{L^2((\mathbb{R}^3)^N)}.$$

2 Fractional Laplacian and related inequalities

For $0 < \alpha < 2$, the fractional Laplacian $|\nabla|^\alpha$ (or $(-\triangle)^{\alpha/2}$) is defined on functions $u : \mathbb{R}^d \to \mathbb{R}$ as a Fourier representation by

$$\mathcal{F}(|\nabla|^\alpha u)(\xi) = |2\pi\xi|^{2\alpha}\mathcal{F}(u)(\xi).$$

In addition, for $\alpha > 2$, the fractional Laplacian $|\nabla|^\alpha$ can be viewed as the composition of $|\nabla|^{\alpha - 2\lfloor\frac{\alpha}{2}\rfloor}$ and $(-\triangle)^{\lfloor\frac{\alpha}{2}\rfloor}$, where $\lfloor x\rfloor$ is the integer part of x.

A function $u \in L^2(\mathbb{R}^d)$ is said to be in $H^\alpha (\alpha > 0)$ if and only if

$$\|u\|^2_{H^\alpha(\mathbb{R}^d)} := \int_{\mathbb{R}^d} (1 + |\xi|^2)^\alpha |\mathcal{F}(u)(\xi)|^2\,\mathrm{d}\xi < \infty.$$

In this note, the operator $\mathcal{L}_{\mathcal{I},\alpha,\beta}$ is defined by the same manner:

$$\mathcal{F}(\mathcal{L}_{\mathcal{I},\alpha,\beta}u)(\xi) = \left(\sum_{l=1}^{q}\left(\prod_{i=1}^{N}(1 + |2\pi\xi_i|^2)^{\beta/2}\right)\left(\prod_{j\in\mathcal{I}_l}(1 + |2\pi\xi_j|^2)^{\alpha/2}\right)\right)^{1/2}\mathcal{F}(u)(\xi).$$

If we apply the Fourier transform to solve the Poisson equation

$$|\nabla|^\alpha u = f \quad \text{in}\,\mathbb{R}^d,$$

we find that $|2\pi\xi|^\alpha\mathcal{F}(u)(\xi) = \mathcal{F}(f)(\xi)$. The inverse of the fractional Laplacian, or negative power of the Laplacian $|\nabla|^{-\alpha}, s > 0$, is defined for $f \in \mathcal{S}(\mathbb{R}^d)$ as

$$\mathcal{F}(|\nabla|^{-\alpha}u)(\xi) = |2\pi\xi|^{-\alpha}\mathcal{F}(u)(\xi) \qquad \text{for}\, k \neq 0.$$

In principle, we need the restriction $0 < \alpha < d$ because when $\alpha \geqslant d$ the multiplier $|k|^{-\alpha}$ does not define a tempered distribution (for more details, see for example [Sti19]).

On the other hand, the term $\frac{1}{|x|^\alpha}$ is a tempered distribution for $0 < \alpha < d$ with Fourier transform

$$b_\alpha\mathcal{F}(|\cdot|^{-\alpha})(\xi) = b_{d-\alpha}|\xi|^{-d+\alpha}, \qquad b_\alpha = \pi^{-\alpha/2}\Gamma(\alpha/2), \tag{4}$$

(see for example [LL01]). Hence, if $0 < \alpha < d$, the operator $|\nabla|^{\alpha}$ can be represented by

$$|\nabla|^{-\alpha} u(x) = \frac{b_{d-\alpha}}{(2\pi)^{\alpha} b_{\alpha}} \int_{\mathbb{R}^d} |x-y|^{-d+\alpha} u(y)\, \mathrm{d}y. \tag{5}$$

Suppose that $0 < \alpha < d$, then $|\nabla|^{\alpha}|x|^{\beta}$ is a $L^1_{\mathrm{loc}}(\mathbb{R}^d)$-function for $0 < \beta < d - \alpha$ and

$$|\nabla|^{\alpha}|x|^{-\beta} = \frac{b_{\alpha+\beta} b_{d-\beta}}{b_{d-\alpha-\beta} b_{\beta}} |x|^{-\alpha-\beta}. \tag{6}$$

And $|\nabla|^{-\alpha}|x|^{-\beta}$ is equally a $L^1_{\mathrm{loc}}(\mathbb{R}^d)$-function for $0 < \alpha < \beta < d$ and

$$|\nabla|^{-\alpha}|x|^{-\beta} = \frac{b_{\beta-\alpha} b_{d-\beta}}{b_{d+\alpha-\beta} b_{\beta}} |x|^{\alpha-\beta}. \tag{7}$$

However, in this note, we need to deal with the term $|\nabla|^{\pm\alpha}(|x|^{-\beta}u)$. The first and most important result about it is the famous Herbst's inequality which is based on the Formula (5):

Theorem 2.1. *[Her77] Define the operator C_α on $\mathcal{S}(\mathbb{R}^d)$ by*

$$C_\alpha := |x|^{-\alpha}|\nabla|^{-\alpha}$$

and let $p^{-1} + q^{-1} = 1$. Suppose $\alpha > 0$ and $d\alpha^{-1} > p > 1$. Then C_α extends to a bounded operator on $L^p(\mathbb{R}^d)$ with

$$\|C_\alpha\|_{\mathcal{B}(L^p(\mathbb{R}^d))} = 2^{-\alpha} \frac{\Gamma(\frac{1}{2}(dp^{-1} - \alpha))\Gamma(\frac{1}{2}dq^{-1})}{\Gamma(\frac{1}{2}(dq^{-1} + \alpha))\Gamma(\frac{1}{2}dp^{-1})} \tag{8}$$

If $p \geqslant d\alpha^{-1}$ or $p = 1$, then C_α is unbounded.

Remark 2.2. *Let $v := |\nabla|^{\alpha} u$, then this theorem can be expressed as:*

$$\||x|^{-\alpha} u\|_{L^p(\mathbb{R}^d)} \leqslant \|C_\alpha\|_{\mathcal{B}(L^p(\mathbb{R}^d))} \||\nabla|^{\alpha} u\|_{L^p(\mathbb{R}^d)}.$$

Remark 2.3. *For $1 \leqslant p < d$ $p \neq 2$ and $\alpha = 1$, it is not the Hardy's inequality which is written as:*

$$\||x|^{-1} u\|_{L^p(\mathbb{R}^d)} \leqslant \frac{p}{d-p} \|\nabla u\|_{L^p(\mathbb{R}^d)}.$$

However, for $d > 2$, $p = 2$ and $\alpha = 1$, it is the Hardy's inequality since

$$\||\nabla| u\|_{L^2(\mathbb{R}^d)} = \|\nabla u\|_{L^2(\mathbb{R}^d)},$$

and

$$\|C_\alpha\|_{\mathcal{B}(L^p(\mathbb{R}^d))} = \frac{2}{d-2}.$$

Remark 2.4. *Let $(q)^{-1} + p^{-1} = 1$, then we have that*

$$\|C_\alpha^*\|_{\mathcal{B}(L^q(\mathbb{R}^d))} = \|C_\alpha\|_{\mathcal{B}(L^p(\mathbb{R}^d))}.$$

And particularly, when $p = 2$, we have a special result:

$$\|C_\alpha^*\|_{\mathcal{B}(L^2(\mathbb{R}^d))} = \|C_\alpha\|_{\mathcal{B}(L^2(\mathbb{R}^d))},$$

namely

$$\||\nabla|^{-\alpha} u\|_{L^2(\mathbb{R}^d)} \leqslant \|C_\alpha\|_{\mathcal{B}(L^2(\mathbb{R}^d))} \||x|^{\alpha} u\|_{L^2(\mathbb{R}^d)}.$$

In this note, we only need the case $d = 3$ and $p = 2$. Let

$$c_\alpha := \|C_\alpha\|_{\mathcal{B}(L^2(\mathbb{R}^3))}$$

for $0 < \alpha < 3/2$. And if $\alpha = 0$, then $\|u\|_{L^2(\mathbb{R}^d)} = \|u\|_{L^2(\mathbb{R}^d)}$, we define $c_0 := 1$.

Considering the interaction between electrons, we need to deal with the term $\frac{1}{|x-y|}$:

Lemma 2.5. *Define the operator $C_{\alpha,\beta}$ on $\mathcal{S}(\mathbb{R}^{3\times 3})$ by*

$$C_{\alpha,\beta} := |x-y|^{-\alpha-\beta}|\nabla_x|^{-\alpha}|\nabla_y|^{-\beta}$$

where ∇_x, ∇_y are the gradient for variable $x \in \mathbb{R}^3$ and $y \in \mathbb{R}^3$ respectively.

Suppose that $\alpha, \beta > 0$ and $\alpha + \beta < 3/2$. Then $C_{\alpha,\beta}$ extends to a bounded operator on $L^2(\mathbb{R}^{3\times 3})$ with

$$\|C_{\alpha,\beta}\|_{\mathcal{B}(L^2(\mathbb{R}^{3\times 3}))} \leqslant 2c_{\alpha+\beta}.$$

Proof. Notice that

$$\||x-y|^{-\alpha-\beta}|\nabla_x|^{-\alpha}|\nabla_y|^{-\beta}\|_{\mathcal{B}(L^2(\mathbb{R}^{3\times 3}))} = \||\nabla_x|^{-\alpha}|\nabla_y|^{-\beta}|x-y|^{-\alpha-\beta}\|_{\mathcal{B}(L^2(\mathbb{R}^{3\times 3}))}.$$

Now, for any function $u(x,y) \in L^2(\mathbb{R}^{3\times 3})$, by Fourier transform

$$\||\nabla_x|^{-\alpha}|\nabla_y|^{-\beta}|x-y|^{-\alpha-\beta}u\|_{L^2(\mathbb{R}^{3\times 3})} = (2\pi)^{-\alpha-\beta}\||\xi_x|^{-\alpha}|\xi_y|^{-\beta}\mathcal{F}(|x-y|^{-\alpha-\beta}u)(\xi_x,\xi_y)\|_{L^2(\mathbb{R}^{3\times 3})}.$$

Herein $\xi := (\xi_x, \xi_y)$, and ξ_x, ξ_y are the frequency with respect to x and y respectively. As $|t|^\alpha \leqslant |t|^{\alpha+\beta} + 1$ for $t \in \mathbb{R}$, and let $t = |\xi_x|/|\xi_y|$, we yield

$$|\xi_x|^{-\alpha}|\xi_y|^{-\beta} \leqslant |\xi_x|^{-\alpha-\beta} + |\xi_y|^{-\alpha-\beta}. \tag{9}$$

Thus,

$$\begin{aligned}
&\||\nabla_x|^{-\alpha}|\nabla_y|^{-\beta}|x-y|^{-\alpha-\beta}u\|_{L^2(\mathbb{R}^{3\times 3})}\\
=&(2\pi)^{-\alpha-\beta}\||\xi_x|^{-\alpha}|\xi_y|^{-\beta}\mathcal{F}(|x-y|^{-\alpha-\beta}u)(\xi_x,\xi_y)\|_{L^2(\mathbb{R}^{3\times 3})}\\
\leqslant&(2\pi)^{-\alpha-\beta}\||\xi_x|^{-\alpha-\beta}\mathcal{F}(|x-y|^{-\alpha-\beta}u)(\xi_x,\xi_y)\|_{L^2(\mathbb{R}^{3\times 3})}\\
&+(2\pi)^{-\alpha-\beta}\||\xi_y|^{-\alpha-\beta}\mathcal{F}(|x-y|^{-\alpha-\beta}u)(\xi_x,\xi_y)\|_{L^2(\mathbb{R}^{3\times 3})}\\
=&\||\nabla_x|^{-\alpha-\beta}|x-y|^{-\alpha-\beta}u\|_{L^2(\mathbb{R}^{3\times 3})}\\
&+\||\nabla_y|^{-\alpha-\beta}|x-y|^{-\alpha-\beta}u\|_{L^2(\mathbb{R}^{3\times 3})}.
\end{aligned}$$

For the term $\||\nabla_x|^{-\alpha-\beta}|x-y|^{-\alpha-\beta}u\|_{L^2(\mathbb{R}^{3\times 3})}$, it is an integral with respect to x and y together. Now, we only consider the integral over x and fix y. Changing coordinates $z = x - y$, then

$$\begin{aligned}
&\||\nabla_x|^{-\alpha-\beta}|x-y|^{-\alpha-\beta}u(x,y)\|_{L^2(\mathbb{R}^3_x)}(y)\\
=&\||\nabla_z|^{-\alpha-\beta}|z|^{-\alpha-\beta}u(z+y,y)\|_{L^2(\mathbb{R}^3_z)}(y)\\
\leqslant&c_{\alpha+\beta}\|u(z+y,y)\|_{L^2(\mathbb{R}^3_z)}(y)\\
=&c_{\alpha+\beta}\|u(x,y)\|_{L^2(\mathbb{R}^3_x)}(y).
\end{aligned}$$

Thus,

$$\||\nabla_x|^{-\alpha-\beta}|x-y|^{-\alpha-\beta}u\|_{L^2(\mathbb{R}^{3\times 3})} \leqslant c_{\alpha+\beta}\|u\|_{L^2(\mathbb{R}^{3\times 3})}.$$

Analogously,

$$\||\nabla_y|^{-\alpha-\beta}|x-y|^{-\alpha-\beta}u\|_{L^2(\mathbb{R}^{3\times 3})} \leqslant c_{\alpha+\beta}\|u\|_{L^2(\mathbb{R}^{3\times 3})}.$$

Consequently, we deduce that

$$\||\nabla_x|^{-\alpha}|\nabla_y|^{-\beta}|x-y|^{-\alpha-\beta}u\|_{L^2(\mathbb{R}^{3\times 3})} \leqslant 2c_{\alpha+\beta}\|u\|_{L^2(\mathbb{R}^{3\times 3})},$$

namely,

$$\||x-y|^{-\alpha-\beta}|\nabla_x|^{-\alpha}|\nabla_y|^{-\beta}\|_{\mathcal{B}(L^2(\mathbb{R}^{3\times 3}))} \leqslant 2c_{\alpha+\beta}.$$

□

If $u \in C_0^\infty(\mathbb{R}^3\backslash\{0\})$, for $\alpha > d/2$, we have the following Hardy's type inequality which is the generalization of [Yse04, Lemma 2] with a similar proof:

Lemma 2.6. *[Men19] If $u \in C_0^\infty(\mathbb{R}^3\backslash\{0\})$, then*

$$\left\|\frac{u}{|x|^\alpha}\right\|_{L^2(\mathbb{R}^3)} \leqslant \frac{2}{|2\alpha-3|}\left\|\frac{\nabla u}{|x|^{\alpha-1}}\right\|_{L^2(\mathbb{R}^3)}.$$

for $\alpha \in [1, 3/2) \cup (3/2, 5/2)$.

And the the potential of the interaction between electrons:

Corollary 2.7. *[Men19] If $u \in C_0^\infty(\mathbb{R}^{3\times 3})$ with $u(x,y) = -u(y,x)$ for $x, y \in \mathbb{R}^3$. Then we have the following inequality:*

$$\left\|\frac{u}{|x-y|^\alpha}\right\|_{L^2(\mathbb{R}^{3\times 3})} \leqslant \frac{4}{|2\alpha-5||2\alpha-3|}\left\|\frac{\nabla_x\nabla_y u}{|x-y|^{\alpha-2}}\right\|_{L^2(\mathbb{R}^{3\times 3})}$$

for $\alpha \in [2, 2.5)$.

Combining the Lemma 2.5 with the Corollary 2.7, we have

Corollary 2.8. *If $u \in C_0^\infty(\mathbb{R}^{3\times 3})$ with $u(x,y) = -u(y,x)$ for $x, y \in \mathbb{R}^3$. Then we have the following inequality:*

$$\left\|\frac{u}{|x-y|^\alpha}\right\|_{L^2(\mathbb{R}^{3\times 3})} \leqslant c_k\left\||\nabla_x|^{\alpha/2}|\nabla_y|^{\alpha/2}u\right\|_{L^2(\mathbb{R}^{3\times 3})}$$

with $c_\alpha = \frac{8c_{\alpha-2}}{(5-2\alpha)(2\alpha-3)}$ and $\alpha \in [2, 2.5)$.

3 Properties of the interaction potentials

In the proof of the mixed regularity, the study of the potential plays the core role. In this section, we analyse the regularity of the interaction potentials. And we split firstly the potentials into two types: nucleus-electron interaction potentials and electron-electron interaction potentials.

3.1 Nucleus-electron interaction potential

Lemma 3.1. *Let* $\mathcal{K} = (1+|\nabla|^2)^{\alpha/2}(1+|\nabla|^\alpha)^{-1}$, *then for any* $0 \leqslant \alpha \leqslant 2$

$$\|\mathcal{K}\|_{\mathcal{B}(L^2(\mathbb{R}^3))} \leqslant 1.$$

Proof. For any $0 \leqslant \alpha \leqslant 2$, $u \in L^2(\mathbb{R}^3)$,

$$\|\mathcal{K}u\|_{L^2(\mathbb{R}^3)} = \|(1+|2\pi\xi|^2)^{\alpha/2}(1+|2\pi\xi|^\alpha)^{-1}\mathcal{F}(u)\|_{L^2(\mathbb{R}^3)}.$$

As $(1+|2\pi\xi|^2)^{\alpha/2} \leqslant (1+|2\pi\xi|^\alpha)$, we know that

$$\|\mathcal{K}u\|_{L^2(\mathbb{R}^3)} \leqslant \|\mathcal{F}(u)\|_{L^2(\mathbb{R}^3)} = \|u\|_{L^2(\mathbb{R}^3)}.$$

Now we get the conclusion. □

Lemma 3.2. *For* $0 < \alpha < 1$, *and* $u \in H^{1-\alpha}(\mathbb{R}^3)$,

$$\left\| |\nabla|^{-\alpha} \frac{u}{|x-a_\nu|} \right\|_{L^2(\mathbb{R}^3)} \leqslant c_\alpha c_{1-\alpha} \||\nabla|^{1-\alpha} u\|_{L^2(\mathbb{R}^3)}.$$

And for $0.5 < \beta < 1.5$, *and* $u \in H^{2-\beta}(\mathbb{R}^3)$,

$$\||\nabla|^{-\beta}(\nabla|x-a_\nu|^{-1})u\|_{L^2(\mathbb{R}^3)} \leqslant c_\beta c_{2-\beta} \||\nabla|^{2-\beta} u\|_{L^2(\mathbb{R}^3)}.$$

Proof. Here we use Theorem 2.1 twice. And for convenience, let $a_\nu = 0$. Notice that by Theorem 2.1,

$$\||\nabla|^{-\alpha}|x|^{-\alpha}\|_{\mathcal{B}(L^2(\mathbb{R}^3))} = \||x|^{-\alpha}|\nabla|^{-\alpha}\|_{\mathcal{B}(L^2(\mathbb{R}^3))} = c_\alpha.$$

Then,

$$\left\| |\nabla|^{-\alpha} \frac{u}{|x|} \right\|_{L^2(\mathbb{R}^3)} \leqslant c_\alpha \||x|^{\alpha-1} u\|_{L^2(\mathbb{R}^3)}.$$

And

$$\||x|^{\alpha-1}u\|_{L^2(\mathbb{R}^3)} = \||x|^{\alpha-1}|\nabla|^{\alpha-1}|\nabla|^\alpha u\|_{L^2(\mathbb{R}^3)} \leqslant c_{1-\alpha} \||\nabla|^\alpha u\|_{L^2(\mathbb{R}^3)}.$$

Now we get

$$\left\| |\nabla|^{-\alpha} \frac{u}{|x-a_\nu|} \right\|_{L^2(\mathbb{R}^3)} \leqslant c_\alpha c_{1-\alpha} \||\nabla|^{1-\alpha} u\|_{L^2(\mathbb{R}^3)}.$$

And for the second inequality, similarly, as $0 < \beta < 1.5$ we get that

$$\left\| |\nabla|^{-\beta} \frac{u}{|x|} \right\|_{L^2(\mathbb{R}^3)} \leqslant c_\beta \||x|^\beta (\nabla|x|^{-1})u\|_{L^2(\mathbb{R}^3)}.$$

As $|\nabla|x|^{-1}| = |x|^{-2}$, we have that

$$\||x|^\beta(\nabla|x|^{-1})u\|_{L^2(\mathbb{R}^3)} = \||x|^{\beta-2}u\|_{L^2(\mathbb{R}^3)}.$$

Besides $0 < 2-\beta < 1.5$, by Theorem 2.1 again,

$$\||x|^{\beta-2}u\|_{L^2(\mathbb{R}^3)} \leqslant c_{2-\beta} \||\nabla|^{2-\beta} u\|_{L^2(\mathbb{R}^3)}.$$

Thus,

$$\||\nabla|^{-\beta}(\nabla|x-a_\nu|^{-1})u\|_{L^2(\mathbb{R}^3)} \leqslant c_\beta c_{2-\beta} \||\nabla|^{2-\beta} u\|_{L^2(\mathbb{R}^3)}.$$

□

Lemma 3.3. *For $0 < \alpha < 0.5$, and $u \in H^{1+\alpha}(\mathbb{R}^3)$,*

$$\left\| |\nabla|^\alpha \frac{u}{|x - a_\nu|} \right\|_{L^2(\mathbb{R}^3)} \leqslant (c_{1+\alpha} + c_\alpha) c_{1-\alpha} \| |\nabla|^{1+\alpha} u \|_{L^2(\mathbb{R}^3)}.$$

Proof. Similarly, for convenience, let $a_\nu = 0$. Notice that

$$\left\| |\nabla|^\alpha \frac{u}{|x|} \right\|_{L^2(\mathbb{R}^3)} = \left\| \nabla |\nabla|^{\alpha-1} \frac{u}{|x - a|} \right\|_{L^2(\mathbb{R}^3)}.$$

Thus,

$$\left\| |\nabla|^\alpha \frac{u}{|x|} \right\|_{L^2(\mathbb{R}^3)} \leqslant \left\| |\nabla|^{\alpha-1} (\nabla |x|^{-1}) u \right\|_{L^2(\mathbb{R}^3)} + \left\| |\nabla|^{\alpha-1} |x|^{-1} (\nabla u) \right\|_{L^2(\mathbb{R}^3)}.$$

By Lemma 3.2, we get

$$\left\| |\nabla|^{\alpha-1} (\nabla |x|^{-1}) u \right\|_{L^2(\mathbb{R}^3)} \leqslant c_{1-\alpha} c_{1+\alpha} \| |\nabla|^{1+\alpha} u \|_{L^2(\mathbb{R}^3)},$$

and

$$\left\| |\nabla|^{\alpha-1} |x|^{-1} (\nabla u) \right\|_{L^2(\mathbb{R}^3)} \leqslant c_{1-\alpha} c_\alpha \| |\nabla|^{1+\alpha} u \|_{L^2(\mathbb{R}^3)}.$$

Consequently,

$$\left\| |\nabla|^\alpha \frac{u}{|x - a_\nu|} \right\|_{L^2(\mathbb{R}^3)} \leqslant (c_{1+\alpha} + c_\alpha) c_{1-\alpha} \| |\nabla|^{1+\alpha} u \|_{L^2(\mathbb{R}^3)}.$$

□

Combining Hardy's inequality with Lemma 3.2 and Lemma 3.3, we have the following corollary:

Corollary 3.4. *For $-1 < \alpha < 0.5$, and $u \in H^{1+\alpha}(\mathbb{R}^3)$, then*

$$\left\| |\nabla|^\alpha \frac{u}{|x - a_\nu|} \right\|_{L^2(\mathbb{R}^3)} \leqslant C_\alpha \| |\nabla|^{1+\alpha} u \|_{L^2(\mathbb{R}^3)},$$

where $C_\alpha = (c_{1+\alpha} + c_\alpha) c_{1-\alpha}$ if $\alpha > 0$; $C_0 = 2$; $C_\alpha = c_{-\alpha} c_{1+\alpha}$ if $-1 < \alpha < 0$.

Now, the main estimate in this subsection is

Lemma 3.5. *For $u, v \in C_0^\infty(\mathbb{R}^3)$ and for any $0 < \alpha < 1.5$, then*

$$\begin{aligned} &\left| \left\langle (1 + |\nabla|^2)^{\alpha/2} \frac{u}{|x - a_\nu|}, (1 + |\nabla|^2)^{\alpha/2} v \right\rangle \right| \\ \leqslant &(C_{\alpha-1} + 2) \| (1 + |\nabla|^2)^{\alpha/2} u \|_{L^2(\mathbb{R}^3)} \| \nabla (1 + |\nabla|^2)^{\alpha/2} v \|_{L^2(\mathbb{R}^3)}. \end{aligned}$$

Proof. As $(1 + |\nabla|^2)^{\alpha/2} = (1 + |\nabla|^\alpha)\mathcal{K}$, we know that

$$\begin{aligned} &\left\langle (1 + |\nabla|^2)^{\alpha/2} \frac{u}{|x - a_\nu|}, (1 + |\nabla|^2)^{\alpha/2} v \right\rangle \\ = &\left\langle \mathcal{K} \frac{u}{|x - a_\nu|}, (1 + |\nabla|^2)^{\alpha/2} v \right\rangle + \left\langle |\nabla|^\alpha \mathcal{K} \frac{u}{|x - a_\nu|}, (1 + |\nabla|^2)^{\alpha/2} v \right\rangle. \end{aligned} \tag{10}$$

For the first term in the right-hand side, by Hölder inequality,

$$\left|\left\langle \mathcal{K}\frac{u}{|x-a_\nu|}, (1+|\nabla|^2)^{\alpha/2}v \right\rangle\right| \leqslant \|u\|_{L^2(\mathbb{R}^3)} \left\|\frac{1}{|x-a_\nu|}\mathcal{K}(1+|\nabla|^2)^{\alpha/2}v\right\|_{L^2(\mathbb{R}^3)}.$$

By Hardy's inequality or Herbst's inequality, we know that

$$\left\|\frac{1}{|x-a_\nu|}\mathcal{K}(1+|\nabla|^2)^{\alpha/2}v\right\|_{L^2(\mathbb{R}^3)} \leqslant 2\left\|\nabla\mathcal{K}(1+|\nabla|^2)^{\alpha/2}v\right\|_{L^2(\mathbb{R}^3)}.$$

And as

$$\left\|\nabla\mathcal{K}(1+|\nabla|^2)^{\alpha/2}v\right\|_{L^2(\mathbb{R}^3)} = \left\|\mathcal{K}\nabla(1+|\nabla|^2)^{\alpha/2}v\right\|_{L^2(\mathbb{R}^3)} \leqslant \left\|\nabla(1+|\nabla|^2)^{\alpha/2}v\right\|_{L^2(\mathbb{R}^3)},$$

by Lemma 3.1, we know that

$$\left\|\frac{1}{|x-a_\nu|}\mathcal{K}(1+|\nabla|^2)^{\alpha/2}v\right\|_{L^2(\mathbb{R}^3)} \leqslant 2\left\|\nabla(1+|\nabla|^2)^{\alpha/2}v\right\|_{L^2(\mathbb{R}^3)}.$$

And obviously

$$\|u\|_{L^2(\mathbb{R}^3)} \leqslant \|(1+|\nabla|^2)^{\alpha/2}u\|_{L^2(\mathbb{R}^3)}.$$

Thus,

$$\left|\left\langle \mathcal{K}\frac{u}{|x-a_\nu|}, (1+|\nabla|^2)^{\alpha/2}v \right\rangle\right| \leqslant 2\|(1+|\nabla|^2)^{\alpha/2}u\|_{L^2(\mathbb{R}^3)}\left\|\nabla(1+|\nabla|^2)^{\alpha/2}v\right\|_{L^2(\mathbb{R}^3)}.$$

For the second term in the right-hand side of equation (10), by Hölder's inequality again

$$\left|\left\langle |\nabla|^\alpha\mathcal{K}\frac{u}{|x-a_\nu|}, (1+|\nabla|^2)^{\alpha/2}v \right\rangle\right| \leqslant \left\||\nabla|^{\alpha-1}\mathcal{K}\frac{u}{|x-a_\nu|}\right\|_{L^2(\mathbb{R}^3)}\|\nabla(1+|\nabla|^2)^{\alpha/2}v\|_{L^2(\mathbb{R}^3)}.$$

And we have that

$$\left\||\nabla|^{\alpha-1}\mathcal{K}\frac{u}{|x-a_\nu|}\right\|_{L^2(\mathbb{R}^3)} \leqslant \left\||\nabla|^{\alpha-1}\frac{u}{|x-a_\nu|}\right\|_{L^2(\mathbb{R}^3)}.$$

By Corollary 3.4,

$$\left\||\nabla|^{\alpha-1}\frac{u}{|x-a_\nu|}\right\|_{L^2(\mathbb{R}^3)} \leqslant C_{\alpha-1}\||\nabla|^\alpha u\|_{L^2(\mathbb{R}^3)} \leqslant C_{\alpha-1}\|(1+|\nabla|^2)^{\alpha/2}u\|_{L^2(\mathbb{R}^3)}.$$

Consequently,

$$\begin{aligned}&\left|\left\langle (1+|\nabla|^2)^{\alpha/2}\frac{u}{|x-a_\nu|}, (1+|\nabla|^2)^{\alpha/2}v \right\rangle\right| \\ \leqslant&(C_{\alpha-1}+2)\|(1+|\nabla|^2)^{\alpha/2}u\|_{L^2(\mathbb{R}^3)}\|\nabla(1+|\nabla|^2)^{\alpha/2}v\|_{L^2(\mathbb{R}^3)}.\end{aligned}$$

□

3.2 Electron-electron interaction potential

Lemma 3.6. *For $0 < \beta \leqslant \alpha$, $1 \leqslant \alpha + \beta < 1.5$ and $u(x,y) \in C_0^\infty(\mathbb{R}^{3\times 3})$, then*

$$\||\nabla_x|^{\alpha+\beta-1}|x-y|^{-1}u\|_{L^2(\mathbb{R}^{3\times 3})} \leqslant b_{\alpha,\beta}\||\nabla_x|^\alpha|\nabla_y|^\beta u\|_{L^2(\mathbb{R}^{3\times 3})}.$$

with $b_{\alpha,\beta} := 2((2\pi)^{\alpha+\beta-1}\pi^{-1}b_{\alpha+\beta}c_{\alpha+\beta}/b_{3-\alpha-\beta}+2)$

Proof. If $\alpha+\beta=1$, then by Lemma 2.5, we obtain directly

$$\||x-y|^{-1}u\|_{L^2(\mathbb{R}^{3\times 3})} \leqslant 2c_1\||\nabla_x|^\alpha|\nabla_y|^\beta u\|_{L^2(\mathbb{R}^{3\times 3})} = 4\||\nabla_x|^\alpha|\nabla_y|^\beta u\|_{L^2(\mathbb{R}^{3\times 3})},$$

where $c_1 = 4$. By virtue of Formula (4) and as $\mathcal{F}(f(\cdot+z))(\xi) = e^{2\pi i z\cdot\xi}\mathcal{F}(u)(\xi)$, we obtain that for $0<t<3$,

$$\mathcal{F}\left(\frac{u(x,y)}{|x-y|^t}\right)(\xi_x,\xi_y) = \frac{b_{3-t}}{b_t}\int_{\mathbb{R}^3}\frac{\mathcal{F}(u)(\xi_x-l,\xi_y+l)}{|l|^{3-t}}\,\mathrm{d}l. \tag{11}$$

In particular $\frac{b_2}{b_1} = \pi^{-1}$. Thus, for $\alpha+\beta>1$, by Plancherel's Theorem

$$\begin{aligned}
&\||\nabla_x|^{\alpha+\beta-1}|x-y|^{-1}u\|_{L^2(\mathbb{R}^{3\times 3})}\\
=&(2\pi)^{\alpha+\beta-1}\pi^{-1}\left\||\xi_x|^{\alpha+\beta-1}\int_{\mathbb{R}^3}\frac{\mathcal{F}(u)(\xi_x-l,\xi_y+l)}{|l|^2}\,\mathrm{d}l\right\|_{L^2(\mathbb{R}^{3\times 3})}\\
\leqslant&(2\pi)^{\alpha+\beta-1}\pi^{-1}\left\||\xi_x|^{\alpha+\beta-1}\int_{\mathbb{R}^3}\frac{|\mathcal{F}(u)(\xi_x-l,\xi_y+l)|}{|l|^2}\,\mathrm{d}l\right\|_{L^2(\mathbb{R}^{3\times 3})}.
\end{aligned}$$

For any l, $|\xi_x|^{\alpha+\beta-1} \leqslant |l|^{\alpha+\beta-1} + |\xi_x-l|^{\alpha+\beta-1}$, we yield

$$\begin{aligned}
&\||\nabla_x|^{\alpha+\beta-1}|x-y|^{-1}u\|_{L^2(\mathbb{R}^{3\times 3})}\\
\leqslant&(2\pi)^{\alpha+\beta-1}\pi^{-1}\left\|\int_{\mathbb{R}^3}\frac{|\mathcal{F}(u)(\xi_x-l,\xi_y+l)|}{|l|^{3-\alpha-\beta}}\,\mathrm{d}l\right\|_{L^2(\mathbb{R}^{3\times 3})}\\
&+(2\pi)^{\alpha+\beta-1}\pi^{-1}\left\|\int_{\mathbb{R}^3}\frac{||\xi_x-l|^{\alpha+\beta-1}\mathcal{F}(u)(\xi_x-l,\xi_y+l)|}{|l|^2}\,\mathrm{d}l\right\|_{L^2(\mathbb{R}^{3\times 3})}.
\end{aligned}$$

Using the Formula (11) again, for the first term, we get

$$\left\|\int_{\mathbb{R}^3}\frac{|\mathcal{F}(u)(\xi_x-l,\xi_y+l)|}{|l|^{3-\alpha-\beta}}\,\mathrm{d}l\right\|_{L^2(\mathbb{R}^{3\times 3})} = \frac{b_{\alpha+\beta}}{b_{3-\alpha-\beta}}\left\||x-y|^{-\alpha-\beta}\mathcal{F}^{-1}(|\mathcal{F}(u)|)\right\|_{L^2(\mathbb{R}^{3\times 3})}.$$

By Lemma 2.5, we obtain

$$\begin{aligned}
&\left\||x-y|^{-\alpha-\beta}\mathcal{F}^{-1}(|\mathcal{F}(u)|)\right\|_{L^2(\mathbb{R}^{3\times 3})}\\
\leqslant&2c_{\alpha+\beta}\||\nabla_x|^\alpha|\nabla_y|^\beta\mathcal{F}^{-1}(|\mathcal{F}(u)|)\|_{L^2(\mathbb{R}^{3\times 3})}\\
=&2c_{\alpha+\beta}\||\nabla_x|^\alpha|\nabla_y|^\beta u\|_{L^2(\mathbb{R}^{3\times 3})}.
\end{aligned}$$

For the second term, similarly

$$\begin{aligned}
&(2\pi)^{\alpha+\beta-1}\pi^{-1}\left\|\int_{\mathbb{R}^3}\frac{||\xi_x-l|^{\alpha+\beta-1}\mathcal{F}(u)(\xi_x-l,\xi_y+l)|}{|l|^2}\,\mathrm{d}l\right\|_{L^2(\mathbb{R}^{3\times 3})}\\
=&\||x-y|^{-1}\mathcal{F}^{-1}(|\mathcal{F}(|\nabla_x|^{\alpha+\beta-1}u)|)\|_{L^2(\mathbb{R}^{3\times 3})},
\end{aligned}$$

and as $\beta \leqslant \alpha$, then $\beta < 0.75$, thus

$$\begin{aligned}
&\||x-y|^{-1}\mathcal{F}^{-1}(|\mathcal{F}(|\nabla_x|^{\alpha+\beta-1}u)|)\|_{L^2(\mathbb{R}^{3\times 3})}\\
\leqslant& 2c_1\||\nabla_x|^{1-\beta}|\nabla_y|^{\beta}\mathcal{F}^{-1}(|\mathcal{F}(|\nabla_x|^{\alpha+\beta-1}u)|)\|_{L^2(\mathbb{R}^{3\times 3})}\\
=& 4\||\nabla_x|^{\alpha}|\nabla_y|^{\beta}u\|_{L^2(\mathbb{R}^{3\times 3})},
\end{aligned}$$

where $c_1 = 4$. Consequently, for $0 < \beta \leqslant \alpha$ and $1 < \alpha + \beta < 1.5$, we deduce

$$\begin{aligned}
&\||\nabla_x|^{\alpha+\beta-1}|x-y|^{-1}u\|_{L^2(\mathbb{R}^{3\times 3})}\\
\leqslant& 2((2\pi)^{\alpha+\beta-1}\pi^{-1}b_{\alpha+\beta}c_{\alpha+\beta}/b_{3-\alpha-\beta}+2)\||\nabla_x|^{\alpha}|\nabla_y|^{\beta}u\|_{L^2(\mathbb{R}^{3\times 3})}.
\end{aligned}$$

Combing these two cases together, as $b_1/b_2 = \pi$ and $4 < 2((2\pi)^{\alpha+\beta-1}\pi^{-1}b_{\alpha+\beta}c_{\alpha+\beta}/b_{3-\alpha-\beta}+2)$ if $\alpha + \beta = 1$, we conclude

$$\begin{aligned}
&\||\nabla_x|^{\alpha+\beta-1}|x-y|^{-1}u\|_{L^2(\mathbb{R}^{3\times 3})}\\
\leqslant& 2((2\pi)^{\alpha+\beta-1}\pi^{-1}b_{\alpha+\beta}c_{\alpha+\beta}/b_{3-\alpha-\beta}+2)\||\nabla_x|^{\alpha}|\nabla_y|^{\beta}u\|_{L^2(\mathbb{R}^{3\times 3})}.
\end{aligned}$$

□

Lemma 3.7. *For $u(x,y), v(x,y) \in C_0^\infty(\mathbb{R}^{3\times 3})$, and define*

$$\||v\||_{\alpha,\beta} := \left\|(1+|\nabla_x|^2)^{\alpha/2}(1+|\nabla_y|^2)^{\beta/2}v\right\|_{L^2(\mathbb{R}^{3\times 3})}.$$

If $0 < \alpha, \beta$ and $\alpha + \beta < 1.5$, then

$$\begin{aligned}
&\left|\left\langle(1+|\nabla_x|^2)^{\alpha/2}(1+|\nabla_y|^2)^{\beta/2}|x-y|^{-1}u, (1+|\nabla_x|^2)^{\alpha/2}(1+|\nabla_y|^2)^{\beta/2}v\right\rangle\right|\\
\leqslant& D_{\alpha,\beta}\||u\||_{\alpha,\beta}(\||\nabla_x v\||_{\alpha,\beta}+\||\nabla_y v\||_{\alpha,\beta}).
\end{aligned}$$

with

$$D_{\alpha,\beta} := \begin{cases} 1 + C_{\alpha-1} + C_{\beta-1} + 2c_{\alpha+\beta}c_{1-\alpha-\beta} & \text{if} \quad 0 < \alpha, \beta, \alpha+\beta < 1;\\ 1 + C_{\alpha-1} + C_{\beta-1} + b_{\alpha,\beta} & \text{if} \quad 0 < \alpha, \beta, 1 \leqslant \alpha+\beta < 1.5. \end{cases}$$

Furthermore, if u is anti-symmetric ($u(x,y) = -u(y,x)$), then for $1 \leqslant \alpha < 1.25$,

$$\begin{aligned}
&\left|\left\langle(1+|\nabla_x|^2)^{\alpha/2}(1+|\nabla_y|^2)^{\alpha/2}|x-y|^{-1}u, (1+|\nabla_x|^2)^{\alpha/2}(1+|\nabla_y|^2)^{\alpha/2}v\right\rangle\right|\\
\leqslant& D_{\alpha,\alpha}\||u\||_{\alpha,\beta}(\||\nabla_x v\||_{\alpha,\alpha}+\||\nabla_y v\||_{\alpha,\alpha}).
\end{aligned}$$

with if $1 \leqslant \alpha < 1.25$,

$$D_{\alpha,\alpha} := 1 + 2C_{\alpha-1} + 2(c_{2\alpha-2} + 2c_{2\alpha-1} + \sqrt{6}c_{2\alpha})c_{3-2\alpha}.$$

Proof. Similar to Lemma 3.5, we introduce the operator $\mathcal{K}_{\alpha,x}$ defined by

$$\mathcal{K}_{\alpha,x} := (1+|\nabla_x|^2)^{\alpha/2}(1+|\nabla_x|^\alpha)^{-1}.$$

Now,

$$\begin{aligned}
&\left\langle(1+|\nabla_x|^2)^{\alpha/2}(1+|\nabla_y|^2)^{\beta/2}|x-y|^{-1}u, (1+|\nabla_x|^2)^{\alpha/2}(1+|\nabla_y|^2)^{\beta/2}v\right\rangle\\
=&\left\langle(1+|\nabla_x|^\alpha)(1+|\nabla_y|^\beta)\mathcal{K}_{\alpha,x}\mathcal{K}_{\beta,y}|x-y|^{-1}u, (1+|\nabla_x|^2)^{\alpha/2}(1+|\nabla_y|^2)^{\beta/2}v\right\rangle\\
=&\left\langle\mathcal{K}_{\alpha,x}\mathcal{K}_{\beta,y}|x-y|^{-1}u, (1+|\nabla_x|^2)^{\alpha/2}(1+|\nabla_y|^2)^{\beta/2}v\right\rangle\\
&+\left\langle(|\nabla_x|^\alpha+|\nabla_y|^\beta)\mathcal{K}_{\alpha,x}\mathcal{K}_{\beta,y}|x-y|^{-1}u, (1+|\nabla_x|^2)^{\alpha/2}(1+|\nabla_y|^2)^{\beta/2}v\right\rangle\\
&+\left\langle|\nabla_x|^\alpha|\nabla_y|^\beta\mathcal{K}_{\alpha,x}\mathcal{K}_{\beta,y}|x-y|^{-1}u, (1+|\nabla_x|^2)^{\alpha/2}(1+|\nabla_y|^2)^{\beta/2}v\right\rangle
\end{aligned} \tag{12}$$

Now, we calculate every term in the right-hand side of this equation separately.

Steps 1. *For the first term.*

$$\begin{aligned}&\left|\left\langle \mathcal{K}_{\alpha,x}\mathcal{K}_{\beta,y}|x-y|^{-1}u,(1+|\nabla_x|^2)^{\alpha/2}(1+|\nabla_y|^2)^{\beta/2}v\right\rangle\right|\\ \leqslant&\|u\|_{L^2(\mathbb{R}^{3\times3})}\left\||x-y|^{-1}\mathcal{K}_{\alpha,x}\mathcal{K}_{\beta,y}(1+|\nabla_x|^2)^{\alpha/2}(1+|\nabla_y|^2)^{\beta/2}v\right\|_{L^2(\mathbb{R}^{3\times3})}.\end{aligned}$$

Using Hardy's inequality for x and y respectively and by Lemma 3.1, we get

$$\begin{aligned}&\left\||x-y|^{-1}\mathcal{K}_{\alpha,x}\mathcal{K}_{\beta,y}(1+|\nabla_x|^2)^{\alpha/2}(1+|\nabla_y|^2)^{\beta/2}v\right\|_{L^2(\mathbb{R}^{3\times3})}\\ \leqslant&\||\nabla_x\mathcal{K}_{\alpha,x}\mathcal{K}_{\beta,y}v\|_{\alpha,\beta}+\||\nabla_y\mathcal{K}_{\alpha,x}\mathcal{K}_{\beta,y}v\|_{\alpha,\beta}\\ \leqslant&\||\nabla_x v\|_{\alpha,\beta}+\||\nabla_y v\|_{\alpha,\beta}.\end{aligned}$$

As $\|u\|_{L^2(\mathbb{R}^{3\times3})}\leqslant\||u\|_{\alpha,\beta}$, then

$$\begin{aligned}&\left|\left\langle \mathcal{K}_{\alpha,x}\mathcal{K}_{\beta,y}|x-y|^{-1}u,(1+|\nabla_x|^2)^{\alpha/2}(1+|\nabla_y|^2)^{\beta/2}v\right\rangle\right|\\ \leqslant&\||u\|_{\alpha,\beta}(\||\nabla_x|v\|_{\alpha,\beta}+\||\nabla_y v\|_{\alpha,\beta}).\end{aligned}$$

Steps 2. *For the second term.*

$$\begin{aligned}&\left|\left\langle(|\nabla_x|^\alpha+|\nabla_y|^\beta)\mathcal{K}_{\alpha,x}\mathcal{K}_{\beta,y}|x-y|^{-1}u,(1+|\nabla_x|^2)^{\alpha/2}(1+|\nabla_y|^2)^{\beta/2}v\right\rangle\right|\\ \leqslant&\left|\left\langle|\nabla_x|^\alpha\mathcal{K}_{\alpha,x}\mathcal{K}_{\beta,y}|x-y|^{-1}u,(1+|\nabla_x|^2)^{\alpha/2}(1+|\nabla_y|^2)^{\beta/2}v\right\rangle\right|\\ &+\left|\left\langle|\nabla_y|^\beta\mathcal{K}_{\alpha,x}\mathcal{K}_{\beta,y}|x-y|^{-1}u,(1+|\nabla_x|^2)^{\alpha/2}(1+|\nabla_y|^2)^{\beta/2}v\right\rangle\right|.\end{aligned}$$

As $1=|\nabla_x|^{-1}|\nabla_x|$, we have that

$$\begin{aligned}&\left|\left\langle|\nabla_x|^\alpha\mathcal{K}_{\alpha,x}\mathcal{K}_{\beta,y}|x-y|^{-1}u,(1+|\nabla_x|^2)^{\alpha/2}(1+|\nabla_y|^2)^{\beta/2}v\right\rangle\right|\\ =&\left|\left\langle|\nabla_x|^{\alpha-1}\mathcal{K}_{\alpha,x}\mathcal{K}_{\beta,y}|x-y|^{-1}u,|\nabla_x|(1+|\nabla_x|^2)^{\alpha/2}(1+|\nabla_y|^2)^{\beta/2}v\right\rangle\right|\\ \leqslant&\left\||\nabla_x|^{\alpha-1}\mathcal{K}_{\alpha,x}\mathcal{K}_{\beta,y}|x-y|^{-1}u\right\|_{L^2(\mathbb{R}^{3\times3})}\||\nabla_x v\|_{\alpha,\beta}\end{aligned}$$

By Lemma 3.1,

$$\left\||\nabla_x|^{\alpha-1}\mathcal{K}_{\alpha,x}\mathcal{K}_{\beta,y}|x-y|^{-1}u\right\|_{L^2(\mathbb{R}^{3\times3})}\leqslant\left\||\nabla_x|^{\alpha-1}|x-y|^{-1}u\right\|_{L^2(\mathbb{R}^{3\times3})}.$$

Only considering the integral over $x\in\mathbb{R}^3$ and fixing $y\in\mathbb{R}^3$, by Corollary 3.4 for $0<\alpha<1.5$, we obtain

$$\left\||\nabla_x|^{\alpha-1}|x-y|^{-1}u\right\|_{L^2(\mathbb{R}^3_x)}(y)\leqslant C_{\alpha-1}\left\||\nabla_x|^\alpha u\right\|_{L^2(\mathbb{R}^3_x)}(y).$$

Thus,

$$\left\||\nabla_x|^{\alpha-1}|x-y|^{-1}u\right\|_{L^2(\mathbb{R}^{3\times3})}\leqslant C_{\alpha-1}\left\||\nabla_x|^\alpha u\right\|_{L^2(\mathbb{R}^{3\times3})}.$$

Since $\||\nabla_x|^\alpha u\|_{L^2(\mathbb{R}^{3\times3})}\leqslant\||u\|_{\alpha,\beta}$, we yield

$$\left\||\nabla_x|^{\alpha-1}|x-y|^{-1}u\right\|_{L^2(\mathbb{R}^{3\times3})}\leqslant C_{\alpha-1}\||u\|_{\alpha,\beta}.$$

Consequently,

$$\left|\left\langle|\nabla_x|^{\alpha}\mathcal{K}_{\alpha,x}\mathcal{K}_{\beta,y}|x-y|^{-1}u,(1+|\nabla_x|^2)^{\alpha/2}(1+|\nabla_y|^2)^{\beta/2}v\right\rangle\right|\leqslant C_{\alpha-1}\||u\|\|_{\alpha,\beta}\||\nabla_x v\|\|_{\alpha,\beta}.$$

Analogously, for $0<\beta<1.5$,

$$\left|\left\langle|\nabla_y|^{\beta}\mathcal{K}_{\alpha,x}\mathcal{K}_{\beta,y}|x-y|^{-1}u,(1+|\nabla_x|^2)^{\alpha/2}(1+|\nabla_y|^2)^{\beta/2}v\right\rangle\right|\leqslant C_{\beta-1}\||u\|\|_{\alpha,\beta}\||\nabla_y v\|\|_{\alpha,\beta}.$$

Thus,

$$\begin{aligned}&\left|\left\langle(|\nabla_x|^{\alpha}+|\nabla_y|^{\beta})\mathcal{K}_{\alpha,x}\mathcal{K}_{\beta,y}|x-y|^{-1}u,(1+|\nabla_x|^2)^{\alpha/2}(1+|\nabla_y|^2)^{\beta/2}v\right\rangle\right|\\ \leqslant&(C_{\alpha-1}+C_{\beta-1})\||u\|\|_{\alpha,\beta}(\||\nabla_x v\|\|_{\alpha,\beta}+\||\nabla_y v\|\|_{\alpha,\beta}).\end{aligned}$$

Steps 3. *For the last term without anti-symmetry.*

Assume that $\beta\leqslant\alpha$, thus $\beta<0.75$ and $0<\alpha-\beta<0.5$. If not, we can exchange the notation α,β and x,y respectively, then $\beta\leqslant\alpha$.

We have that

$$\begin{aligned}&\left|\left\langle|\nabla_x|^{\alpha}|\nabla_y|^{\beta}\mathcal{K}_{\alpha,x}\mathcal{K}_{\beta,y}|x-y|^{-1}u,(1+|\nabla_x|^2)^{\alpha/2}(1+|\nabla_y|^2)^{\beta/2}v\right\rangle\right|\\ =&\left|\left\langle|\nabla_x|^{\alpha+\beta-1}\mathcal{K}_{\alpha,x}\mathcal{K}_{\beta,y}|x-y|^{-1}u,|\nabla_x|^{1-\beta}|\nabla_y|^{\beta}(1+|\nabla_x|^2)^{\alpha/2}(1+|\nabla_y|^2)^{\beta/2}v\right\rangle\right|\end{aligned}$$

Since $|z|^{\beta}\leqslant 1+|z|$, let $z=|\xi_y/\xi_x|$, then

$$|\xi_x|^{1-\beta}|\xi_y|^{\beta}\leqslant|\xi_x|+|\xi_y|,$$

thus

$$\||\nabla_y|^{1-\beta}|\nabla_y|^{\beta}v\|\|_{\alpha,\beta}\leqslant(\||\nabla_x v\|\|_{\alpha,\beta}+\||\nabla_y v\|\|_{\alpha,\beta}).$$

Now, we yield

$$\begin{aligned}&\left|\left\langle|\nabla_x|^{\alpha}|\nabla_y|^{\beta}\mathcal{K}_{\alpha,x}\mathcal{K}_{\beta,y}|x-y|^{-1}u,(1+|\nabla_x|^2)^{\alpha/2}(1+|\nabla_y|^2)^{\beta/2}v\right\rangle\right|\\ \leqslant&\left\||\nabla_x|^{\alpha+\beta-1}|x-y|^{-1}u\right\|_{L^2(\mathbb{R}^{3\times3})}(\||\nabla_x v\|\|_{\alpha,\beta}+\||\nabla_y v\|\|_{\alpha,\beta}).\end{aligned}\tag{13}$$

If $\alpha+\beta<1$, by Theorem 2.1

$$\left\||\nabla_x|^{\alpha+\beta-1}|x-y|^{-1}u\right\|_{L^2(\mathbb{R}^{3\times3})}\leqslant c_{1-\alpha-\beta}\||x-y|^{-\alpha-\beta}u\|_{L^2(\mathbb{R}^{3\times3})}.$$

And by Lemma 2.5,

$$\left\||\nabla_x|^{\alpha+\beta-1}|x-y|^{-1}u\right\|_{L^2(\mathbb{R}^{3\times3})}\leqslant 2c_{1-\alpha-\beta}c_{\alpha+\beta}\||\nabla_x|^{\alpha}|\nabla_y|^{\beta}u\|_{L^2(\mathbb{R}^{3\times3})}.$$

If $\alpha+\beta\geqslant1$, then by Lemma 3.6 we get

$$\left\||\nabla_x|^{\alpha+\beta-1}|x-y|^{-1}u\right\|_{L^2(\mathbb{R}^{3\times3})}\leqslant b_{\alpha,\beta}\||\nabla_x|^{\alpha}|\nabla_y|^{\beta}u\|_{L^2(\mathbb{R}^{3\times3})}.$$

Finally, let $C_{\alpha,\beta}:=2c_{1-\alpha-\beta}c_{\alpha+\beta}$ if $\alpha+\beta<1$, and $C_{\alpha,\beta}:=b_{\alpha,\beta}$ if $\alpha+\beta\geqslant1$, then

$$\begin{aligned}&\left|\left\langle|\nabla_x|^{\alpha}|\nabla_y|^{\beta}\mathcal{K}_{\alpha,x}\mathcal{K}_{\beta,y}|x-y|^{-1}u,(1+|\nabla_x|^2)^{\alpha/2}(1+|\nabla_y|^2)^{\beta/2}v\right\rangle\right|\\ \leqslant&C_{\alpha,\beta}\||u\|\|_{\alpha,\beta}(\||\nabla_x v\|\|_{\alpha,\beta}+\||\nabla_y v\|\|_{\alpha,\beta}).\end{aligned}$$

Steps 4. *For the last term with anti-symmetry.*
For $\alpha = 1$, it has been proved in [Yse04], with

$$\begin{aligned}&\left|\left\langle|\nabla_x||\nabla_y||x-y|^{-1}u, |\nabla_x||\nabla_y|v\right\rangle\right|\\ \leqslant&(5+4\sqrt{6})\||u\||_{\alpha,\alpha}(\||\nabla_x v\||_{\alpha,\alpha}+\||\nabla_y v\||_{\alpha,\alpha}).\end{aligned}$$

Thus,

$$\begin{aligned}&\left|\left\langle|\nabla_x|^\alpha|\nabla_y|^\alpha\mathcal{K}_{\alpha,x}\mathcal{K}_{\alpha,y}|x-y|^{-1}u, (1+|\nabla_x|^2)^{\alpha/2}(1+|\nabla_y|^2)^{\alpha/2}v\right\rangle\right|\\ \leqslant&(5+4\sqrt{6})\||u\||_{\alpha,\alpha}(\||\nabla_x v\||_{\alpha,\alpha}+\||\nabla_y v\||_{\alpha,\alpha}).\end{aligned}$$

If $\alpha > 1$, we have that

$$\begin{aligned}&\left|\left\langle|\nabla_x|^\alpha|\nabla_y|^\alpha\mathcal{K}_{\alpha,x}\mathcal{K}_{\alpha,y}|x-y|^{-1}u, (1+|\nabla_x|^2)^{\alpha/2}(1+|\nabla_y|^2)^{\alpha/2}v\right\rangle\right|\\ =&\left|\left\langle|\nabla_x|^{\alpha-1/2}|\nabla_y|^{\alpha-1/2}\mathcal{K}_{\alpha,x}\mathcal{K}_{\alpha,y}|x-y|^{-1}u, |\nabla_x|^{1/2}|\nabla_y|^{1/2}(1+|\nabla_x|^2)^{\alpha/2}(1+|\nabla_y|^2)^{\alpha/2}v\right\rangle\right|\end{aligned}$$

As $|\xi_x|^{1/2}|\xi_y|^{1/2} \leqslant 1/2(|\xi_x|+|\xi_y|)$, we get

$$\begin{aligned}&\left|\left\langle|\nabla_x|^\alpha|\nabla_y|^\alpha\mathcal{K}_{\alpha,x}\mathcal{K}_{\alpha,y}|x-y|^{-1}u, (1+|\nabla_x|^2)^{\alpha/2}(1+|\nabla_y|^2)^{\alpha/2}v\right\rangle\right|\\ \leqslant&1/2\left\||\nabla_x|^{\alpha-1/2}|\nabla_y|^{\beta-1/2}|x-y|^{-1}u\right\|_{L^2(\mathbb{R}^{3\times3})}(\||\nabla_x v\||_{\alpha,\beta}+\||\nabla_y v\||_{\alpha,\beta}).\end{aligned}\tag{14}$$

Notice that

$$\begin{aligned}&\left\||\nabla_x|^{\alpha-1/2}|\nabla_y|^{\alpha-1/2}|x-y|^{-1}u\right\|_{L^2(\mathbb{R}^{3\times3})}\\ =&\left\|\nabla_x\nabla_y|\nabla_x|^{\alpha-3/2}|\nabla_y|^{\alpha-3/2}|x-y|^{-1}u\right\|_{L^2(\mathbb{R}^{3\times3})}\\ \leqslant&\left\||\nabla_x|^{\alpha-3/2}|\nabla_y|^{\alpha-3/2}|x-y|^{-1}(\nabla_x\nabla_y u)\right\|_{L^2(\mathbb{R}^{3\times3})}\\ &+\left\||\nabla_x|^{\alpha-3/2}|\nabla_y|^{\alpha-3/2}(\nabla_x|x-y|^{-1})(\nabla_y u)\right\|_{L^2(\mathbb{R}^{3\times3})}\\ &+\left\||\nabla_x|^{\alpha-3/2}|\nabla_y|^{\alpha-3/2}(\nabla_y|x-y|^{-1})(\nabla_x u)\right\|_{L^2(\mathbb{R}^{3\times3})}\\ &+\left\||\nabla_x|^{\alpha-3/2}|\nabla_y|^{\alpha-3/2}(\nabla_x\nabla_y|x-y|^{-1})u\right\|_{L^2(\mathbb{R}^{3\times3})}\end{aligned}$$

Now, we use Lemma 2.5 again. For the first term:

$$\left\||\nabla_x|^{\alpha-3/2}|\nabla_y|^{\alpha-3/2}|x-y|^{-1}(\nabla_x\nabla_y u)\right\|_{L^2(\mathbb{R}^{3\times3})} \leqslant 2c_{3-2\alpha}\left\||x-y|^{2-2\alpha}(\nabla_x\nabla_y u)\right\|_{L^2(\mathbb{R}^{3\times3})},$$

and as $0 < 2\alpha - 2 < 0.5$

$$\left\||x-y|^{2-2\alpha}(\nabla_x\nabla_y u)\right\|_{L^2(\mathbb{R}^{3\times3})} \leqslant 2c_{2\alpha-2}\||\nabla_x|^\alpha|\nabla_y|^\alpha u\|_{L^2(\mathbb{R}^{3\times3})}.$$

Thus,

$$\left\||\nabla_x|^{\alpha-3/2}|\nabla_y|^{\alpha-3/2}|x-y|^{-1}(\nabla_x\nabla_y u)\right\|_{L^2(\mathbb{R}^{3\times3})} \leqslant 4c_{3-2\alpha}c_{2\alpha-2}\||u\||_{\alpha,\alpha}.$$

For the second term,

$$\begin{aligned}&\left\||\nabla_x|^{\alpha-3/2}|\nabla_y|^{\alpha-3/2}(\nabla_x|x-y|^{-1})(\nabla_y u)\right\|_{L^2(\mathbb{R}^{3\times3})}\\ \leqslant&2c_{3-2\alpha}\||x-y|^{3-2\alpha}(\nabla_x|x-y|^{-1})(\nabla_y u)\|_{L^2(\mathbb{R}^{3\times3})}\\ =&2c_{3-2\alpha}\||x-y|^{1-2\alpha}\nabla_y u\|_{L^2(\mathbb{R}^{3\times3})}.\end{aligned}$$

As $0 < 2\alpha - 1 < 1.5$,

$$\left\| |x-y|^{1-2\alpha} \nabla_y u \right\|_{L^2(\mathbb{R}^{3\times 3})} \leqslant 2c_{2\alpha-1} \| |\nabla_x|^\alpha |\nabla_y|^\alpha u \|_{L^2(\mathbb{R}^{3\times 3})}.$$

Hence,

$$\left\| |\nabla_x|^{\alpha-3/2} |\nabla_y|^{\alpha-3/2} (\nabla_x |x-y|^{-1})(\nabla_y u) \right\|_{L^2(\mathbb{R}^{3\times 3})} \leqslant 4c_{3-2\alpha} c_{2\alpha-1} \|u\|_{\alpha,\alpha}.$$

And,

$$\left\| |\nabla_x|^{\alpha-3/2} |\nabla_y|^{\alpha-3/2} (\nabla_y |x-y|^{-1})(\nabla_x u) \right\|_{L^2(\mathbb{R}^{3\times 3})} \leqslant 4c_{3-2\alpha} c_{2\alpha-1} \|u\|_{\alpha,\alpha}.$$

For the last term, as $|\nabla_x \nabla_y |x-y|^{-1}|^2 = 6|x-y|^{-6}$,

$$\begin{aligned}
&\left\| |\nabla_x|^{\alpha-3/2} |\nabla_y|^{\alpha-3/2} (\nabla_x \nabla_y |x-y|^{-1}) u \right\|_{L^2(\mathbb{R}^{3\times 3})} \\
\leqslant & 2c_{3-2\alpha} \| |x-y|^{3-2\alpha} (\nabla_x \nabla_y |x-y|^{-1}) u \|_{L^2(\mathbb{R}^{3\times 3})} \\
= & 2\sqrt{6} c_{3-2\alpha} \| |x-y|^{-2\alpha} u \|_{L^2(\mathbb{R}^{3\times 3})}.
\end{aligned}$$

And since $u \in C_0^\infty$, $u(x,y) = -u(y,x)$, and $2 < 2\alpha < 2.5$, by Corollary 2.8,

$$\begin{aligned}
&\left\| |\nabla_x|^{\alpha-3/2} |\nabla_y|^{\alpha-3/2} (\nabla_x \nabla_y |x-y|^{-1}) u \right\|_{L^2(\mathbb{R}^{3\times 3})} \\
\leqslant & 2\sqrt{6} c_{3-2\alpha} c_{2\alpha} \| |\nabla_x|^\alpha |\nabla_y|^\alpha u \|_{L^2(\mathbb{R}^{3\times 3})}.
\end{aligned}$$

Consequently, if $\alpha > 1$,

$$\begin{aligned}
&\left| \left\langle |\nabla_x|^\alpha |\nabla_y|^\alpha \mathcal{K}_{\alpha,x} \mathcal{K}_{\alpha,y} |x-y|^{-1} u, (1+|\nabla_x|^2)^{\alpha/2} (1+|\nabla_y|^2)^{\alpha/2} v \right\rangle \right| \\
\leqslant & 2(c_{2\alpha-2} + 2c_{2\alpha-1} + \sqrt{6} c_{2\alpha}) c_{3-2\alpha} \|u\|_{\alpha,\alpha} (\| |\nabla_x v\|_{\alpha,\alpha} + \| |\nabla_y v\|_{\alpha,\alpha}).
\end{aligned}$$

As $c_0 = 1, c_1 = 2$ and $c_2 = 8$, we know that $5 + 4\sqrt{6} < 2(c_0 + 2c_1 + \sqrt{6}c_2)c_1)$. Finally for $1 \leqslant \alpha < 1.25$,

$$\begin{aligned}
&\left| \left\langle |\nabla_x|^\alpha |\nabla_y|^\alpha \mathcal{K}_{\alpha,x} \mathcal{K}_{\alpha,y} |x-y|^{-1} u, (1+|\nabla_x|^2)^{\alpha/2} (1+|\nabla_y|^2)^{\alpha/2} v \right\rangle \right| \\
\leqslant & 2(c_{2\alpha-2} + 2c_{2\alpha-1} + \sqrt{6} c_{2\alpha}) c_{3-2\alpha} \|u\|_{\alpha,\alpha} (\| |\nabla_x v\|_{\alpha,\alpha} + \| |\nabla_y v\|_{\alpha,\alpha}).
\end{aligned}$$

Steps 5. *Conclusion.*

Combining the first three steps, we conclude that there is a constant $D_{\alpha,\beta}$, such that

$$\begin{aligned}
&\left| \left\langle (1+|\nabla_x|^2)^{\alpha/2} (1+|\nabla_y|^2)^{\beta/2} |x-y|^{-1} u, (1+|\nabla_x|^2)^{\alpha/2} (1+|\nabla_y|^2)^{\beta/2} v \right\rangle \right| \\
\leqslant & D_{\alpha,\beta} \|u\|_{\alpha,\beta} (\| |\nabla_x v\|_{\alpha,\beta} + \| |\nabla_y v\|_{\alpha,\beta}),
\end{aligned}$$

with

$$D_{\alpha,\beta} := \begin{cases} 1 + C_{\alpha-1} + C_{\beta-1} + 2c_{1-\alpha-\beta} c_{\alpha+\beta} & \text{if} \quad 0 < \alpha, \beta, 0 < \alpha + \beta < 1; \\ 1 + C_{\alpha-1} + C_{\beta-1} + b_{\alpha,\beta} & \text{if} \quad 0 < \alpha, \beta, 1 \leqslant \alpha + \beta < 1.5. \end{cases}$$

Furthermore if $u(x,y) = -u(y,x)$, for $1 \leqslant \alpha < 1.25$,

$$\begin{aligned}
&\left| \left\langle (1+|\nabla_x|^2)^{\alpha/2} (1+|\nabla_y|^2)^{\alpha/2} |x-y|^{-1} u, (1+|\nabla_x|^2)^{\alpha/2} (1+|\nabla_y|^2)^{\alpha/2} v \right\rangle \right| \\
\leqslant & D_{\alpha,\alpha} \|u\|_{\alpha,\alpha} (\| |\nabla_x v\|_{\alpha,\alpha} + \| |\nabla_y v\|_{\alpha,\alpha}),
\end{aligned}$$

with if $1 \leqslant \alpha < 1.25$,

$$D_{\alpha,\alpha} := 1 + 2C_{\alpha-1} + 2(c_{2\alpha-2} + 2c_{2\alpha-2} + \sqrt{6} c_{2\alpha}) c_{3-2\alpha}.$$

□

Lemma 3.8. *For the condition $\alpha+\beta<1.5$ (or $\alpha<1.25$ if u is anti-symmetric) in Lemma 3.7, the bound 1.5 (or 1.25 respectively) can neither be reached nor surpassed.*

Proof. By estimate (13), we only need

$$\left\||\nabla_x|^{\alpha+\beta-1}|x-y|^{-1}u\right\|_{L^2(\mathbb{R}^{3\times 3})}<\infty.$$

Let $r_1=x-y$ and $r_2=x+y$, then for the gradient ∇_1,∇_2 corresponding to r_1,r_2 respectively we have that

$$\nabla_x=\nabla_1+\nabla_2,\qquad \nabla_y=\nabla_2-\nabla_1.$$

As $u\in C_0^\infty(\mathbb{R}^{3\times 3})$, by cusp analysis, $u(r_1,r_2)\sim\mathcal{O}(r_1/|r_1|)$ and $|r_1|^{-1}u\sim\mathcal{O}(|r_1|^{-1})$ when $|r_1|\to 0$. And $|\nabla_x|^{\alpha+\beta-1}=|\nabla_1+\nabla_2|^{\alpha+\beta-1}\sim|\nabla_1|^{\alpha+\beta-1}$ as $|r_1|\to 0$. Consequently, in a neighborhood of $|r_1|=0$ small enough, by Formula (6)

$$|\nabla_x|^{\alpha+\beta-1}|x-y|^{-1}u\sim\mathcal{O}(|\nabla_1|^{\alpha+\beta-1}|r_1|^{-1})=\mathcal{O}(|r_1|^{-\alpha-\beta}).$$

Thus if $\alpha+\beta\geqslant 1.5$,

$$\||\nabla_x|^{\alpha+\beta-1}|x-y|^{-1}u\|_{L^2(\mathbb{R}^{3\times 3})}=\infty.$$

For u is anti-symmetric, notice that $u\sim\mathcal{O}(|r_1|)$ when $|r_1|\to 0$. Then, $u/|r_1|\sim\mathcal{O}(r_1/|r_1|)$. As $|\nabla_x|^{\alpha-1/2}|\nabla_y|^{\alpha-1/2}\sim|\nabla_1|^{2\alpha-1}$, we get

$$|\nabla_x|^{2\alpha-1}|x-y|^{-1}u\sim\mathcal{O}(|\nabla_1|^{2\alpha-1}r_1/|r_1|)=\mathcal{O}(|r_1|^{1-2\alpha}).$$

Thus, if $\alpha\geqslant 1.25$,

$$\||\nabla_x|^{\alpha-1/2}|\nabla_y|^{\alpha-1/2}|x-y|^{-1}u\|_{L^2(\mathbb{R}^{3\times 3})}=\infty.$$

□

Remark 3.9. *In the above lemma, we can not replace $\mathcal{O}(r_1/|r_1|)$ by $\mathcal{O}(1)$, since $|\nabla_1 1|=0$ while $|\nabla_1(r_1/|r_1|)|=\mathcal{O}(|r_1|^{-1})$.*

3.3 For the Coulomb system

For convenience, we define another operator $\mathcal{L}_{\mathcal{I},l,\alpha,\beta}$ by

$$\mathcal{L}_{\mathcal{I},l,\alpha,\beta}:=\left(\prod_{i\in\mathcal{I}_l}(1+|\nabla_i|^2)^{\alpha/2}\right)\left(\prod_{j\in\mathcal{I}\setminus\mathcal{I}_l}(1+|\nabla_j|^2)^{\beta/2}\right).$$

Obviously,

$$\mathcal{L}^2_{\mathcal{I},\alpha,\beta}=\sum_{l=1}^{q}\mathcal{L}^2_{\mathcal{I},l,\alpha,\beta}.$$

And recall that

$$V_{ne}=\sum_{i=1}^{N}\sum_{\nu=1}^{M}\frac{Z_\nu}{|x_i-a_\nu|},\qquad V_{ee}=\frac{1}{2}\sum_{i\neq j}\frac{1}{|x_i-x_j|}.$$

By Lemma 3.5, we know that if $0 < \alpha, \beta < 1.5$, for $\forall u, v \in \mathcal{D}_{\mathcal{I}}$,

$$\left|\left\langle \mathcal{L}_{\mathcal{I},l,\alpha,\beta}\frac{u}{|x_i - a_\nu|}, \mathcal{L}_{\mathcal{I},l,\alpha,\beta}v\right\rangle\right| \leqslant C'_{\alpha,\beta}\|\mathcal{L}_{\mathcal{I},l,\alpha,\beta}u\|_{L^2((\mathbb{R}^3)^N)}\|\nabla_i\mathcal{L}_{\mathcal{I},l,\alpha,\beta}v\|_{L^2((\mathbb{R}^3)^N)},$$

with $C'_{\alpha,\beta} = \max\{C_{\alpha-1}, C_{\beta-1}\} + 2$. Thus,

$$|\langle\mathcal{L}_{\mathcal{I},l,\alpha,\beta}V_{ne}u, \mathcal{L}_{\mathcal{I},l,\alpha,\beta}v\rangle| \leqslant C'_{\alpha,\beta}ZN^{1/2}\|\mathcal{L}_{\mathcal{I},l,\alpha,\beta}u\|_{L^2((\mathbb{R}^3)^N)}\|\nabla\mathcal{L}_{\mathcal{I},l,\alpha,\beta}v\|_{L^2((\mathbb{R}^3)^N)},$$

where $Z = \sum_{\nu=1}^{M} Z_\nu$, $\nabla := (\nabla_1, \cdots, \nabla_N)$ and

$$\|\nabla v\|^2_{L^2((\mathbb{R}^3)^N)} = \sum_{i=1}^{N}\|\nabla_i v\|^2_{L^2((\mathbb{R}^3)^N)}.$$

Consequently,

$$|\langle\mathcal{L}_{\mathcal{I},\alpha,\beta}V_{ne}u, \mathcal{L}_{\mathcal{I},\alpha,\beta}v\rangle| \leqslant C'_{\alpha,\beta}ZN^{1/2}\|\mathcal{L}_{\mathcal{I},\alpha,\beta}u\|_{L^2((\mathbb{R}^3)^N)}\|\nabla\mathcal{L}_{\mathcal{I},\alpha,\beta}v\|_{L^2((\mathbb{R}^3)^N)},$$

Now, we need to consider the different cases: (A)-(C). For case (B), if $i, j \in \mathcal{I}_l$, u satisfies the equation (3). And for $1 \leqslant \alpha < 1.25$ (or $0 < \alpha < 0.75$), by Lemma 3.7,

$$\begin{aligned}&\left|\left\langle \mathcal{L}_{\mathcal{I},l,\alpha,\beta}\frac{u}{|x_i - x_j|}, \mathcal{L}_{\mathcal{I},l,\alpha,\beta}v\right\rangle\right|\\ \leqslant& D_{\alpha,\alpha}\|\mathcal{L}_{\mathcal{I},l,\alpha,\beta}u\|_{L^2((\mathbb{R}^3)^N)}\left(\|\nabla_i\mathcal{L}_{\mathcal{I},l,\alpha,\beta}v\|_{L^2((\mathbb{R}^3)^N)} + \|\nabla_j\mathcal{L}_{\mathcal{I},l,\alpha,\beta}v\|_{L^2((\mathbb{R}^3)^N)}\right).\end{aligned}$$

If $i \in \mathcal{I}_l$ and $j \notin \mathcal{I}_l$, for $1 \leqslant \alpha$ (or $0 < \alpha < 0.75$), $0 < \beta$ and $\alpha + \beta < 1.5$, by Lemma 3.7,

$$\begin{aligned}&\left|\left\langle \mathcal{L}_{\mathcal{I},l,\alpha,\beta}\frac{u}{|x_i - x_j|}, \mathcal{L}_{\mathcal{I},l,\alpha,\beta}v\right\rangle\right|\\ \leqslant& D_{\alpha,\beta}\|\mathcal{L}_{\mathcal{I},l,\alpha,\beta}u\|_{L^2((\mathbb{R}^3)^N)}\left(\|\nabla_i\mathcal{L}_{\mathcal{I},l,\alpha,\beta}v\|_{L^2((\mathbb{R}^3)^N)} + \|\nabla_j\mathcal{L}_{\mathcal{I},l,\alpha,\beta}v\|_{L^2((\mathbb{R}^3)^N)}\right).\end{aligned}$$

And if $i, j \notin I_l$, for $0 < \beta < 0.75$,

$$\begin{aligned}&\left|\left\langle \mathcal{L}_{\mathcal{I},l,\alpha,\beta}\frac{u}{|x_i - x_j|}, \mathcal{L}_{\mathcal{I},l,\alpha,\beta}v\right\rangle\right|\\ \leqslant& D_{\beta,\beta}\|\mathcal{L}_{\mathcal{I},l,\alpha,\beta}u\|_{L^2((\mathbb{R}^3)^N)}\left(\|\nabla_i\mathcal{L}_{\mathcal{I},l,\alpha,\beta}v\|_{L^2((\mathbb{R}^3)^N)} + \|\nabla_j\mathcal{L}_{\mathcal{I},l,\alpha,\beta}v\|_{L^2((\mathbb{R}^3)^N)}\right).\end{aligned}$$

Finally, we yield

$$\begin{aligned}&|\langle\mathcal{L}_{\mathcal{I},l,\alpha,\beta}V_{ee}u, \mathcal{L}_{\mathcal{I},l,\alpha,\beta}v\rangle|\\ \leqslant& D'_{\alpha,\beta}N\sum_{i=1}^{N}\|\mathcal{L}_{\mathcal{I},l,\alpha,\beta}u\|_{L^2((\mathbb{R}^3)^N)}\|\nabla_i\mathcal{L}_{\mathcal{I},l,\alpha,\beta}v\|_{L^2((\mathbb{R}^3)^N)}\\ \leqslant& D'_{\alpha,\beta}N^{3/2}\|\mathcal{L}_{\mathcal{I},l,\alpha,\beta}u\|_{L^2((\mathbb{R}^3)^N)}\|\nabla\mathcal{L}_{\mathcal{I},l,\alpha,\beta}v\|_{L^2((\mathbb{R}^3)^N)}.\end{aligned}$$

with $D'_{\alpha,\beta} = \max\{D_{\alpha,\beta}, D_{\alpha,\alpha}, D_{\beta,\beta}\}$.

Consequently, for $1 \leqslant \alpha < 1.25$ (or $0 < \alpha < 0.75$), $0 < \beta < 0.75$ and $\alpha + \beta < 1.5$:

$$|\langle\mathcal{L}_{\mathcal{I},\alpha,\beta}V_{ee}u, \mathcal{L}_{\mathcal{I},\alpha,\beta}v\rangle| \leqslant D'_{\alpha,\beta}N^{3/2}\|\mathcal{L}_{\mathcal{I},\alpha,\beta}u\|_{L^2((\mathbb{R}^3)^N)}\|\nabla\mathcal{L}_{\mathcal{I},\alpha,\beta}v\|_{L^2((\mathbb{R}^3)^N)}.$$

Analogously, for case (A), and for $0 < \beta < 0.75$ we have that

$$|\langle \mathcal{L}_{\mathcal{I},\beta} V_{ee} u, \mathcal{L}_{\mathcal{I},\beta} v\rangle| \leqslant D'_{\beta,\beta} N^{3/2} \|\mathcal{L}_{\mathcal{I},\beta} u\|_{L^2((\mathbb{R}^3)^N)} \|\nabla \mathcal{L}_{\mathcal{I},\beta} v\|_{L^2((\mathbb{R}^3)^N)}.$$

And for case (C), and for $1 \leqslant \alpha < 1.25$ (or $0 < \alpha < 0.75$), we have that

$$|\langle \mathcal{L}_{\mathcal{I},\alpha} V_{ee} u, \mathcal{L}_{\mathcal{I},\alpha} v\rangle| \leqslant D'_{\alpha,\alpha} N^{3/2} \|\mathcal{L}_{\mathcal{I},\alpha} u\|_{L^2((\mathbb{R}^3)^N)} \|\nabla \mathcal{L}_{\mathcal{I},\alpha} v\|_{L^2((\mathbb{R}^3)^N)}.$$

Now we conclude:

Lemma 3.10.

- *For case (A), if* $0 < \beta < 0.75$,

$$\begin{aligned} &|\langle \mathcal{L}_{\mathcal{I},\beta,}(V_{ne} + V_{ee}) u, \mathcal{L}_{\mathcal{I},\beta,} v\rangle| \\ \leqslant &(C'_{\beta,\beta} Z + D'_{\beta,\beta} N) N^{1/2} \|\mathcal{L}_{\mathcal{I},\beta,} u\|_{L^2((\mathbb{R}^3)^N)} \|\nabla \mathcal{L}_{\mathcal{I},\beta} v\|_{L^2((\mathbb{R}^3)^N)}. \end{aligned} \tag{15}$$

- *For case (B), if* $1 \leqslant \alpha < 1.25$ *(or* $0 < \alpha < 0.75$*),* $0 < \beta < 0.75$ *and* $\alpha + \beta < 1.5$,

$$\begin{aligned} &|\langle \mathcal{L}_{\mathcal{I},\alpha,\beta}(V_{ne} + V_{ee}) u, \mathcal{L}_{\mathcal{I},\alpha,\beta} v\rangle| \\ \leqslant &(C'_{\alpha,\beta} Z + D'_{\alpha,\beta} N) N^{1/2} \|\mathcal{L}_{\mathcal{I},\alpha,\beta} u\|_{L^2((\mathbb{R}^3)^N)} \|\nabla \mathcal{L}_{\mathcal{I},\alpha,\beta} v\|_{L^2((\mathbb{R}^3)^N)}. \end{aligned} \tag{16}$$

- *For case (C), if* $1 \leqslant \alpha < 1.25$ *(or* $0 < \alpha < 0.75$*),*

$$\begin{aligned} &|\langle \mathcal{L}_{\mathcal{I},\alpha}(V_{ne} + V_{ee}) u, \mathcal{L}_{\mathcal{I},\alpha} v\rangle| \\ \leqslant &(C'_{\alpha,\alpha} Z + D'_{\alpha,\alpha} N) N^{1/2} \|\mathcal{L}_{\mathcal{I},\alpha} u\|_{L^2((\mathbb{R}^3)^N)} \|\nabla \mathcal{L}_{\mathcal{I},\alpha} v\|_{L^2((\mathbb{R}^3)^N)}. \end{aligned} \tag{17}$$

4 The Regularity of Solutions

Repeating the proof in [Yse07], we split the eigenfunctions into the high-frequency part and the low frequency part and estimate the high-frequency part by the low frequency part. Let P_Ω be the projector to the high frequency part, with

$$\mathcal{F}(P_\Omega u)(\xi) := \mathbb{1}_{|\xi| \geqslant \Omega} \mathcal{F}(u)(\xi).$$

where

$$|\xi|^2 = \sum_{i=1}^{N} |\xi_i|^2.$$

And let

$$u_H := P_\Omega u, \quad u_L := (1 - P_\Omega) u.$$

Hence $u_L \in H^1_{\mathcal{I}}$ is well-defined. And we only need to prove the existence of u_H. We have that

$$\|u_H\|_{L^2((\mathbb{R}^3)^N)} \leqslant (2\pi\Omega)^{-1} \|\nabla u_H\|_{L^2((\mathbb{R}^3)^N)}.$$

For case (B), taking $v_H \in P_\Omega X_{\mathcal{I},\alpha,\beta}((\mathbb{R}^3)^N)$ (or $v_H \in P_\Omega X_{\mathcal{I},\alpha,\alpha}((\mathbb{R}^3)^N)$ for case (A) and case (C)), then for the existence of mixed regularity we need to study:

$$\langle \mathcal{L}_{\mathcal{I},\alpha,\beta} H u, \mathcal{L}_{\mathcal{I},\alpha,\beta} v_H\rangle - \lambda \langle \mathcal{L}_{\mathcal{I},\alpha,\beta} u, \mathcal{L}_{\mathcal{I},\alpha,\beta} v_H\rangle = 0$$

Decomposing u by u_H and u_L, we have

$$\begin{aligned}
&\langle \mathcal{L}_{\mathcal{I},\alpha,\beta}(H-\lambda)u_H, \mathcal{L}_{\mathcal{I},\alpha,\beta}v_H\rangle \\
=&1/2\,\langle \nabla\mathcal{L}_{\mathcal{I},\alpha,\beta}u_H, \nabla\mathcal{L}_{\mathcal{I},\alpha,\beta}v_H\rangle + \langle \mathcal{L}_{\mathcal{I},\alpha,\beta}(V_{ne}+V_{ee})u_H, \mathcal{L}_{\mathcal{I},\alpha,\beta}v_H\rangle \\
&-\lambda\,\langle \mathcal{L}_{\mathcal{I},\alpha,\beta}u_H, \mathcal{L}_{\mathcal{I},\alpha,\beta}v_H\rangle \\
=&\,\langle \mathcal{L}_{\mathcal{I},\alpha,\beta}(V_{ne}+V_{ee})u_L, \mathcal{L}_{\mathcal{I},\alpha,\beta}v_H\rangle\,.
\end{aligned}$$

Let

$$\Omega \geqslant (2\pi)^{-1}(C'_{\alpha,\beta}Z + D'_{\alpha,\alpha}N)N^{1/2} \geqslant 1, \tag{18}$$

then

$$\begin{aligned}
&|\langle \mathcal{L}_{\mathcal{I},\alpha,\beta}(V_{ne}+V_{ee})u_H, \mathcal{L}_{\mathcal{I},\alpha,\beta}v_H\rangle| \leqslant 1/4\|\nabla\mathcal{L}_{\mathcal{I},\alpha,\beta}u_H\|_{L^2((\mathbb{R}^3)^N)}\|\nabla\mathcal{L}_{\mathcal{I},\alpha,\beta}v_H\|_{L^2((\mathbb{R}^3)^N)}, \\
&\|\mathcal{L}_{\mathcal{I},\alpha,\beta}u_H\|_{L^2((\mathbb{R}^3)^N)} \leqslant \|\nabla\mathcal{L}_{\mathcal{I},\alpha,\beta}u_H\|_{L^2((\mathbb{R}^3)^N)}\,.
\end{aligned}$$

As the eigenvalues of problem 2 are negatives, therefore we have the coercivity

$$\langle \mathcal{L}_{\mathcal{I},\alpha,\beta}(H-\lambda)u_H, \mathcal{L}_{\mathcal{I},\alpha,\beta}u_H\rangle \geqslant 1/8\|u_H\|^2_{\mathcal{I},\alpha,\beta}, \tag{19}$$

the continuity

$$|\langle \mathcal{L}_{\mathcal{I},\alpha,\beta}(H-\lambda)u_H, \mathcal{L}_{\mathcal{I},\alpha,\beta}v_H\rangle| \leqslant \|u_H\|_{\mathcal{I},\alpha,\beta}\|v_H\|_{\mathcal{I},\alpha,\beta}, \tag{20}$$

and the continuity of the term $\langle \mathcal{L}_{\mathcal{I},\alpha,\beta}(V_{ne}+V_{ee})\psi, \mathcal{L}_{\mathcal{I},\alpha,\beta}v_H\rangle$

$$|\langle \mathcal{L}_{\mathcal{I},\alpha,\beta}(V_{ne}+V_{ee})\psi, \mathcal{L}_{\mathcal{I},\alpha,\beta}v_H\rangle| \leqslant (C'_{\alpha,\beta}Z + D'_{\alpha,\alpha}N)N^{1/2}\|\mathcal{L}_{\mathcal{I},\alpha,\beta}\psi\|_{L^2((\mathbb{R}^3)^N)}\|v_H\|_{\mathcal{I},\alpha,\beta}, \tag{21}$$

And now, we prove the regularity of the eigenfunctions.

Sketch Proof of the Theorem 1.1. This proof is similar to the proof in [Yse04, Yse11]. So we just give the sketch of proof, and only consider the case (B), the proof of other cases is same.

Step 1. For the frequency bounds Ω as in (18), the equation

$$\langle \mathcal{L}_{\mathcal{I},\alpha,\beta}(H-\lambda)u_H, \mathcal{L}_{\mathcal{I},\alpha,\beta}v_H\rangle = \langle \mathcal{L}_{\mathcal{I},\alpha,\beta}(V_{ne}+V_{ee})\psi, \mathcal{L}_{\mathcal{I},\alpha,\beta}v_H\rangle\,,\ \forall v_H \in P_\Omega X_{\mathcal{I},\alpha,\beta}((\mathbb{R}^3)^N) \tag{22}$$

possesses a unique solution $u_H \in P_\Omega X_{\mathcal{I},\alpha,\beta}((\mathbb{R}^3)^N)$ for all given functions $\psi \in X_{\mathcal{I},\alpha,\beta}((\mathbb{R}^3)^N)$ by using the Lax-Milgram theorem, and combining the estimate (19) with the estimate (16) for ψ.

Step 2. For the frequency bounds Ω as in (18), the equation

$$\langle (H-\lambda)u_H, \chi_H\rangle = \langle (V_{ne}+V_{ee})\psi, \chi_H\rangle\,,\ \forall \chi_H \in P_\Omega H^1((\mathbb{R}^3)^N) \tag{23}$$

possesses a unique solution $u_H \in P_\Omega X_{\mathcal{I},\alpha,\beta}((\mathbb{R}^3)^N)$ for all given functions $\psi \in H^1((\mathbb{R}^3)^N)$, see [Yse04, Yse07].

Step 3. For all $\chi_H \in P_\Omega H^1((\mathbb{R}^3)^N)$, there is a unique high-frequency function $v_H \in P_\Omega X_{\mathcal{I},\alpha,\beta}((\mathbb{R}^3)^N)$ such that $\mathcal{L}^2_{\mathcal{I},\alpha,\beta}v_H = \chi_H$.

By Fourier transform, we have

$$\sum_{l=1}^{q}\left(\prod_{i\in\mathcal{I}_l}(1+|2\pi\xi_i|^2)^{\alpha}\right)\left(\prod_{m\in\mathcal{I}\setminus\mathcal{I}_l}(1+|2\pi\xi_j|^2)^{\beta}\right)\widehat{v_H}(\omega)=\widehat{\chi_H}(\omega),$$

Thus we know that $P_\Omega H^1\subset\mathcal{L}^2_{\mathcal{I},\alpha,\beta}P_\Omega X_{\mathcal{I},\alpha,\beta}((\mathbb{R}^3)^N)$.

Step 4. We rewrite the equation (22) as

$$\left\langle(H-\lambda)u_H,\mathcal{L}^2_{\mathcal{I},\alpha,\beta}v_H\right\rangle=\left\langle(V_{ne}+V_{ee})\psi,\mathcal{L}^2_{\mathcal{I},\alpha,\beta}v_H\right\rangle,\ \forall v_H\in P_\Omega X_{\mathcal{I},\alpha,\beta}((\mathbb{R}^3)^N).$$

And by the step 3, we know the solution of equation (22) satisfies the original equation (23) for all $\chi_H\in P_\Omega H^1((\mathbb{R}^3)^N)$. Hence for all $\mathcal{L}_{\mathcal{I},\alpha,\beta}\psi\in L^2((\mathbb{R}^3)^N)$, by the uniqueness of solution, we yield that the solution of problem (23) $u_H\in X_{\mathcal{I},\alpha,\beta}((\mathbb{R}^3)^N)$.

Step 5. Since the low-frequency part u_L of the solution is contained in $\mathcal{D}_\mathcal{I}$, we know the solution $u\in X_{\mathcal{I},\alpha,\beta}((\mathbb{R}^3)^N)$. And by Lemma 3.8, we know the condition $\alpha\geqslant 1.25$, $\alpha+\beta\geqslant 1.5$ or $\beta\geqslant 0.75$ can not be reached or surpassed. In this sense, our results are optimal. □

Proof of Corollary 1.2. Recall that

$$\mathcal{L}_{\mathcal{I},l,\alpha,\beta}:=\left(\prod_{i\in\mathcal{I}_l}(1+|\nabla_i|^2)^{\alpha/2}\right)\left(\prod_{j\in\mathcal{I}\setminus\mathcal{I}_l}(1+|\nabla_j|^2)^{\beta/2}\right).$$

Since $u\in X_{\mathcal{I},\alpha,\beta}((\mathbb{R}^3)^N)$, we know that

$$\|\mathcal{L}_{\mathcal{I},l,\alpha,\beta}u\|_{H^1((\mathbb{R}^3)^N))}<\infty.$$

Assume that $u\in X_{\mathcal{I},\alpha_1,\beta_1}((\mathbb{R}^3)^N)\bigcap X_{\mathcal{I},\alpha_2,\beta_2}((\mathbb{R}^3)^N)$, then for any $0\leqslant s\leqslant 1$,

$$\begin{aligned}&\|\mathcal{L}_{\mathcal{I},l,s\alpha_1+(1-s)\alpha_2,s\beta_1+(1-s)\beta_2}u\|_{H^1((\mathbb{R}^3)^N))}\\=&\|\mathcal{L}^s_{\mathcal{I},l,\alpha_1,\beta_1}\mathcal{L}^{(1-s)}_{\mathcal{I},l,\alpha_2,\beta_2}u\|_{H^1((\mathbb{R}^3)^N))}\\\leqslant&\|\mathcal{L}_{\mathcal{I},l,\alpha_1,\beta_1}u\|_{H^1((\mathbb{R}^3)^N))}+\|\mathcal{L}_{\mathcal{I},l,\alpha_2,\beta_2}u\|_{H^1((\mathbb{R}^3)^N))}\\<&\infty.\end{aligned}$$

Now, we get conclusion. □

5 Numerical analysis

In this part, we study the hyperbolic cross space approximation, which is almost same with [Yse07] except Theorem 9 in it. So we just give the sketch, and only consider the case (B).

Let $\psi=u_L$ and $v_H=u_H$, then by estimates (19) and (21), we get

$$1/8\|u_H\|^2_{\mathcal{I},\alpha,\beta}\leqslant(C'_{\alpha,\beta}Z+D'_{\alpha,\alpha}N)N^{1/2}\|\mathcal{L}_{\mathcal{I},\alpha,\beta}u_L\|_{L^2((\mathbb{R}^3)^N)}\|u_H\|_{\mathcal{I},\alpha,\beta}.$$

Thus,

$$\begin{aligned}\pi\Omega/4\|\mathcal{L}_{\mathcal{I},\alpha,\beta}u_H\|_{L^2((\mathbb{R}^3)^N)} \leqslant & 1/8\|\nabla\mathcal{L}_{\mathcal{I},\alpha,\beta}u_H\|_{L^2((\mathbb{R}^3)^N)}\\ \leqslant & (C'_{\alpha,\beta}Z + D'_{\alpha,\alpha}N)N^{1/2}\|\mathcal{L}_{\mathcal{I},\alpha,\beta}u_L\|_{L^2((\mathbb{R}^3)^N)}.\end{aligned}$$

Let $\Omega \geqslant 32\pi^{-1}(C'_{\alpha,\beta}Z + D'_{\alpha,\alpha}N)N^{1/2}$ large enough, then

$$\|\mathcal{L}_{\mathcal{I},\alpha,\beta}u_H\|_{L^2((\mathbb{R}^3)^N)} \leqslant \sqrt{2}\|\mathcal{L}_{\mathcal{I},\alpha,\beta}u_L\|_{L^2((\mathbb{R}^3)^N)}, \tag{24}$$

and

$$\|\nabla\mathcal{L}_{\mathcal{I},\alpha,\beta}u_H\|_{L^2} \leqslant \sqrt{2}\Omega\|\mathcal{L}_{\mathcal{I},\alpha,\beta}u_L\|_{L^2}. \tag{25}$$

We take the following norm:

$$\||u|\|^2_{\mathcal{I},\alpha,\beta,1} = \sum_{l=1}^{q}\int\left(\sum_{i=1}^{N}\left|\frac{\xi_i}{\Omega}\right|^2\right)\left(\prod_{k\in\mathcal{I}_l}\left(1+\left|\frac{\xi_i}{\Omega}\right|^2\right)^{\alpha}\right)\left(\prod_{j\in\mathcal{I}\setminus\mathcal{I}_l}\left(1+\left|\frac{\xi_i}{\Omega}\right|^2\right)^{\beta}\right)|\mathcal{F}(u)|^2\,\mathrm{d}\xi,$$

and

$$\||u|\|^2_{\mathcal{I},\alpha,\beta,0} = \sum_{l=1}^{q}\int\left(\prod_{k\in\mathcal{I}_l}\left(1+\left|\frac{\xi_i}{\Omega}\right|^2\right)^{\alpha}\right)\left(\prod_{j\in\mathcal{I}\setminus\mathcal{I}_l}\left(1+\left|\frac{\xi_i}{\Omega}\right|^2\right)^{\beta}\right)|\mathcal{F}(u)|^2\,\mathrm{d}\xi.$$

Lemma 5.1. *For scaling parameters $\Omega \geqslant 2\pi^{-1}(C'_{\alpha,\beta}Z + D'_{\alpha,\alpha}N)N^{1/2}$ large enough, the eigenfunction $u \in X_{\mathcal{I},\alpha,\beta}$ satisfies the estimates*

$$\||u|\|_{\mathcal{I},\alpha,\beta,0} \leqslant \sqrt{2q}e^{0.625}\|u\|_{L^2((\mathbb{R}^3)^N)},\ \ \||u|\|_{\mathcal{I}_l,\alpha,\beta,1} \leqslant \sqrt{2q}e^{0.625}\|u\|_{L^2((\mathbb{R}^3)^N)}.$$

Proof. The proof is similar with [Yse07, Theorem 9]. By estimate (24), replace u by $u((2\pi\Omega)^{-1}x)$, then

$$\||u|\|_{\mathcal{I},\alpha,\beta,0} \leqslant \sqrt{2}\||u_L|\|_{\mathcal{I},\alpha,\beta,0},$$

with

$$\||u_L|\|^2_{\mathcal{I},\alpha,\beta,0} = \sum_{l=1}^{q}\int\left(\prod_{k\in\mathcal{I}_l}\left(1+\left|\frac{\xi_i}{\Omega}\right|^2\right)^{\alpha}\right)\left(\prod_{j\in\mathcal{I}\setminus\mathcal{I}_l}\left(1+\left|\frac{\xi_i}{\Omega}\right|^2\right)^{\beta}\right)|\mathcal{F}(u)|^2\,\mathrm{d}\xi.$$

As $0 < \beta \leqslant \alpha < 1.25$,

$$\left(\prod_{k\in\mathcal{I}_l}\left(1+\left|\frac{\xi_i}{\Omega}\right|^2\right)^{\alpha}\right)\left(\prod_{j\in\mathcal{I}\setminus\mathcal{I}_l}\left(1+\left|\frac{\xi_i}{\Omega}\right|^2\right)^{\beta}\right). \leqslant \exp\left(\alpha\sum_{i=1}^{N}\left|\frac{\xi_i}{\Omega}\right|^2\right).$$

Thus,

$$\begin{aligned}&\||u_L|\|^2_{\mathcal{I},\alpha,\beta,0}\\ \leqslant & \sum_{l=1}^{q}\int_{|\xi|\leqslant\Omega}\exp\left(\alpha\sum_{i=1}^{N}\left|\frac{\xi_i}{\Omega}\right|^2\right)|\mathcal{F}(u)|^2\,\mathrm{d}\xi\\ \leqslant & qe^{1.25}\int|\mathcal{F}(u)|^2\,\mathrm{d}\xi.\end{aligned}$$

Finally,

$$\||u|\|_{\mathcal{I},\alpha,\beta,0} \leqslant \sqrt{2q}e^{0.625}\|u\|_{L^2((\mathbb{R}^3)^N)}.$$

The other case can repeated equally. □

Proof of Theorem 1.4. Thus, we know that

$$\|u - P_R u\|_{L^2((\mathbb{R}^3)^N)} \leqslant \frac{1}{R}\||u - P_R u\||_{\mathcal{I},\alpha,\beta,0} \leqslant \frac{1}{R}\||u\||_{\mathcal{I},\alpha,\beta,0} \leqslant \frac{\sqrt{2q}}{R} e^{0.625}\|u\|_{L^2((\mathbb{R}^3)^N)}.$$

And for the other term,

$$\|\nabla(u - P_R u)\|_{L^2((\mathbb{R}^3)^N)} \leqslant \frac{\sqrt{2q}}{R} e^{0.625}\Omega\|u\|_{L^2((\mathbb{R}^3)^N)}.$$

□

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References

[FHOHOS02] Søren Fournais, Maria Hoffmann-Ostenhof, Thomas Hoffmann-Ostenhof, and T Østergaard Sørensen. The electron density is smooth away from the nuclei. *Communications in Mathematical Physics*, 228(3):401–415, 2002.

[FHOHOS05] Søren Fournais, Maria Hoffmann-Ostenhof, Thomas Hoffmann-Ostenhof, and Thomas Østergaard Sørensen. Sharp regularity results for coulombic many-electron wave functions. *Communications in mathematical physics*, 255(1):183–227, 2005.

[FHOHOS09] Søren Fournais, Maria Hoffmann-Ostenhof, Thomas Hoffmann-Ostenhof, and Thomas Østergaard Sørensen. Analytic structure of many-body coulombic wave functions. *Communications in Mathematical Physics*, 289(1):291–310, 2009.

[Her77] Ira W Herbst. Spectral theory of the operator (p 2+ m 2) 1/2- ze 2/r. *Communications in Mathematical Physics*, 53(3):285–294, 1977.

[HOHOLT08] M Hoffmann-Ostenhof, Th Hoffmann-Ostenhof, Ari Laptev, and Jesper Tidblom. Many-particle hardy inequalities. *Journal of the London Mathematical Society*, 77(1):99–115, 2008.

[HOHOS94] Maria Hoffmann-Ostenhof, Thomas Hoffmann-Ostenhof, and Hanns Stremnitzer. Local properties of coulombic wave functions. *Communications in mathematical physics*, 163(1):185–215, 1994.

[HOHOS01] Maria Hoffmann-Ostenhof, Thomas Hoffmann-Ostenhof, and Thomas Østergaard Sørensen. Electron wavefunctions and densities for atoms. In *Annales Henri Poincaré*, volume 2, pages 77–100. Springer, 2001.

[HS00] Walter Hunziker and Israel Michael Sigal. The quantum n-body problem. *Journal of Mathematical Physics*, 41(6):3448–3510, 2000.

[Kat57] Tosio Kato. On the eigenfunctions of many-particle systems in quantum mechanics. *Communications on Pure and Applied Mathematics*, 10(2):151–177, 1957.

[KY12] Hans-Christian Kreusler and Harry Yserentant. The mixed regularity of electronic wave functions in fractional order and weighted sobolev spaces. *Numerische Mathematik*, 121(4):781–802, 2012.

[LBL05] Claude Le Bris and Pierre-Louis Lions. From atoms to crystals: a mathematical journey. *Bulletin of the American Mathematical Society*, 42(3):291–363, 2005.

[LL01] Elliott H Lieb and Michael Loss. *Analysis*, volume 14. American Mathematical Soc., 2001.

[Men19] Long Meng. Regularity of many-body schrödinger evolution equation and its application to numerical analysis. *HAL preprint hal-02129838*, 2019.

[Sti19] Pablo Raúl Stinga. User's guide to the fractional laplacian and the method of semigroups. *Fractional Differential Equations*, pages 235–266, 2019.

[Yse04] Harry Yserentant. On the regularity of the electronic schrödinger equation in hilbert spaces of mixed derivatives. *Numerische Mathematik*, 98(4):731–759, 2004.

[Yse07] Harry Yserentant. The hyperbolic cross space approximation of electronic wavefunctions. *Numerische Mathematik*, 105(4):659–690, 2007.

[Yse11] Harry Yserentant. The mixed regularity of electronic wave functions multiplied by explicit correlation factors. *ESAIM: Mathematical Modelling and Numerical Analysis*, 45(5):803–824, 2011.