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ON THE MIXED REGULARITY OF N-BODY COULOMBIC WAVEFUNCTIONS

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Abstract. In this paper, we prove a new mixed regularity of Coulombic wavefunction taking into account the Pauli exclusion principle. We also study the hyperbolic cross space approximation of eigenfunctions associated with this new regularity, and deduce the corresponding error estimates in L^2-norm and H^1-semi-norm. The proofs are based on the study of extended Hardy-type inequalities for Coulomb-type potentials.

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1. Introduction

In most applications of molecular simulation, a molecule is described by an assembly of M static nuclei equipped with N electrons, with M, N in $\mathbb{N}_+$. We assume that the nuclei are fixed, according to the Born-Oppenheimer approximation, while the electrons are modeled quantum mechanically through a wavefunction and the N-body Hamiltonian operator:

$$H = -\frac{1}{2}\sum_{i=1}^{N} \triangle_i - V_{ne} + V_{ee} \tag{1.1}$$

with

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

and

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

where $a_1, \cdots, a_M \in \mathbb{R}^3$ are the positions of nuclei with respective charges $Z_1, \cdots, Z_M \in \mathbb{N}_+$ (in atomic units), and $x_1, \cdots, x_N \in \mathbb{R}^3$ are the coordinates of given N electrons. We denote $Z := \sum_{\nu=1}^{M} Z_\nu$ the total nuclear charge. The right-hand side terms in (1.1) model the kinetic energy, the Coulomb attraction between nuclei and electrons V_{ne} and the Coulomb repulsion between electrons V_{ee}, respectively.

Keywords and phrases. Mixed regularity, N-body problem, hyperbolic cross approximation.

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Mathematically, the electronic ground – or excited – state problem can be expressed by the Euler–Lagrange equation of the eigenvalue problem of the operator (1.1):

$$Hu = \lambda u, \tag{1.2}$$

where $u \in H^1((\mathbb{R}^3)^N)$ and $\|u\|_{L^2((\mathbb{R}^3)^N)} = 1$.

Remark 1.1. It is shown in [18] that any eigenvalue of (1.2) is negative.

The eigenvalue problem (1.2) is well-explored mathematically (see for example [11], as well as the regularity properties of eigenfunctions of problem (1.2) [3–5, 8–10, 12]).

In quantum mechanics, in addition to the spatial coordinates, a particle may have internal degrees of freedom, the most important one being the spin. Electrons, for example, have two kinds of spins $\widetilde{\sigma}$ with value $1, 2$. If a particle has q kinds of spins, we shall say that the particle has q spin states and we label them by the integer

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

From the mathematical point of view, it is interesting to consider an arbitrary q spin states in our system. For this reason, in this article, we will study the wavefunctions of N identical particles with q spin states instead of the electronic wavefunctions.

A wavefunction Ψ of identical N particles with q spin states can be written as

$$\Psi : \left(\mathbb{R}^3\right)^N \times \{1, \cdots, q\}^N \to \mathbb{C}, \quad (x, \sigma) \mapsto \Psi(x, \sigma), \tag{1.3}$$

where $x := (x_1, \cdots, x_N)$ and $\sigma := (\sigma_1, \cdots, \sigma_N)$ with $x_i \in \mathbb{R}^3$ and $\sigma_i \in \{1, \cdots, q\}$.

There are two kinds of particles: fermions and bosons. Fermions, among them electrons, satisfy the Pauli exclusion principle: the sign of the wavefunction Ψ changes sign under an exchange of the space coordinates x_i, x_j, and the spins σ_i, σ_j of two identical fermions i, j. More precisely, Pauli exclusion principle writes:

$$\Psi\left(P_{i,j}^{(x)} x, P_{i,j}^{(\sigma)} \sigma\right) = -\Psi(x, \sigma) \tag{1.4}$$

where $P_{i,j}^{(x)}$ and $P_{i,j}^{(\sigma)}$ the permutation operators which exchange the space coordinates x_i, x_j and the spins σ_i, σ_j respectively, *i.e.*,

$$P_{i,j}^{(x)}(\cdots, x_i, \cdots, x_j, \cdots) := (\cdots, x_j, \cdots, x_i, \cdots), \tag{1.5}$$

and

$$P_{i,j}^{(\sigma)}(\cdots, \sigma_i, \cdots, \sigma_j, \cdots) := (\cdots, \sigma_j, \cdots, \sigma_i, \cdots). \tag{1.6}$$

On the other hand, bosons satisfy the Bose–Einstein statistics in which the particles occupy symmetric quantum states. Thus the bosonic wavefunctions Ψ satisfies (1.4) when the sign $-$ is replaced by $+$.

Now we are going to fix the spin σ, and only consider the antisymmetry of the fermionic wavefunction with respect to x. As the eigenvalue problem (1.2) does not act upon the spin variables, for every fixed spin σ, the wavefunction $\Psi(x, \sigma)$ in (1.3) can be represented by the wavefunction $u(x)$ which is defined by

$$u : (\mathbb{R}^3)^N \to \mathbb{C}, \quad x \mapsto \Psi(x, \sigma). \tag{1.7}$$

Furthermore, for every fixed spin σ, the particles can be categorized into q subsets according to their spin states:

$$I_l := \{i \in \{1, \cdots, N\}; \sigma_i = l\}, \quad l = 1, \cdots, q, \quad \text{and} \quad \mathcal{I}_\sigma := \{I_1, \cdots, I_q\}. \tag{1.8}$$

In particular, if $\sigma_i \neq l$ for any $i = 1, \cdots, N$, we set $I_l = \varnothing$ and $|I_l| = 0$. If $i, j \in I$ with $I \in \mathcal{I}_\sigma$ and $|I| > 1$, then $\sigma_i = \sigma_j$. Thus

$$P_{i,j}^{(\sigma)}\sigma = \sigma.$$

Therefore, the permutation operator $P_{i,j}^{(\sigma)}$ keeps the spin σ invariant if the i-th and j-th electrons have the same spin. Hence for every fixed σ and for any $i, j \in I$ with $I \in \mathcal{I}_\sigma$ and $|I| > 1$, equation (1.4) implies the fermionic wavefunction u is antisymmetric with respect to x_i, x_j, *i.e.*,

$$u\Big(P_{i,j}^{(x)}x\Big) = -u(x). \tag{1.9}$$

In particular, if $x_i = x_j$ then $u(x) = 0$: thanks to the antisymmetry, the fermionic wavefunctions can counterbalance the singularity of the interaction potential $\frac{1}{|x_i - x_j|}$.

Relying on this observation, a new regularity result about eigenfunctions of problem (1.2) has been proven in [17, 18] which can help to break the complexity barriers in computational quantum mechanics. More precisely, it is shown in [17, 18] that, for every fixed spin σ, any eigenfunction u_* of problem (1.2) satisfies

$$\int_{(\mathbb{R}^3)^N} \left(1 + \sum_{i=1}^N |2\pi\xi_i|^2\right)\left(\sum_{I\in\mathcal{I}_\sigma}\prod_{k\in I}\Big(1 + |2\pi\xi_k|^2\Big)\right)|\widehat{u}_*(\xi)|^2\, \mathrm{d}\xi < +\infty, \tag{1.10}$$

where $\widehat{u}_*(\xi) := \mathcal{F}_{x_1,\cdots,x_N}(u_*)(\xi) = \int_{(\mathbb{R}^3)^N} u_*(x)e^{-2\pi i\xi\cdot x}dx$ is the Fourier transform of u with $\xi := (\xi_1, \cdots, \xi_N)$ and $\xi_i \in \mathbb{R}^3$, $i = 1, \cdots, N$. The proof is based on a Hardy-type inequality for the Coulomb system in the scalar product. Then based on this Hardy-type inequality, a hyperbolic cross space approximation of any eigenfunction of (1.2) has been studied. The convergence of this approximation is proven in [18]. The hyperbolic cross space approximation is defined by (2.10) below.

Later, by using $r12$-methods and interpolation of Sobolev spaces, H.C. Kreusler and H. Yserentant [13] proved that any eigenfunction u_* of problem (1.2) satisfies

$$\int_{(\mathbb{R}^3)^N} \left(1 + \sum_{i=1}^N |2\pi\xi_i|^2\right)^s \left(\prod_{k=1}^N (1 + |2\pi\xi_k|^2)\right)^t |\widehat{u}_*(\xi)|^2\, \mathrm{d}\xi < +\infty, \tag{1.11}$$

for $s = 0$ and $t = 1$ or $s = 1$ and $t < 3/4$. Notice that this regularity is independent of the choice of σ. It is shown in [13] that the bound $3/4$ is the best possible: it can neither be reached nor surpassed except for the totally antisymmetric eigenfunctions. However, lacking Hardy-type inequalities associated with the new type of mixed regularity, they could not prove the convergence of the corresponding hyperbolic cross space approximation of eigenfunctions.

In this article, we are going to improve the results of [13, 18] in two directions: (a) we prove the convergence of the hyperbolic cross space approximation of eigenfunctions associated with the regularity (1.11); (b) due to the Pauli exclusion principle, taking the antisymmetry of the wavefunctions into account, we prove a better mixed regularity of eigenfunctions and prove the convergence of the corresponding hyperbolic cross space approximation.

We generalize the concept of the antisymmetric functions such that, under this new definition, non-antisymmetric functions can also be regarded as special antisymmetric functions.

Definition 1.2 (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 $i, j \in I$,

$$u\Big(P_{i,j}^{(x)}x\Big) = -u(x),$$

where $P_{i,j}^{(x)}$ is defined by (1.5). When $|I| = 1$, every wavefunction u is antisymmetric with respect to I.

Remark 1.3. According to (1.8), (1.9) and above definition, wavefunction u defined by (1.7) with q spin states and the fixed spin σ is antisymmetric with respect to I for any $I \in \mathcal{I}_\sigma$.

Let u_* given by (1.7) with q spin states and the fixed spin σ be an eigenfunction of (1.2). The main results of this paper (Thm. 2.3 and Cor. 2.4) then state that

$$\int_{(\mathbb{R}^3)^N} \left(1+\sum_{i=1}^N |2\pi\xi_i|^2\right) \sum_{I\in\mathcal{I}_\sigma} \left(\prod_{j\in I}\left(1+|2\pi\xi_j|^2\right)\right)^{\alpha_I} \left(\prod_{k\in I^c}\left(1+|2\pi\xi_k|^2\right)\right)^{\beta_I} |\widehat{u}_*(\xi)|^2 \,\mathrm{d}\xi < +\infty. \tag{1.12}$$

Here and below $I^c = \{1,\cdots,N\}\backslash I$, $\alpha_I \in [0,5/4), \beta_I \in [0,3/4)$ and $\alpha_I+\beta_I < 3/2$.

As mentioned above, this result improves the results in [17,18]. Actually, if we take $\alpha_I = 1$ and $\beta_I = 0$, then (1.12) becomes (1.10). Thus the regularity (1.10) is a special case of (1.12). Furthermore, we can choose $\alpha_I \approx \frac{5}{4}$ and $\beta_I \approx \frac{1}{4}$ in (1.12) which are much larger than the ones in (1.10).

If we assume in particular that, for the fixed spin σ, there exists l such that $I_l = \{1,\cdots,N\}$ with I_l given by (1.8), then u_* is totally antisymmetric (*i.e.*, u_* is antisymmetric w.r.t. $\{1,\cdots,N\}$) and (1.12) becomes

$$\int_{(\mathbb{R}^3)^N} \left(1+\sum_{i=1}^N |2\pi\xi_i|^2\right) \left(\prod_{j=1}^N\left(1+|2\pi\xi_j|^2\right)\right)^{\alpha} |\widehat{u}_*(\xi)|^2 \,\mathrm{d}\xi < +\infty$$

with any $0 \leqslant \alpha < \frac{5}{4}$. Then (1.12) is better than (1.10) and (1.11) for the totally antisymmetric case.

Now we choose $\alpha_I = \beta_I$. Then if u_* is not totally antisymmetric, the condition on α_I and β_I shows that $0 \leqslant \alpha_I = \beta_I < \frac{3}{4}$, and (1.12) becomes

$$\int_{(\mathbb{R}^3)^N} \left(1+\sum_{i=1}^N |2\pi\xi_i|^2\right) \left(\prod_{j=1}^N\left(1+|2\pi\xi_j|^2\right)\right)^{\beta} |\widehat{u}_*(\xi)|^2 \,\mathrm{d}\xi < +\infty \tag{1.13}$$

with any $0 \leqslant \beta < \frac{3}{4}$. This is exactly (1.11) with $s = 1$ and $t < \frac{3}{4}$, and this regularity is independent of the choice of the spin σ and of the antisymmetry of the eigenfunctions. Thus we provide an alternative proof for (1.11). As mentioned above and shown in [19], our regularity is optimal in this case except for the totally antisymmetric eigenfunctions.

The proof of this new mixed regularity is based on a generalization of the Hardy-type inequality for Coulomb system in [17] (*i.e.*, Thm. 2.2) for any α_I and β_I as in (1.12). As in [18], from this new Hardy-type inequality, we can obtain the corresponding hyperbolic cross space approximation (*i.e.*, Thm. 2.5). In particular, concerning the case $\alpha_I = \beta_I < \frac{3}{4}$, we prove the convergence of the hyperbolic cross space approximation of eigenfunctions associated with the regularity (1.11).

2. Set-up and main results

In this section, we introduce first the operators and functional spaces used in this paper, then we present our main results and give the main ideas of the proof.

2.1. Operators and functional spaces

For every set $I \subset \{1,\cdots,N\}$, we define the Hilbert spaces $L^2_I((\mathbb{R}^3)^N)$ and $H^1_I((\mathbb{R}^3)^N)$ of the wavefunctions which are antisymmetric with respect to I by

$$L^2_I\left(\left(\mathbb{R}^3\right)^N\right) := \left\{u \in L^2\left(\left(\mathbb{R}^3\right)^N\right);\, u \text{ is antisymmetric with respect to } I\right\}, \tag{2.1}$$

and

$$H^1_I\left(\left(\mathbb{R}^3\right)^N\right) := \left\{u \in H^1\left(\left(\mathbb{R}^3\right)^N\right);\, u \text{ is antisymmetric with respect to } I\right\}, \tag{2.2}$$

respectively. It is easy to see that, when $|I| = 1$, $H^1_I((\mathbb{R}^3)^N) = H^1((\mathbb{R}^3)^N)$ and $L^2_I((\mathbb{R}^3)^N) = L^2((\mathbb{R}^3)^N)$. However when $|I| > 1$, we have $L^2_I((\mathbb{R}^3)^N) \subsetneq L^2((\mathbb{R}^3)^N)$ and $H^1_I((\mathbb{R}^3)^N) \subsetneq H^1((\mathbb{R}^3)^N)$.

Now we are going to define the new mixed Sobolev space like (1.11) in consideration of the antisymmetry with respect to I. Before going further, we define some fractional Laplacian-type operators associated with I. Define the operator $\mathcal{L}_{I,\alpha,\beta}$ by

$$\mathcal{L}_{I,\alpha,\beta} := \left(\prod_{j\in I}\left(1+|\nabla_j|^2\right)^{\alpha/2}\right)\left(\prod_{i\in I^c}\left(1+|\nabla_i|^2\right)^{\beta/2}\right), \tag{2.3}$$

where $I^c = \{1,\cdots,N\}\backslash I$ and ∇_i is the gradient with respect to the coordinate $x_i \in \mathbb{R}^3$. This operator is defined with the help of the Fourier transform (see Sect. 3 for details). In particular, when $I = \{1,\cdots,N\}$, then

$$\mathcal{L}_{I,\alpha,\beta} = \prod_{j=1}^{N}\left(1+|\nabla_j|^2\right)^{\alpha/2}$$

is indeed independent of the choice of β.

In addition to the operator $\mathcal{L}_{I,\alpha,\beta}$, the following operators will be useful,

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

and

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

Thus,

$$\mathcal{L}_{I,\alpha,\beta} = \left(1+|\nabla_i|^2\right)^{\gamma_i/2}\mathcal{L}^{(i)}_{I,\alpha,\beta}, \quad \mathcal{L}_{I,\alpha,\beta} = \left(1+|\nabla_i|^2\right)^{\gamma_i/2}\left(1+|\nabla_j|^2\right)^{\gamma_j/2}\mathcal{L}^{(i,j)}_{I,\alpha,\beta}, \tag{2.4}$$

where $\gamma_k = \alpha$ if $k \in I$, and $\gamma_k = \beta$ if $k \in I^c$.

We next introduce the corresponding functional spaces $X_{I,\alpha,\beta}$ defined by

$$X_{I,\alpha,\beta} := \left\{u \in H^1_I;\, \|\mathcal{L}_{I,\alpha,\beta}u\|_{H^1\left((\mathbb{R}^3)^N\right)} < +\infty\right\}, \tag{2.5}$$

endowed with the norm

$$\|u\|_{I,\alpha,\beta} := \|\mathcal{L}_{I,\alpha,\beta}u\|_{H^1\left((\mathbb{R}^3)^N\right)}. \tag{2.6}$$

We also define the following norm and semi-norm respectively,

$$\|u\|_{0,I,\alpha,\beta} := \|\mathcal{L}_{I,\alpha,\beta}u\|_{L^2\left((\mathbb{R}^3)^N\right)}, \quad \|u\|_{1,I,\alpha,\beta} := \|\nabla\mathcal{L}_{I,\alpha,\beta}u\|_{L^2\left((\mathbb{R}^3)^N\right)}. \tag{2.7}$$

Here $\nabla := (\nabla_1,\cdots,\nabla_N)$ is the gradient with respect to $x \in (\mathbb{R}^3)^N$. Obviously, $\|u\|^2_{I,\alpha,\beta} = \|u\|^2_{0,I,\alpha,\beta} + \|u\|^2_{1,I,\alpha,\beta}$.

2.2. Main results

Before going further, we need some assumptions on α and β.

Assumption 2.1. *We assume that* $\alpha \in [0, 5/4)$, $\beta \in [0, 3/4)$ *and* $\alpha + \beta < 3/2$.

The key tool to prove the regularity of eigenfunctions is the following.

Theorem 2.2 (Hardy-type inequality for Coulomb system in the scalar product)**.** *For every* $I \subset \{1, \cdots, N\}$, *and under Assumption 2.1 on* α, β, *there is a constant* $C_{\text{mix},\alpha,\beta}$ *independent of* N, Z *such that for any* $u, v \in X_{I,\alpha,\beta}$,

$$|\langle \mathcal{L}_{I,\alpha,\beta}(V_{ne} + V_{ee})u, \mathcal{L}_{I,\alpha,\beta}v\rangle| \leqslant C_{\text{mix},\alpha,\beta}\sqrt{N}\max\{Z, N\}\|u\|_{0,I,\alpha,\beta}\|v\|_{1,I,\alpha,\beta}. \tag{2.8}$$

It is shown in [17] that (2.8) holds for $\alpha = 1$ and $\beta = 0$. Based on this inequality, the regularity of eigenfunction u_* and the corresponding hyperbolic cross space approximation are also proven therein.

Our main result on the new mixed regularity of the wavefunction is the following.

Theorem 2.3 (Mixed regularity of eigenfunctions)**.** *Let* $I \subset \{1, \cdots, N\}$, *and let* $u_* \in H_I^1((\mathbb{R}^3)^N)$ *be a solution to the eigenvalue problem* (1.2). *Then, under Assumption 2.1 on* α *and* β, $u_* \in X_{I,\alpha,\beta}$.

This proof is postponed until Section 5.

According to Remark 1.3, we know that u given by (1.7) is situated in $\bigcap_{I\in\mathcal{I}_\sigma} H_I^1((\mathbb{R}^3)^N)$. Then we have

Corollary 2.4. *Let* u *given by* (1.7) *be an eigenfunction of the eigenvalue problem* (1.2) *with* q *spin states and a fixed spin* σ. *Then* $u_* \in \bigcap_{I\in\mathcal{I}_\sigma} X_{I,\alpha_I,\beta_I}$ *where* α_I *and* β_I *satisfy Assumption 2.1.*

We first recall the definition of the hyperbolic cross space approximation. Let Ω be a scaling parameter which will be given in Theorem 2.5. Let $\mathcal{H}_{I,\alpha,\beta}(R,\Omega)$ be a region defined by

$$\mathcal{H}_{I,\alpha,\beta}(R,\Omega) := \left\{(\omega_1, \cdots, \omega_N) \in \left(\mathbb{R}^3\right)^N; \prod_{i\in I}\left(1 + \left|\frac{\omega_i}{\Omega}\right|^2\right)^\alpha \prod_{j\in I^c}\left(1 + \left|\frac{\omega_j}{\Omega}\right|^2\right)^\beta \leqslant R^2\right\}. \tag{2.9}$$

Note that this region can be considered as cartesian product of hyperboloid-like regions, from which the notion hyperbolic cross space approximation originates. Then we define the projector

$$\left(\mathcal{P}_{I,\alpha,\beta}^{R,\Omega}u\right)(x) := \int_{(\mathbb{R}^3)^N} \chi_{I,\alpha,\beta}^{R,\Omega}(\xi)\widehat{u}(\xi)\exp\left(2\pi i\xi\cdot x\right)\mathrm{d}\xi \tag{2.10}$$

where $\chi_{I,\alpha,\beta}^{R,\Omega}$ is the characteristic function of the domain $\mathcal{H}_{I,\alpha,\beta}(R,\Omega)$. The approximation (2.10) of u is called the *hyperbolic cross space approximation.*

In [18], based on the mixed regularity (1.10), the convergence of hyperbolic cross space approximation of eigenfunctions is proven. Now we are going to prove the convergence of the hyperbolic cross space approximation of eigenfunctions associated with the regularity proven in Theorem 2.3.

Based on Theorem 2.2, we get the following.

Theorem 2.5 (Hyperbolic cross space approximation)**.** *Let* $I \subset \{1, \cdots, N\}$. *For any eigenfunction* $u_* \in H_I^1$ *of* (1.2), *and every* $\Omega \geqslant \frac{2}{\pi}C_{\text{mix},\alpha,\beta}\sqrt{N}\max\{Z, N\}$, *under Assumption 2.1 on* α, β, *we have*

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

and

$$\left\|\nabla\left(u_* - \mathcal{P}_{I,\alpha,\beta}^{R,\Omega}u_*\right)\right\|_{L^2\left((\mathbb{R}^3)^N\right)} \leqslant \frac{2\sqrt{2}\pi e^{5/8}}{R}\Omega\|u_*\|_{L^2((\mathbb{R}^3)^N)}.$$

Here the constant $C_{\text{mix},\alpha,\beta}$ *is defined in Theorem 2.2.*

This proof is provided in Section 6.

2.3. Main ideas of the proof of Theorem 2.2

As mentioned in Introduction, the extension of the results in [17–19] is based on Theorem 2.2. Once Theorem 2.2 is proven, following the proofs in [17, 18] line by line, we can prove Theorems 2.3 and 2.5, respectively. Thus this paper is devoted mainly to the proof of Theorem 2.2. As the proof of Theorem 2.2 is quite technical, before entering the details, let us try to explain the main ideas and the main improvements with respect to the existing results.

Let

$$L_I := \bigotimes_{j\in I} \nabla_j, \quad L_I^{(i)} := \bigotimes_{j\in I\backslash\{i\}} \nabla_j \quad \text{and} \quad L_I^{(i,j)} := \bigotimes_{k\in I\backslash\{i,j\}} \nabla_k.$$

The Hardy-type inequality used in [17, 18] can be expressed in the following way.

Theorem 2.6 ([17, 18])**.** *For every $I \subset \{1, \cdots, N\}$, there is a constant C_I independent of N, Z such that for any $u, v \in X_{I,1,0}$,*

$$|\langle L_I(V_{ne} + V_{ee})u, L_I v\rangle| \leqslant C_I\sqrt{N} \max\{Z, N\}\|u\|_{0,I,\alpha,\beta}\|v\|_{1,I,\alpha,\beta}. \tag{2.11}$$

One can essentially recover Theorem 2.2 with our Theorem 2.6 by setting $\alpha = 1$ and $\beta = 0$.

Remark 2.7. Actually, Theorem 2.2 is optimal at least for the case $\alpha = \beta$ if the wavefunction u is not totally antisymmetric. Otherwise, if (2.8) holds for some $\alpha = \beta \geqslant \frac{3}{4}$, then following the proofs in [17, 18] as in Section 5 in this paper, Theorem 2.3 and Corollary 2.4 will also hold for these α and β. This means that for any eigenfunction u_* which is not totally antisymmetric, $u_* \in X_{I,\alpha,\beta}$ with some $\alpha = \beta \geqslant \frac{3}{4}$. However, Yserentant [19] (see also (1.11) and (1.13) in this paper) shows that $\alpha = \beta < \frac{3}{4}$ is optimal. Then we reach a contradiction. Thus (2.8) is optimal for the case $\alpha = \beta$ if the wavefunction u is not totally antisymmetric.

Now we compare these two inequalities technically. We first give a glimpse into the formulae on the left-hand side of (2.8) and (2.11):

$$\mathcal{L}_{I,\alpha,\beta}V_{ne}u = \sum_{i=1}^{N}\sum_{\nu=1}^{M}\Big(1+|\nabla_i|^2\Big)^{\gamma_i/2}\Big(\frac{Z_\nu}{|x_i-a_\nu|}\mathcal{L}_{I,\alpha,\beta}^{(i)}u\Big), \tag{2.12}$$

$$L_I V_{ne}u = \sum_{i=1}^{N}\sum_{\nu=1}^{M}\nabla_i\Big(\frac{Z_\nu}{|x_i-a_\nu|}L_I^{(i)}u\Big), \tag{2.13}$$

$$\mathcal{L}_{I,\alpha,\beta}V_{ee}u = \frac{1}{2}\sum_{i\neq j}\Big(1+|\nabla_i|^2\Big)^{\gamma_i/2}\Big(1+|\nabla_j|^2\Big)^{\gamma_j/2}\Big(\frac{1}{|x_i-x_j|}\mathcal{L}_{I,\alpha,\beta}^{(i,j)}u\Big), \tag{2.14}$$

and

$$L_I V_{ee}u = \frac{1}{2}\sum_{i\neq j}\nabla_i^{\gamma_i'}\bigotimes\nabla_j^{\gamma_j'}\Big(\frac{1}{|x_i-x_j|}L_I^{(i,j)}u\Big), \tag{2.15}$$

where $\gamma_k = \alpha$, $\gamma_k' = 1$ if $k \in I$; and $\gamma_k = \beta$, $\gamma_k' = 0$ if $k \in I^c$.

Notice that by the Leibniz rule, $\nabla_y(\frac{1}{|y|}f(y)) = -\frac{y}{|y|^3}f(y) + \frac{1}{|y|}\nabla_y f$. Then from (2.13), (2.15) and by using Hardy inequality and its antisymmetric version (see *e.g.*, Cor. 3.8 with $s = 1$), one can deduce (2.11) directly.

We can not prove Theorem 2.2 as for Theorem 2.6 since the Leibniz rule fails for fractional Laplacian operators. In addition, the optimality of Theorem 2.2 for the case $\alpha = \beta$ and the singularity of the Coulomb potential make the proof of (2.8) in Theorem 2.2 much more delicate than the one of (2.11) in Theorem 2.6.

To prove Theorem 2.2, we need first to study the relationship between the fractional operator $(1 + |\nabla_i|^2)^{\gamma_i/2}$ and the Coulomb type potentials. In this paper, this is equivalent to the study of the relationship between

$|\nabla_i|^{\gamma_i}$ and the Coulomb type potentials by introducing a bounded operator $\mathcal{K}_{s,y} := (1+|\nabla_y|^2)^{s/2}(1+|\nabla_y|^s)^{-1}$ in Section 3.1.

The main tool of this paper is the following Hardy-type inequality (*i.e.*, Thm. 3.3):

$$\left\||y|^{-s}|\nabla_y|^{-s}f\right\|_{L^2(\mathbb{R}^3)} \lesssim_s \|f\|_{L^2(\mathbb{R}^3)}, \quad 0 \leqslant s < \frac{3}{2},$$

and its dual form:

$$\left\||\nabla_y|^{-s}|y|^{-s}f\right\|_{L^2(\mathbb{R}^3)} \lesssim_s \|f\|_{L^2(\mathbb{R}^3)}, \quad 0 \leqslant s < \frac{3}{2}.$$

This is the most important inequality used in this paper and this gives the tool to study the electron-nucleus term V_{ne} immediately (see (2.12)).

Concerning the electron-electron term V_{ee} in (2.14), we need a corresponding version of Hardy-type inequality for two particles. From the above Hardy-type inequality, one can deduce the following (see Lem. 3.6):

$$\left\||y-z|^{-s-t}|\nabla_y|^{-s}|\nabla_z|^{-t}f\right\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)} \lesssim_{s,t} \|f\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)}, \quad s,t \geqslant 0,\ s+t < \frac{3}{2}.$$

This gives the condition that $\beta < \frac{3}{4}$ and $\alpha + \beta < \frac{3}{2}$ in Assumption 2.1.

Thanks to antisymmetry, we can also generalize the standard Hardy inequality for two particles since the antisymmetry will counterbalance the singularity of the potential $\frac{1}{|x_i-x_j|}$. More precisely, for any function $g \in C_0^\infty(\mathbb{R}^3\times\mathbb{R}^3)$ satisfying $g(x,y) = -g(y,x)$, it is easy to see that $g(x,y) = 0$ for $x = y$. Thus $|g(x,y)| \leqslant C|x-y|$ in any compact neighborhood of the set $\{x = y\}$. As a result,

$$\left\|\frac{g}{|y-z|^{2s}}\right\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)} < +\infty, \quad 0 \leqslant s < \frac{5}{4}.$$

Then arguing as for the standard Hardy inequality, we show in Corollary 3.8 and Lemma 3.9 the following inequalities with antisymmetry:

$$\left\|\frac{g}{|y-z|^{2s}}\right\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)} \lesssim_s \left\|\frac{\nabla_y\nabla_z g}{|y-z|^{2s-2}}\right\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)} \lesssim_s \||\nabla_y|^s|\nabla_z|^s g\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)}, \qquad 1 \leqslant s < \frac{5}{4}.$$

Returning back to (2.8) and (2.14), we will use the following extension of the Hardy-type inequality for two particles with antisymmetry in Lemma 4.5:

$$\left\||\nabla_y|^{s-1/2}|\nabla_y|^{s-1/2}|y-z|^{-1}g\right\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)} \lesssim_s \||\nabla_y|^s|\nabla_z|^s g\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)}, \quad 0 \leqslant s < \frac{5}{4}.$$

This gives the condition $\alpha < \frac{5}{4}$ in Assumption 2.1. In addition, this estimate shows that spatial antisymmetry implies regularity.

Once the fractional Laplacian operator is defined and the above inequalities and their extensions are established, we can obtain Theorem 2.2 immediately.

This paper is organised as follows. As mentioned above, we will use the fractional Laplacian operator. Thus in Section 3, we will first study the fractional Laplacian. Then based on Hardy-type inequalities, we will deduce the above inequalities. In Section 4, we will use the above inequalities to prove Theorem 2.2. Then in Sections 5 and 6, following the proofs in [18], we will prove Theorems 2.3 and 2.5, respectively.

3. Fractional Laplacian operators and related inequalities

In the following, we denote the gradients ∇_y and ∇_z corresponding to the variables y and z in $\mathbb{R}^3$, respectively.

In the next subsection, we study the fractional Laplacian operator $(1+|\nabla_y|^2)^{s/2}$ on $\mathbb{R}^3$. Actually, we rather study the fractional Laplacian operator $|\nabla_y|^s$. The relationship between $|\nabla_y|^s$ and $(1+|\nabla_y|^2)^{s/2}$ will be studied equally. Then, for some $s,t > 0$, we will study some Hardy-type inequalities associated with the operators $|\nabla_y|^{-s}|y|^{-s}$ and $|\nabla_y|^{-s}|\nabla_z|^{-t}|y-z|^{-s-t}$.

3.1. Fractional Laplacian

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

$$\mathcal{F}_y(f)(\xi_y) := \int_{\mathbb{R}^3} f(y)e^{-2\pi i \xi_y \cdot y}\,\mathrm{d}y, \quad \mathcal{F}_{y,z}(g)(\xi_y,\xi_z) := \mathcal{F}_z \circ \mathcal{F}_y(g)(\xi_y,\xi_z),$$

and

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

For $s > 0$, a function $f \in L^2(\mathbb{R}^3)$ is said to be in $H^s(\mathbb{R}^3)$ if and only if

$$\|f\|^2_{H^s(\mathbb{R}^3)} := \int_{\mathbb{R}^3} \left(1 + |\xi_y|^2\right)^s |\mathcal{F}_y(f)(\xi_y)|^2\,\mathrm{d}\xi_y < +\infty.$$

The fractional Laplacian $|\nabla_y|^s$ (or $(-\triangle_y)^{s/2}$) is defined on functions $f \in H^s(\mathbb{R}^3)$ by the Fourier representation:

$$\mathcal{F}_y(|\nabla_y|^s f)(\xi_y) := |2\pi\xi_y|^s \mathcal{F}_y(f)(\xi_y).$$

Similarly, $(1 + |\nabla_y|^2)^{s/2}$ is defined by

$$\mathcal{F}_y\left(\left(1 + |\nabla_y|^2\right)^{s/2} f\right)(\xi_y) := \left(1 + |2\pi\xi_y|^2\right)^{s/2} \mathcal{F}_y(f)(\xi_y).$$

The operator $\mathcal{L}_{I,\alpha,\beta}$ which is defined on functions $u \in X_{I,\alpha,\beta}$ can be regarded as a composition of fractional Laplacian operators on $\mathbb{R}^3$ in the following manner:

$$\mathcal{L}_{I,\alpha,\beta} u := \left(1 + |\nabla_1|^2\right)^{\gamma_1/2} \circ \cdots \circ \left(1 + |\nabla_N|^2\right)^{\gamma_N/2} u,$$

where $\gamma_k = \alpha$ if $k \in I$, and $\gamma_k = \beta$ if $k \in I^c$.

Applying the Fourier transform to solve the Poisson equation

$$|\nabla_y|^s f_1(y) = f_2(y) \quad \text{in} \quad \mathbb{R}^3,$$

we find that $|2\pi\xi_y|^s \mathcal{F}_y(f_1)(\xi_y) = \mathcal{F}_y(f_2)(\xi_y)$. The inverse of the fractional Laplacian, or negative power of the Laplacian $|\nabla_y|^{-s}$ with $s > 0$ is defined on functions f in the Schwartz space $\mathcal{S}(\mathbb{R}^3)$ by

$$\mathcal{F}_y\left(|\nabla_y|^{-s} f\right)(\xi_y) = |2\pi\xi_y|^{-s} \mathcal{F}_y(f)(\xi_y) \qquad \text{for} \quad \xi_y \neq 0.$$

In principle, we need the restriction $0 < s < 3$ because when $s \geqslant 3$ the multiplier $|\xi_y|^{-s}$ does not define a tempered distribution (for more details, see *e.g.*, [16]).

On the other hand, the term $\frac{1}{|y|^s}$ is a tempered distribution for $0 < s < 3$ with Fourier transform

$$b_s \mathcal{F}_y\left(|\cdot|^{-s}\right)(\xi_y) = b_{3-s}|\xi_y|^{-3+s}, \qquad b_s = \pi^{-s/2}\Gamma(s/2), \tag{3.1}$$

where Γ is the Gamma function. For the detail, see *e.g.*, equation (3.3) of [6] (the difference of the definition of b_s therein is because of the different definition of the Fourier transform) or Theorem 5.9 of [14] by using the fact that $\mathcal{F}_y(fg) = \mathcal{F}_y(f) * \mathcal{F}_y(g)$. Hence, if $0 < s < 3$, the operator $|\nabla_y|^{-s}$ can be rewritten as

$$|\nabla_y|^{-s} f(y) = \frac{b_{3-s}}{(2\pi)^s b_s} \int_{\mathbb{R}^3} |z - y|^{-3+s} f(z)\,\mathrm{d}z, \quad f \in \mathcal{S}\big(\mathbb{R}^3\big). \tag{3.2}$$

Suppose that $0 < s < 3$, then $|\nabla_y|^s |y|^{-t}$ is an $L^1_{\text{loc}}(\mathbb{R}^3)$-function for $0 < t < 3-s$ and, using (3.1),

$$|\nabla_y|^s |y|^{-t} = \mathcal{F}_y^{-1}\big(|2\pi\xi_y|^s \mathcal{F}_y\big(|\cdot|^{-t}\big)\big) = \frac{(2\pi)^s b_{3-t}}{b_t}\mathcal{F}_y^{-1}\big(|\cdot|^{-3+t+s}\big) = \frac{(2\pi)^s b_{s+t} b_{3-t}}{b_{3-s-t} b_t}|y|^{-s-t}. \tag{3.3}$$

This equation can also be found in equations (3.4) and (3.5) from [6]. Also, $|\nabla_y|^{-s}|y|^{-t}$ is a $L^1_{\text{loc}}(\mathbb{R}^3)$-function for $0 < s < t < 3$ and

$$|\nabla_y|^{-s}|y|^{-t} = \mathcal{F}_y^{-1}\Big(|2\pi\xi_y|^{-s}\mathcal{F}_y\big(|\cdot|^{-t}\big)\Big) = \frac{b_{t-s} b_{3-t}}{(2\pi)^s b_{3+s-t} b_t}|y|^{s-t}. \tag{3.4}$$

We end this subsection by studying the relationship between $(1 + |\nabla_y|^2)^{s/2}$ and $|\nabla_y|^s$, then in the next subsections we will study Hardy-type inequalities associated with the fractional Laplacian operator $|\nabla_y|^s$.

Let

$$\mathcal{K}_{s,y} := \Big(1 + |\nabla_y|^2\Big)^{s/2}\big(1 + |\nabla_y|^s\big)^{-1}, \tag{3.5}$$

which is defined by the Fourier transform:

$$\mathcal{F}_y(\mathcal{K}_{s,y} f)(\xi_y) := \frac{\big(1 + |2\pi\xi|^2\big)^{s/2}}{1 + |2\pi\xi|^s}\mathcal{F}_y(f)(\xi_y).$$

By the Fourier transform, it is easy to see that

$$\mathcal{K}^*_{s,y} = \mathcal{K}_{s,y}. \tag{3.6}$$

Then we have the following.

Lemma 3.1. *For any* $0 \leqslant s \leqslant 2$,

$$\|\mathcal{K}_{s,y}\|_{L^2(\mathbb{R}^3)\to L^2(\mathbb{R}^3)} \leqslant 1.$$

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

$$\|\mathcal{K}_{s,y} f\|_{L^2(\mathbb{R}^3)} = \left\|\Big(1 + |2\pi\xi_y|^2\Big)^{s/2}\big(1 + |2\pi\xi_y|^s\big)^{-1}\mathcal{F}_y(f)\right\|_{L^2(\mathbb{R}^3)}.$$

As $0 \leqslant s/2 \leqslant 1$, $(1 + |2\pi\xi_y|^2)^{s/2} \leqslant (1 + |2\pi\xi_y|^s)$. Thus,

$$\|\mathcal{K}_{s,y} f\|_{L^2(\mathbb{R}^3)} \leqslant \|\mathcal{F}_y(f)\|_{L^2(\mathbb{R}^3)} = \|f\|_{L^2(\mathbb{R}^3)}.$$

Hence the lemma. □

Remark 3.2. Actually, the operator $\mathcal{K}_{s,y}$ is also bounded from below. One can use the inequalities $(a^p + b^p) \leqslant (a+b)^p \leqslant 2^p(a^p + b^p)$ for $a, b \geqslant 0$. (We thank one of the referees for this remark.)

3.2. Hardy-type inequalities for a single particle

We now consider the term $|\nabla_y|^{-s}|y|^{-s} f(y)$ with $f \in L^2(\mathbb{R}^3)$. Actually, $|\nabla_y|^{-s}|y|^{-s}$ is the adjoint of the operator $|y|^{-s}|\nabla_y|^{-s}$ which has been well studied in [7] (see equally [2], Thm. 1.7.1). The following holds.

Theorem 3.3 (Hardy-type inequality [7])**.** *Let* $p^{-1} + q^{-1} = 1$. *Suppose* $s > 0$ *and* $3s^{-1} > p > 1$. *Then*

$$\Big\||y|^{-s}|\nabla_y|^{-s} f\Big\|_{L^p(\mathbb{R}^3)} \leqslant C_{s,p}\|f\|_{L^p(\mathbb{R}^3)} \tag{3.7}$$

where

$$C_{s,p} := 2^{-s}\frac{\Gamma\big(\frac{1}{2}(3p^{-1} - s)\big)\Gamma\big(\frac{3}{2}q^{-1}\big)}{\Gamma\big(\frac{3}{2}(q^{-1} + s)\big)\Gamma\big(\frac{1}{2}3p^{-1}\big)}.$$

If $p \geqslant 3s^{-1}$ *or* $p = 1$, *then* $C_{s,p}$ *is unbounded.*

Remark 3.4. It is shown in [7] that the constant $C_{s,p}$ is optimal. When $p = 2$, equation (3.7) is equally proven in Theorem 2.58 of [1] but without the optimal constant $C_{s,p}$.

Remark 3.5. Replacing $f(y)$ by $|\nabla_y|^s g(y)$ in (3.7), then (3.7) can be rewritten as:

$$\big\||y|^{-s}g\big\|_{L^p(\mathbb{R}^3)} \leqslant C_{s,p}\||\nabla_y|^s g\|_{L^p(\mathbb{R}^3)}. \tag{3.8}$$

When $p = 2$ and $s = 1$, (3.7) is indeed the Hardy inequality with the optimal constant $C_{1,2} = 2$. When $p = 2$ and $s = \frac{1}{2}$, (3.7) is the Kato inequality with the optimal constant $C_{\frac{1}{2},2} = \frac{\sqrt{\pi}}{\sqrt{2}}$ (see *e.g.*, [2], Formula (1.7.7)).

In this paper, we only use the case $p = 2$. By duality, we also have the following: for $0 < s < \frac{3}{2}$

$$\Big\||\nabla_y|^{-s}|y|^{-s}f\Big\|_{L^2(\mathbb{R}^3)} \leqslant C_{s,2}\|f\|_{L^2(\mathbb{R}^3)}.$$

Notice that $|\nabla_y|^s[f(y+a)] = [|\nabla_y|^s f](y+a)$. Then from Theorem 3.3, for any $a \in \mathbb{R}^3$ and $0 < s < \frac{3}{2}$,

$$\Big\||\cdot - a|^{-s}f\Big\|_{L^2(\mathbb{R}^3)} \leqslant C_{s,2}\||\nabla_y|^s f\|_{L^2(\mathbb{R}^3)}. \tag{3.9}$$

By Fubini's Theorem and for any $h(y,z) \in L^2(\mathbb{R}^3 \times \mathbb{R}^3)$, we have

$$\big\||y-z|^{-s}h(y,z)\big\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)} \leqslant C_{s,2}\||\nabla_y|^s h\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)}. \tag{3.10}$$

The dual version of (3.9) and (3.10) can be represented respectively as follows: for $a \in \mathbb{R}^3$ and $0 < s < 3/2$,

$$\Big\||\nabla_y|^{-s}|\cdot - a|^{-s}f\Big\|_{L^2(\mathbb{R}^3)} \leqslant C_{s,2}\|f\|_{L^2(\mathbb{R}^3)} \tag{3.11}$$

and

$$\Big\||\nabla_y|^{-s}|y-z|^{-s}f\Big\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)} \leqslant C_{s,2}\|f\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)}. \tag{3.12}$$

3.3. Hardy-type inequalities for two particles

The rest of this section is devoted to Hardy-type inequalities for $|\nabla_y|^{-s}|\nabla_z|^{-t}|z-y|^{-s-t}$ terms for some $s, t \geqslant 0$. By using Theorem 3.3, we have the following.

Lemma 3.6. *For $s, t \geqslant 0$, $s + t < 3/2$, and $f \in L^2(\mathbb{R}^3 \times \mathbb{R}^3)$, we have*

$$\Big\||\nabla_y|^{-s}|\nabla_z|^{-t}|y-z|^{-s-t}f\Big\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)} \leqslant 2c_{s+t}\|f\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)} \tag{3.13}$$

and

$$\Big\||y-z|^{-s-t}|\nabla_y|^{-s}|\nabla_z|^{-t}f\Big\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)} \leqslant 2c_{s+t}\|f\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)}, \tag{3.14}$$

with $c_0 := 1$ and, for $0 < s < 3/2$, $c_s := C_{s,2}$ where $C_{s,2}$ is defined in Theorem 3.3.

Proof. For simplicity, we use the shorthand $\|f\|_{L^2}$ for $\|f\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)}$. We prove first

$$\Big\||\nabla_y|^{-s}|\nabla_z|^{-t}|y-z|^{-s-t}f\Big\|_{L^2} \leqslant 2c_{s+t}\|f\|_{L^2}.$$

If $s = t = 0$, then $\|f\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)} \leqslant 2c_0\|f\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)}$ where $c_0 = 1$.

Now we assume $s = 0$ and $t \neq 0$. Thanks to (3.12), we have

$$\left\| |\nabla_z|^{-t} |y - z|^{-t} f \right\|_{L^2} \leqslant c_t \|f\|_{L^2} \leqslant 2c_t \|f\|_{L^2}.$$

The case $t = 0$ and $s \neq 0$ can be treated in the same manner. Now we only need to consider the case $s, t > 0$. For any function $u(y, z) \in L^2(\mathbb{R}^3 \times \mathbb{R}^3)$, by Fourier transform on $\mathbb{R}^3 \times \mathbb{R}^3$, we have

$$\left\| |\nabla_y|^{-s} |\nabla_z|^{-t} |y - z|^{-s-t} f \right\|_{L^2} = (2\pi)^{-s-t} \left\| |\xi_y|^{-s} |\xi_z|^{-t} \mathcal{F}_{y,z}\big(|y - z|^{-s-t} f\big)(\xi_y, \xi_z) \right\|_{L^2}.$$

Notice that $|\tau|^t \leqslant |\tau|^{s+t} + 1$ for $\tau \in \mathbb{R}$. Then for $\tau = |\xi_y|/|\xi_z|$, we have

$$|\xi_y|^{-s} |\xi_z|^{-t} \leqslant |\xi_y|^{-s-t} + |\xi_z|^{-s-t}.$$

Thus,

$$\begin{aligned}
&\left\| |\xi_y|^{-s} |\xi_z|^{-t} \mathcal{F}_{y,z}\big(|y - z|^{-s-t} f\big)(\xi_x, \xi_y) \right\|_{L^2} \\
&\quad \leqslant \left\| |\xi_y|^{-s-t} \mathcal{F}_{y,z}\big(|y - z|^{-s-t} f\big)(\xi_y, \xi_z) \right\|_{L^2} + \left\| |\xi_z|^{-s-t} \mathcal{F}_{y,z}\big(|y - z|^{-s-t} f\big)(\xi_y, \xi_z) \right\|_{L^2} \\
&\quad = (2\pi)^{s+t} \left\| |\nabla_y|^{-s-t} |y - z|^{-s-t} f \right\|_{L^2} + (2\pi)^{s+t} \left\| |\nabla_z|^{-s-t} |y - z|^{-s-t} f \right\|_{L^2}.
\end{aligned}$$

As $0 < s + t < 3/2$, by (3.12), we have

$$\left\| |\nabla_y|^{-s-t} |y - z|^{-s-t} f \right\|_{L^2} \leqslant c_{s+t} \|f\|_{L^2},$$

and

$$\left\| |\nabla_z|^{-s-t} |y - z|^{-s-t} f \right\|_{L^2} \leqslant c_{s+t} \|f\|_{L^2}.$$

Consequently, we deduce

$$\left\| |\nabla_y|^{-s} |\nabla_z|^{-t} |x - y|^{-s-t} f \right\|_{L^2} \leqslant 2c_{s+t} \|f\|_{L^2}.$$

By duality, equation (3.14) follows. □

For the wavefunction u, the antisymmetry with respect to I will counterbalance the singularities of the potential between electrons. Based on this observation, Lemma 3.6 can be extended in consideration of the antisymmetry. In Theorem 2.2, we only focus on the case $t = s$. The extension is based on the following.

Lemma 3.7. *Let $a \in \mathbb{R}^3$ and $k \in [1, 3/2) \cup (3/2, 5/2)$. If $f \in C_0^\infty(\mathbb{R}^3)$ for $k \in [1, 3/2)$, or if $f \in C_0^\infty(\mathbb{R}^3 \backslash \{a\})$ for $k \in (3/2, 5/2)$, we have*

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

The proof is inspired by Lemma 2 of [17].

Proof. We have the relationship:

$$(2k - 1) \frac{1}{|y - a|^{2k}} = -\nabla \frac{1}{|y - a|^{2k-1}} \cdot \nabla |y - a|.$$

Under the assumption on f, we have $\int_{\mathbb{R}^3} \frac{|f(y)|^2}{|y-a|^{2k}} \, \mathrm{d}y < +\infty$. Then by integration by parts, we obtain

$$(2k - 1) \int_{\mathbb{R}^3} \frac{|f|^2}{|y - a|^{2k}} \, \mathrm{d}y = \int_{\mathbb{R}^3} \frac{\nabla_y \cdot \big(|f|^2 \nabla |y - a|\big)}{|y - a|^{2k-1}} \, \mathrm{d}y.$$

Using $\triangle|y-a| = \frac{2}{|y-a|}$ on the right-hand side, then

$$(2k-1)\int_{\mathbb{R}^3} \frac{|f|^2}{|y-a|^{2k}}\,\mathrm{d}y = 2\Re\int_{\mathbb{R}^3} \frac{\overline{f}\nabla_y f\cdot\nabla|y-a|}{|y-a|^{2k-1}}\,\mathrm{d}y + 2\int_{\mathbb{R}^3} \frac{|f|^2}{|y-a|^{2k}}\,\mathrm{d}y,$$

by the Cauchy–Schwarz inequality, we obtain

$$\left|\frac{2k-3}{2}\right|\int_{\mathbb{R}^3} \frac{|f|^2}{|y-a|^{2k}}\,\mathrm{d}y \leqslant \left(\int_{\mathbb{R}^3} \frac{|f|^2}{|y-a|^{2k}}\,\mathrm{d}y\right)^{1/2}\left(\int_{\mathbb{R}^3} \frac{|\nabla|y-a|\cdot\nabla f|^2}{|y-a|^{2k-2}}\,\mathrm{d}y\right)^{1/2}.$$

As $|\nabla|y-a|\cdot\nabla f| \leqslant \big|\nabla|y-a|\big||\nabla f| \leqslant |\nabla f|$, we finally get the conclusion:

$$\frac{|2k-3|^2}{4}\int_{\mathbb{R}^3} \frac{|f|^2}{|y-a|^{2k}}\,\mathrm{d}y \leqslant \int_{\mathbb{R}^3} \frac{|\nabla f|^2}{|y-a|^{2k-2}}\,\mathrm{d}y.$$

This ends the proof. □

Using Fubini's theorem and Lemma 3.7, the following holds for antisymmetric functions.

Corollary 3.8. *For $s \in [1, 5/4)$ and $f \in C_0^\infty(\mathbb{R}^3\times\mathbb{R}^3)$ with $f(y,z) = -f(z,y)$, we have*

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

Proof. This is a generalization of equation (3.9) from [17]. We first fix $z \in \mathbb{R}^3$, and let $g_z(y) = f(y,z)$. As $f(y,z) = -f(z,y)$ and $f \in C_0^\infty(\mathbb{R}^3\times\mathbb{R}^3)$, we know that $g_z \in C_0^\infty(\mathbb{R}^3\backslash\{z\})$. Thus Lemma 3.7 shows that for any $z \in \mathbb{R}^3$

$$\left\|\frac{g_z}{|\cdot-z|^{2s}}\right\|_{L^2(\mathbb{R}^3_y)} \leqslant \frac{2}{|4s-3|}\left\|\frac{\nabla_y g_z}{|\cdot-z|^{2s-1}}\right\|_{L^2(\mathbb{R}^3_y)}.$$

Taking L^2-norm with respect to z in the above inequality, we get

$$\left\|\frac{f(y,z)}{|y-z|^{2s}}\right\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)} \leqslant \frac{2}{|4s-3|}\left\|\frac{\nabla_y f(y,z)}{|y-z|^{2s-1}}\right\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)}.$$

Now $1 \leqslant 2s-1 < \frac{3}{2}$ and $\nabla_y f(y,\cdot) \in C^\infty(\mathbb{R}^3)$ for any fixed $y \in \mathbb{R}^3$. Arguing as above, fixing $y \in \mathbb{R}^3$, and using Lemma 3.7 again, we infer

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

This ends the proof. □

Combining Lemma 3.6 with Corollary 3.8, we have the following.

Lemma 3.9. *For $s \in [1, 5/4)$ and $f \in C_0^\infty(\mathbb{R}^3\times\mathbb{R}^3)$ with $f(y,z) = -f(z,y)$, we have*

$$\left\|\frac{f}{|y-z|^{2s}}\right\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)} \leqslant c_{2s}\||\nabla_y|^s|\nabla_z|^s f\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)} \tag{3.15}$$

where $c_{2s} := \frac{8c_{2s-2}}{(5-4s)(4s-3)}$ and $c_{2s-2} = C_{2s-2,2}$.

Remark 3.10. Denote the functional space $Y_{\mathrm{anti},s}(\mathbb{R}^3\times\mathbb{R}^3)$ by

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

Then $Y_{\mathrm{anti},s}(\mathbb{R}^3\times\mathbb{R}^3)$ is a completion of $C_0^\infty(\mathbb{R}^3\times\mathbb{R}^3)$ with the antisymmetry $f(y,z) = -f(z,y)$. Thus by density, equation (3.15) still holds for $f \in Y_{\mathrm{anti},s}(\mathbb{R}^3\times\mathbb{R}^3)$.

4. Hardy-type inequalities for the Coulomb system

Now, we are going to use these inequalities to prove Theorem 2.2. We will study separately the contribution of the potential V_{ne} in Section 4.1 and the potential V_{ee} in Section 4.2. Theorem 2.2 follows immediately from Lemmas 4.1 and 4.3 with $C_{\mathrm{mix},\alpha,\beta} = C_{1,\mathrm{mix},\alpha,\beta} + C_{2,\mathrm{mix},\alpha,\beta}$ where $C_{1,\mathrm{mix},\alpha,\beta}$ and $C_{2,\mathrm{mix},\alpha,\beta}$ are given in Lemmas 4.1 and 4.3 respectively.

Before going further, we recall that $Z = \sum_{\nu=1}^{M} Z_\nu$ and that the constant c_k is defined by : $c_0 = 1$, $c_k = C_{k,2}$ for $k \in (0, 3/2)$ with $C_{k,p}$ defined in Theorem 3.3, and $c_k = \frac{8c_{k-2}}{(5-2k)(2k-3)}$ for $k \in [2, 5/2)$.

4.1. Contribution of the electrons–nuclei interaction

In this subsection, we are going to prove the following.

Lemma 4.1 (Contribution of V_{ne})**.** *Let $I \subset \{1, \cdots, N\}$. For any $\alpha, \beta \in [0, 3/2)$, there is a constant $C_{1,\mathrm{mix},\alpha,\beta}$ independent of N, Z such that for any $u, v \in X_{I,\alpha,\beta}$,*

$$|\langle \mathcal{L}_{I,\alpha,\beta} V_{ne} u, \mathcal{L}_{I,\alpha,\beta} v\rangle| \leqslant C_{1,\mathrm{mix},\alpha,\beta} \sqrt{N} Z \|u\|_{0,I,\alpha,\beta} \|v\|_{1,I,\alpha,\beta}. \tag{4.1}$$

It is an immediate result of the following.

Lemma 4.2. *For $s \in [-1, 1/2)$, $a \in \mathbb{R}^3$, and $f \in H^{1+s}(\mathbb{R}^3)$, we have*

$$\big\| |\nabla_y|^s | \cdot - a|^{-1} f \big\|_{L^2(\mathbb{R}^3)} \leqslant C_s \| |\nabla_y|^{1+s} f \|_{L^2(\mathbb{R}^3)},$$

where $C_s = (c_{1+s} + c_s) c_{1-s}$ if $s > 0$, $C_0 = c_1 = 2$, $C_s = c_{-s} c_{1+s}$ if $-1 \leqslant s < 0$.

Before proving Lemma 4.2, we use it to prove Lemma 4.1 first.

Proof of Lemma 4.1. Recall that $\mathcal{K}_{s,y} = (1 + |\nabla_y|^2)^{s/2} (1 + |\nabla_y|^s)^{-1}$.

Following (2.12), (3.6) and the formal identity $|\nabla_i||\nabla_i|^{-1} = 1$, we have

$$\begin{aligned}
\langle \mathcal{L}_{I,\alpha,\beta} V_{ne} u, \mathcal{L}_{I,\alpha,\beta} v\rangle &= \sum_{i=1}^{N} \sum_{\nu=1}^{M} Z_\nu \left\langle \left(1 + |\nabla_i|^2\right)^{\gamma_i/2} |x_i - a_\nu|^{-1} \mathcal{L}_{I,\alpha,\beta}^{(i)} u, \mathcal{L}_{I,\alpha,\beta} v \right\rangle \\
&= \sum_{i=1}^{N} \sum_{\nu=1}^{M} Z_\nu \left\langle |\nabla_i|^{-1} (1 + |\nabla_i|^{\gamma_i}) |x_i - a_\nu|^{-1} \mathcal{L}_{I,\alpha,\beta}^{(i)} u, |\nabla_i| \mathcal{K}_{\gamma_i,x_i} \mathcal{L}_{I,\alpha,\beta} v \right\rangle \\
&= \sum_{i=1}^{N} \sum_{\nu=1}^{M} Z_\nu \left\langle |\nabla_i|^{-1} |x_i - a_\nu|^{-1} \mathcal{L}_{I,\alpha,\beta}^{(i)} u, |\nabla_i| \mathcal{K}_{\gamma_i,x_i} \mathcal{L}_{I,\alpha,\beta} v \right\rangle \\
&\quad + \sum_{i=1}^{N} \sum_{\nu=1}^{M} Z_\nu \left\langle |\nabla_i|^{\gamma_i - 1} |x_i - a_\nu|^{-1} \mathcal{L}_{I,\alpha,\beta}^{(i)} u, |\nabla_i| \mathcal{K}_{\gamma_i,x_i} \mathcal{L}_{I,\alpha,\beta} v \right\rangle
\end{aligned}$$

where $\gamma_k = \alpha$ if $k \in I$, and $\gamma_k = \beta$ if $k \in I^c$. By definition (2.7),

$$\|u\|_{1,I,\alpha,\beta}^2 = \sum_{i=1}^{N} \|\nabla_i u\|_{0,I,\alpha,\beta}^2. \tag{4.2}$$

Thus by Lemma 3.1,

$$|\langle \mathcal{L}_{I,\alpha,\beta} V_{ne} u, \mathcal{L}_{I,\alpha,\beta} v\rangle| \leqslant \left(\sum_{i=1}^{N} \left\| \sum_{\nu} Z_\nu |\nabla_i|^{-1} |x_i - a_\nu|^{-1} \mathcal{L}_{I,\alpha,\beta}^{(i)} u \right\|_{L^2\left((\mathbb{R}^3)^N\right)}^2 \right)^{1/2} \|v\|_{1,I,\alpha,\beta}$$

$$+\left(\sum_{i=1}^{N}\left\|\sum_{\nu} Z_\nu |\nabla_i|^{\gamma_i-1}|x_i-a_\nu|^{-1}\mathcal{L}^{(i)}_{I,\alpha,\beta}u\right\|^2_{L^2\left((\mathbb{R}^3)^N\right)}\right)^{1/2}\|v\|_{1,I,\alpha,\beta}.$$

By Lemma 4.2, we have

$$\begin{aligned}\left\|\sum_{\nu} Z_\nu |\nabla_i|^{s-1}|x_i-a_\nu|^{-1}\mathcal{L}^{(i)}_{I,\alpha,\beta}u\right\|_{L^2\left((\mathbb{R}^3)^N\right)} &\leqslant \sum_\nu Z_\nu \||\nabla_i|^{s-1}|x_i-a_\nu|^{-1}\mathcal{L}^{(i)}_{I,\alpha,\beta}u\|_{L^2\left((\mathbb{R}^3)^N\right)}\\ &\leqslant C_{s-1}Z\||\nabla_i|^{s}\mathcal{L}^{(i)}_{I,\alpha,\beta}u\|_{L^2\left((\mathbb{R}^3)^N\right)} \leqslant C_{s-1}Z\|u\|_{0,I,\alpha,\beta},\end{aligned}$$

where $s=0$ or $s=\gamma_i\geqslant 0$ and the last inequality holds since $|2\pi\xi_i|^s\leqslant(1+|2\pi\xi_i|^2)^{\gamma_i/2}$. Using (4.2) again, we finally get

$$|\langle\mathcal{L}_{I,\alpha,\beta}V_{ne}u,\mathcal{L}_{I,\alpha,\beta}v\rangle|\leqslant C_{1,\mathrm{mix},\alpha,\beta}\sqrt{N}Z\|u\|_{0,I,\alpha,\beta}\|v\|_{1,I,\alpha,\beta}.$$

with $C_{1,\mathrm{mix},\alpha,\beta}:=C_0+\max\{C_{\alpha-1},C_{\beta-1}\}$ independent of N,Z. This ends the proof. □

Now, we turn back to prove Lemma 4.2.

Proof of Lemma 4.2. When $s=0$, it is just the Hardy inequality and $C_0=c_1=2$.

When $s\in[-1,0)$, by (3.11), we have

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

Hence Lemma 4.2 for $s\in[-1,0)$ with $C_s=c_{-s}c_{1+s}$.

When $0<s<1/2$, we use the formal identity $|\nabla|^s=|\nabla||\nabla|^{s-1}$. Thus,

$$\begin{aligned}\big\||\nabla_y|^s|y-a|^{-1}f(y)\big\|_{L^2(\mathbb{R}^3)}&=\big\||\nabla_y|^{s-1}\nabla_y|y-a|^{-1}f(y)\big\|_{L^2(\mathbb{R}^3)}\\&\leqslant\big\||\nabla_y|^{s-1}|y-a|^{-1}\nabla_y f(y)\big\|_{L^2(\mathbb{R}^3)}+\big\||\nabla_y|^{s-1}|y-a|^{-3}(y-a)f(y)\big\|_{L^2(\mathbb{R}^3)}.\end{aligned}$$

Using (3.11) again, we get

$$\Big\||\nabla_y|^{s-1}|y-a|^{-1}\nabla_y f(y)\Big\|_{L^2(\mathbb{R}^3)}\leqslant c_{1-s}\big\||y-a|^{-s}\nabla_y f(y)\big\|_{L^2(\mathbb{R}^3)}\leqslant c_{1-s}c_s\big\||\nabla_y|^{1+s}f\big\|_{L^2(\mathbb{R}^3)}.$$

Analogously, as $0<s<1/2$, we have

$$\Big\||\nabla_y|^{s-1}|y-a|^{-3}(y-a)f(y)\Big\|_{L^2(\mathbb{R}^3)}\leqslant c_{1-s}\big\||y-a|^{-1-s}f(y)\big\|_{L^2(\mathbb{R}^3)}\leqslant c_{1-s}c_{1+s}\big\||\nabla_y|^{1+s}f\big\|_{L^2(\mathbb{R}^3)}.$$

We conclude now that, for $s\in(0,1/2)$, Lemma 4.2 holds with $C_s=c_{1-s}(c_s+c_{1+s})$, *i.e.*,

$$\big\||\nabla_y|^s|\cdot-a|^{-1}f\big\|_{L^2(\mathbb{R}^3)}\leqslant C_s\big\||\nabla_y|^{1+s}f\big\|_{L^2(\mathbb{R}^3)},$$

This ends the proof. □

4.2. Contribution of the electron-electron interaction

In this subsection, we are going to prove the following.

Lemma 4.3 (Contribution of V_{ee})**.** *Let $I\subset\{1,\cdots,N\}$. Under Assumption 2.1 on α,β, there is a constant $C_{2,\mathrm{mix},\alpha,\beta}$ independent of N,Z such that for any $u,v\in X_{I,\alpha,\beta}$,*

$$|\langle\mathcal{L}_{I,\alpha,\beta}V_{ee}u,\mathcal{L}_{I,\alpha,\beta}v\rangle|\leqslant C_{2,\mathrm{mix},\alpha,\beta}N^{3/2}\|u\|_{0,I,\alpha,\beta}\|v\|_{1,I,\alpha,\beta}. \tag{4.3}$$

Recall that $b_s = \pi^{-s/2}\Gamma(s/2)$ where $\Gamma(\cdot)$ is the Gamma function and recall that

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

To prove Lemma 4.3, we need the followings.

Lemma 4.4. *Define* $Y_{s,t}(\mathbb{R}^3 \times \mathbb{R}^3) := \{g \in L^2(\mathbb{R}^3 \times \mathbb{R}^3); |\nabla_y|^s|\nabla_z|^t g \in L^2(\mathbb{R}^3 \times \mathbb{R}^3)\}$. *Let* $0 \leqslant t \leqslant s$, $s+t < 3/2$ *and* $f \in Y_{s,t}(\mathbb{R}^3 \times \mathbb{R}^3)$. *Then,*

$$\left\| |\nabla_y|^{s+t-1}|y-z|^{-1} f\right\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)} \leqslant C'_{s,t}\||\nabla_y|^s|\nabla_z|^t f\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)},$$

where $C'_{s,t} := \left(\frac{2^{s+t}\pi^{s+t-2}b_{s+t}c_{s+t}}{b_{3-s-t}} + 2c_1\right)$ *if* $1 < s+t < 3/2$, *and* $C'_{s,t} := 2c_{1-s-t}c_{s+t}$ *if* $0 \leqslant s+t \leqslant 1$.

Lemma 4.5. *Let* $0 \leqslant s < 5/4$ *and* $f \in Y_{\text{anti},s}(\mathbb{R}^3 \times \mathbb{R}^3)$. *Then,*

$$\left\| |\nabla_y|^{s-1/2}|\nabla_z|^{s-1/2}|y-z|^{-1} f\right\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)} \leqslant C_{\text{anti},s}\||\nabla_y|^s|\nabla_z|^s f\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)},$$

where $C_{\text{anti},0} := 2c_1$, $C_{\text{anti},s} := 4c_{3-2s}c_{2s-2} + 4c_{3-2s}c_{2s-1} + 4c_{3-2s}c_{2s}$ *if* $1 \leqslant s < 5/4$, *and* $C_{\text{anti},s} := C_{\text{anti},0}^{1-s}C_{\text{anti},1}^{s}$ *if* $0 < s < 1$.

We prove Lemma 4.3 first. The proof of Lemmas 4.4 and 4.5 are postponed to Sections 4.2.1 and 4.2.2 respectively.

Proof of Lemma 4.3. Recall that $\mathcal{K}_{s,y} := (1+|\nabla_y|^2)^{s/2}(1+|\nabla_y|^s)^{-1}$. Following (2.14) and (3.6), we have

$$\begin{aligned}\langle \mathcal{L}_{I,\alpha,\beta}V_{ee}u, \mathcal{L}_{I,\alpha,\beta}v\rangle &= \frac{1}{2}\sum_{\substack{i,j=1\\ i\neq j}}^{N}\left\langle (1+|\nabla_i|^2)^{\gamma_i/2}(1+|\nabla_j|^2)^{\gamma_j/2}|x_i-x_j|^{-1}\mathcal{L}_{I,\alpha,\beta}^{(i,j)}u, \mathcal{L}_{I,\alpha,\beta}v\right\rangle \\ &= \frac{1}{2}\sum_{i\neq j}\left\langle (1+|\nabla_i|^{\gamma_i})(1+|\nabla_j|^{\gamma_j})|x_i-x_j|^{-1}\mathcal{L}_{I,\alpha,\beta}^{(i,j)}u, \mathcal{K}_{\gamma_i,x_i}\mathcal{K}_{\gamma_j,x_j}\mathcal{L}_{I,\alpha,\beta}v\right\rangle,\end{aligned}$$

where $\gamma_k = \alpha$ if $k \in I$, and $\gamma_k = \beta$ if $k \in I^c$. Then by using the formal identity $|\nabla_k|^{\gamma_k} = |\nabla_k|^{\gamma_k-1}|\nabla_k|$ for $k = i$ or $k = j$, we get

$$\begin{aligned}\langle \mathcal{L}_{I,\alpha,\beta}V_{ee}u, \mathcal{L}_{I,\alpha,\beta}v\rangle &= \frac{1}{2}\sum_{i\neq j}\left\langle \mathcal{L}_{I,\alpha,\beta}^{(i,j)}u, |x_i-x_j|^{-1}\mathcal{K}_{\gamma_i,x_i}\mathcal{K}_{\gamma_j,x_j}\mathcal{L}_{I,\alpha,\beta}v\right\rangle \\ &+ \frac{1}{2}\sum_{i\neq j}\left\langle |\nabla_j|^{\gamma_j-1}|x_i-x_j|^{-1}\mathcal{L}_{I,\alpha,\beta}^{(i,j)}u, |\nabla_j|\mathcal{K}_{\gamma_i,x_i}\mathcal{K}_{\gamma_j,x_j}\mathcal{L}_{I,\alpha,\beta}v\right\rangle \\ &+ \frac{1}{2}\sum_{i\neq j}\left\langle |\nabla_i|^{\gamma_i-1}|x_i-x_j|^{-1}\mathcal{L}_{I,\alpha,\beta}^{(i,j)}u, |\nabla_i|\mathcal{K}_{\gamma_i,x_i}\mathcal{K}_{\gamma_j,x_j}\mathcal{L}_{I,\alpha,\beta}v\right\rangle \\ &+ \frac{1}{2}\sum_{i\neq j}\left\langle |\nabla_i|^{\gamma_i}|\nabla_j|^{\gamma_j}|x_i-x_j|^{-1}\mathcal{L}_{I,\alpha,\beta}^{(i,j)}u, \mathcal{K}_{\gamma_i,x_i}\mathcal{K}_{\gamma_j,x_j}\mathcal{L}_{I,\alpha,\beta}v\right\rangle. \end{aligned} \tag{4.4}$$

For the first term on the right-hand side of (4.4), it follows from (3.7), Lemma 3.1 and the fact $1 \leqslant (1 + |2\pi\xi_k|^2)^{\gamma_k}$ for $k = i$ or $k = j$ that

$$\left|\left\langle \mathcal{L}_{I,\alpha,\beta}^{(i,j)}u, |x_i-x_j|^{-1}\mathcal{K}_{\gamma_i,x_i}\mathcal{K}_{\gamma_j,x_j}\mathcal{L}_{I,\alpha,\beta}v\right\rangle\right| \leqslant \left\|\mathcal{L}_{I,\alpha,\beta}^{(i,j)}u\right\|_{L^2((\mathbb{R}^3)^N)}\left\||x_i-x_j|^{-1}\mathcal{K}_{\gamma_i,x_i}\mathcal{K}_{\gamma_j,x_j}\mathcal{L}_{I,\alpha,\beta}v\right\|_{L^2((\mathbb{R}^3)^N)}$$

$$\leqslant \frac{c_1}{2}\|u\|_{0,I,\alpha,\beta}\Big(\||\nabla_i|\mathcal{L}_{I,\alpha,\beta}v\|_{0,I,\alpha,\beta}+\||\nabla_j|\mathcal{L}_{I,\alpha,\beta}v\|_{0,I,\alpha,\beta}\Big).$$

Thus, according to (4.2), we get

$$\left|\sum_{i\neq j}\Big\langle \mathcal{L}^{(i,j)}_{I,\alpha,\beta}u, |x_i-x_j|^{-1}\mathcal{K}_{\gamma_i,x_i}\mathcal{K}_{\gamma_j,x_j}\mathcal{L}_{I,\alpha,\beta}v\Big\rangle\right| \leqslant c_1 N^{3/2}\|u\|_{0,I,\alpha,\beta}\|v\|_{1,I,\alpha,\beta}. \tag{4.5}$$

For the second term, it follows from Lemmas 3.1, 4.2 and the fact $\gamma_j\in[0,3/2)$ that

$$\begin{aligned}&\left|\Big\langle |\nabla_j|^{\gamma_j-1}|x_i-x_j|^{-1}\mathcal{L}^{(i,j)}_{I,\alpha,\beta}u, |\nabla_j|\mathcal{K}_{\gamma_i,x_i}\mathcal{K}_{\gamma_j,x_j}\mathcal{L}_{I,\alpha,\beta}v\Big\rangle\right|\\ &\quad\leqslant \Big\||\nabla_j|^{\gamma_j-1}|x_i-x_j|^{-1}\mathcal{L}^{(i,j)}_{I,\alpha,\beta}u\Big\|_{L^2((\mathbb{R}^3)^N)}\big\||\nabla_j|\mathcal{K}_{\gamma_i,x_i}\mathcal{K}_{\gamma_j,x_j}\mathcal{L}_{I,\alpha,\beta}v\big\|_{L^2((\mathbb{R}^3)^N)}\\ &\quad\leqslant C_{\gamma_j}\Big\||\nabla_j|^{\gamma_j}\mathcal{L}^{(i,j)}_{I,\alpha,\beta}u\Big\|_{L^2((\mathbb{R}^3)^N)}\||\nabla_j|v\|_{0,I,\alpha,\beta}\leqslant C_{\gamma_j}\|u\|_{0,I,\alpha,\beta}\||\nabla_j|v\|_{0,I,\alpha,\beta},\end{aligned}$$

where the last inequality holds since $|2\pi\xi_j|^{\gamma_j}\leqslant(1+|2\pi\xi_j|^2)^{\gamma_j/2}$. Thus,

$$\left|\sum_{i\neq j}\Big\langle |\nabla_j|^{\gamma_j-1}|x_i-x_j|^{-1}\mathcal{L}^{(i,j)}_{I,\alpha,\beta}u, |\nabla_j|\mathcal{K}_{\gamma_i,x_i}\mathcal{K}_{\gamma_j,x_j}\mathcal{L}_{I,\alpha,\beta}v\Big\rangle\right| \leqslant C_{\alpha,\beta}N^{3/2}\|u\|_{0,I,\alpha,\beta}\|v\|_{1,I,\alpha,\beta} \tag{4.6}$$

with $C_{\alpha,\beta}:=\max\{C_\alpha,C_\beta\}$. Analogously, for the third term,

$$\left|\sum_{i\neq j}\Big\langle |\nabla_i|^{\gamma_i-1}|x_i-x_j|^{-1}\mathcal{L}^{(i,j)}_{I,\alpha,\beta}u, |\nabla_i|\mathcal{K}_{\gamma_i,x_i}\mathcal{K}_{\gamma_j,x_j}\mathcal{L}_{I,\alpha,\beta}v\Big\rangle\right| \leqslant C_{\alpha,\beta}N^{3/2}\|u\|_{0,I,\alpha,\beta}\|v\|_{1,I,\alpha,\beta}. \tag{4.7}$$

Finally, we deal with the last term on the right-hand side of (4.4). It is the most delicate term in (4.4) and Assumption 2.1 on α,β is necessary. Before going further, we assume that $\gamma_j\leqslant\gamma_i$. The case $\gamma_i\leqslant\gamma_j$ can be treated in the same manner.

We first consider the case $\{i,j\}\not\subset I$. Then as $\gamma_j\leqslant\gamma_i$, we have $\gamma_j=\beta\in[0,3/4)$. Thus by using Lemma 3.1 and the formal identity $|\nabla_i|^{\gamma_i}=|\nabla_i|^{\gamma_i+\gamma_j-1}|\nabla_i|^{1-\gamma_j}$,

$$\begin{aligned}&\left|\Big\langle |\nabla_i|^{\gamma_i}|\nabla_j|^{\gamma_j}|x_i-x_j|^{-1}\mathcal{L}^{(i,j)}_{I,\alpha,\beta}u, \mathcal{K}_{\gamma_i,x_i}\mathcal{K}_{\gamma_j,x_j}\mathcal{L}_{I,\alpha,\beta}v\Big\rangle\right|\\ &\quad=\left|\Big\langle |\nabla_i|^{\gamma_i+\gamma_j-1}|x_i-x_j|^{-1}\mathcal{L}^{(i,j)}_{I,\alpha,\beta}u, |\nabla_j|^{\gamma_j}|\nabla_i|^{1-\gamma_j}\mathcal{K}_{\gamma_i,x_i}\mathcal{K}_{\gamma_j,x_j}\mathcal{L}_{I,\alpha,\beta}v\Big\rangle\right|\\ &\quad\leqslant\Big\||\nabla_i|^{\gamma_i+\gamma_j-1}|x_i-x_j|^{-1}\mathcal{L}^{(i,j)}_{I,\alpha,\beta}u\Big\|_{L^2((\mathbb{R}^3)^N)}\Big\||\nabla_j|^{\gamma_j}|\nabla_i|^{1-\gamma_j}v\Big\|_{0,I,\alpha,\beta}.\end{aligned}$$

Notice that $|\tau|^{\gamma_j}\leqslant 1+|\tau|$ for any $\tau\in\mathbb{R}$ and $0\leqslant\gamma_j<3/4$. For $\tau=\frac{|\xi_j|}{|\xi_i|}$, we have

$$|\xi_j|^{\gamma_j}|\xi_i|^{1-\gamma_j}\leqslant|\xi_j|+|\xi_i|.$$

Thus,

$$\Big\||\nabla_j|^{\gamma_j}|\nabla_i|^{1-\gamma_j}v\Big\|_{0,I,\alpha,\beta}\leqslant\||\nabla_i|v\|_{0,I,\alpha,\beta}+\||\nabla_j|v\|_{0,I,\alpha,\beta}.$$

On the other hand, thanks to Lemma 4.4, Assumption 2.1 and the fact $|2\pi\xi_k|^{\gamma_k}\leqslant(1+|2\pi\xi_k|^2)^{\gamma_k/2}$ with $k=i$ or $k=j$, we have

$$\Big\||\nabla_i|^{\gamma_i+\gamma_j-1}|x_i-x_j|^{-1}\mathcal{L}^{(i,j)}_{I,\alpha,\beta}u\Big\|_{L^2((\mathbb{R}^3)^N)}\leqslant C'_{\gamma_i,\gamma_j}\|u\|_{0,I,\alpha,\beta}. \tag{4.8}$$

We conclude that, if $\{i,j\} \not\subset I$, then

$$\left|\left\langle |\nabla_i|^{\gamma_i}|\nabla_j|^{\gamma_j}|x_i-x_j|^{-1}\mathcal{L}^{(i,j)}_{I,\alpha,\beta}u, \mathcal{K}_{\gamma_i,x_i}\mathcal{K}_{\gamma_j,x_j}\mathcal{L}_{I,\alpha,\beta}v\right\rangle\right| \leqslant C'_{\gamma_i,\gamma_j}\|u\|_{0,I,\alpha,\beta}\Big(\||\nabla_i|v\|_{0,I,\alpha,\beta}+\||\nabla_j|v\|_{0,I,\alpha,\beta}\Big).$$

Now we consider the case $\{i,j\} \subset I$. Then $\gamma_i = \gamma_j = \alpha$ with $\alpha \in [0,5/4)$. Besides, the function u is antisymmetric with respect to $\{i,j\}$. We fix the variables $(x_k)_{k\in\{1,\cdots,N\}\setminus\{i,j\}}$, and let $f(x_i,x_j) = u(x)$ with $x = (x_1,\cdots,x_N)$. Thus $f(x_i,x_j) \in Y_{\mathrm{anti},\alpha}(\mathbb{R}^3_{x_i}\times\mathbb{R}^3_{x_j})$, and by Lemma 4.5,

$$\left\||\nabla_i|^{\alpha-1/2}|\nabla_j|^{\alpha-1/2}|x_i-x_j|^{-1}f\right\|_{L^2\left(\mathbb{R}^3_{x_i}\times\mathbb{R}^3_{x_j}\right)} \leqslant C_{\mathrm{anti},\alpha}\||\nabla_i|^{\alpha}|\nabla_j|^{\alpha}f\|_{L^2\left(\mathbb{R}^3_{x_i}\times\mathbb{R}^3_{x_j}\right)}.$$

Finally, for $i,j\in I$, by the formal identity $|\nabla_i|^{\alpha}|\nabla_j|^{\alpha} = |\nabla_i|^{\alpha-1/2}|\nabla_j|^{\alpha-1/2}|\nabla_i|^{1/2}|\nabla_j|^{1/2}$, we get

$$\begin{aligned}
&\left|\left\langle |\nabla_i|^{\alpha}|\nabla_j|^{\alpha}|x_i-x_j|^{-1}\mathcal{L}^{(i,j)}_{I,\alpha,\beta}u, \mathcal{K}_{\alpha,x_i}\mathcal{K}_{\alpha,x_j}\mathcal{L}_{I,\alpha,\beta}v\right\rangle\right| \\
&\quad= \left|\left\langle |\nabla_i|^{\alpha-1/2}|\nabla_j|^{\alpha-1/2}|x_i-x_j|^{-1}\mathcal{L}^{(i,j)}_{I,\alpha,\beta}u, |\nabla_j|^{1/2}|\nabla_i|^{1/2}\mathcal{K}_{\gamma_i,x_i}\mathcal{K}_{\gamma_j,x_j}\mathcal{L}_{I,\alpha,\beta}v\right\rangle\right| \\
&\quad\leqslant \left\||\nabla_i|^{\alpha-1/2}|\nabla_j|^{\alpha-1/2}|x_i-x_j|^{-1}\mathcal{L}^{(i,j)}_{I,\alpha,\beta}u\right\|_{L^2\left((\mathbb{R}^3)^N\right)}\left\||\nabla_j|^{1/2}|\nabla_i|^{1/2}v\right\|_{0,I,\alpha,\beta} \\
&\quad\leqslant \frac{C_{\mathrm{anti},\alpha}}{2}\left\||\nabla_i|^{\alpha}|\nabla_j|^{\alpha}\mathcal{L}^{i,j}_{I,\alpha,\beta}u\right\|_{L^2\left((\mathbb{R}^3)^N\right)}\Big(\||\nabla_i|v\|_{0,I,\alpha,\beta}+\||\nabla_j|v\|_{0,I,\alpha,\beta}\Big) \\
&\quad\leqslant \frac{C_{\mathrm{anti},\alpha}}{2}\|u\|_{0,I,\alpha,\beta}\Big(\||\nabla_i|u\|_{0,I,\alpha,\beta}+\||\nabla_j|v\|_{0,I,\alpha,\beta}\Big).
\end{aligned} \tag{4.9}$$

Let $C''_{\alpha,\beta} := \max\{\frac{C_{\mathrm{anti},\alpha}}{2}, C'_{\alpha,\beta}, C'_{\beta,\beta}\}$. For the last term on the right-hand side of (4.4), under Assumption 2.1 on α,β, we conclude

$$\left|\sum_{i\neq j}\left\langle |\nabla_i|^{\gamma_i}|\nabla_j|^{\gamma_j}|x_i-x_j|^{-1}\mathcal{L}^{(i,j)}_{I,\alpha,\beta}u, \mathcal{K}_{\gamma_i,x_i}\mathcal{K}_{\gamma_j,x_j}\mathcal{L}_{I,\alpha,\beta}v\right\rangle\right| \leqslant C''_{\alpha,\beta}N^{3/2}\|u\|_{0,I,\alpha,\beta}\|v\|_{1,I,\alpha,\beta}. \tag{4.10}$$

Combining (4.5)–(4.7) and (4.10), we finally get

$$|\langle \mathcal{L}_{I,\alpha,\beta}V_{ee}u, \mathcal{L}_{I,\alpha,\beta}v\rangle| \leqslant C_{2,\mathrm{mix},\alpha,\beta}N^{3/2}\|u\|_{0,I,\alpha,\beta}\|v\|_{1,I,\alpha,\beta},$$

with $C_{2,\mathrm{mix},\alpha,\beta} := (c_1 + 2C_{\alpha,\beta} + C''_{\alpha,\beta})/2$ independent of Z, N. This ends the proof. $\square$

4.2.1. Proof of Lemma 4.4

We split the condition $0 \leqslant s+t < 3/2$ into two cases: $0 \leqslant s+t \leqslant 1$ and $1 < s+t < 3/2$. For the case $0 \leqslant s+t \leqslant 1$, by Lemma 3.6, we have

$$\left\||\nabla_y|^{s+t-1}|y-z|^{-1}f\right\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)} \leqslant c_{1-s-t}\||y-z|^{-s-t}f\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)} \leqslant 2c_{1-s-t}c_{s+t}\left\||\nabla_y|^{s}|\nabla_z|^{t}f\right\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)}.$$

Thus, $C'_{s,t} := 2c_{1-s-t}c_{s+t}$ if $0 \leqslant s+t \leqslant 1$.

Now, we turn to prove the case $1 < s+t < 3/2$. It is based on the study of the fractional Laplacian in Section 3.1.

We consider first the Fourier transform of $\frac{f(y,z)}{|y-z|^{\tau}}$. For any function $g(y,z) \in L^2(\mathbb{R}^3\times\mathbb{R}^3)$, we have $\mathcal{F}_{y,z}(g)(\xi_y,\xi_z) = \mathcal{F}_z\circ\mathcal{F}_y(g)(\xi_y,\xi_z)$. Besides, thanks to (3.1), we have $\mathcal{F}_y(|\cdot-z|^{-\tau})(\xi_y) = \frac{b_{3-\tau}}{b_\tau}\frac{e^{-2i\pi z\cdot\xi_y}}{|\xi_y|^{3-\tau}}$. Thus,

$$\mathcal{F}_{y,z}\left(\frac{f}{|y-z|^{\tau}}\right)(\xi_y,\xi_z) = \frac{b_{3-\tau}}{b_\tau}\int_{\mathbb{R}^3}\frac{1}{|l|^{3-\tau}}\mathcal{F}_z\Big(e^{-2i\pi z\cdot l}\mathcal{F}_y(f)(\xi_y-l,z)\Big)\,\mathrm{d}l$$

$$= \frac{b_{3-\tau}}{b_\tau} \int_{\mathbb{R}^3} \frac{1}{|l|^{3-\tau}} \mathcal{F}_{y,z}(f)(\xi_y - l, \xi_z + l)\, \mathrm{d}l. \tag{4.11}$$

Thus for $s+t>1$, by Plancherel's Theorem,

$$\left\| |\nabla_y|^{s+t-1} |y-z|^{-1} f \right\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)} = 2^{s+t-1}\pi^{s+t-2} \left\| \int_{\mathbb{R}^3} \frac{|\xi_y|^{s+t-1} \mathcal{F}_{y,z}(f)(\xi_y - l, \xi_z + l)}{|l|^2}\, \mathrm{d}l \right\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)}.$$

For any $k \in \mathbb{R}^3$ and $1 < s+t < 3/2$, we have $|\xi_y|^{s+t-1} \leqslant |\xi_y - k|^{s+t-1} + |k|^{s+t-1}$. Let $k = l$, thus

$$\begin{aligned} \left\| |\nabla_y|^{s+t-1} |y-z|^{-1} f \right\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)} &\leqslant (2\pi)^{s+t-1}\pi^{-1} \left\| \int_{\mathbb{R}^3} \frac{|\mathcal{F}_{y,z}(f)(\xi_y - l, \xi_z + l)|}{|l|^{3-s-t}}\, \mathrm{d}l \right\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)} \\ &\quad + (2\pi)^{s+t-1}\pi^{-1} \left\| \int_{\mathbb{R}^3} \frac{|\xi_y - l|^{s+t-1} |\mathcal{F}_{y,z}(f)(\xi_y - l, \xi_z + l)|}{|l|^2}\, \mathrm{d}l \right\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)}. \end{aligned} \tag{4.12}$$

Using (4.11) and Plancherel's Theorem again, we get

$$\left\| \int_{\mathbb{R}^3} \frac{|\mathcal{F}_{y,z}(f)(\xi_y - l, \xi_z + l)|}{|l|^{3-s-t}}\, \mathrm{d}l \right\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)} = \frac{b_{s+t}}{b_{3-s-t}} \left\| |y-z|^{-s-t} \mathcal{F}^{-1}_{y,z}(|\mathcal{F}_{y,z}(f)|) \right\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)}.$$

By Lemma 3.6, we finally deduce

$$\begin{aligned} \left\| |y-z|^{-s-t} \mathcal{F}^{-1}_{y,z}(|\mathcal{F}_{y,z}(f)|) \right\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)} &\leqslant 2c_{s+t} \left\| |\nabla_y|^s |\nabla_z|^t \mathcal{F}^{-1}_{y,z}(|\mathcal{F}_{y,z}(f)|) \right\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)} \\ &= 2c_{s+t}(2\pi)^{s+t} \left\| |\xi_y|^s |\xi_z|^t \mathcal{F}_{y,z}(f) \right\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)} \\ &= 2c_{s+t} \left\| |\nabla_y|^s |\nabla_z|^t f \right\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)}. \end{aligned}$$

On the other hand, for the second term on the right-hand side of (4.12), we have

$$\begin{aligned} &\left\| \int_{\mathbb{R}^3} \frac{|\xi_y - l|^{s+t-1} |\mathcal{F}_{y,z}(f)(\xi_y - l, \xi_z + l)|}{|l|^2}\, \mathrm{d}l \right\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)} \\ &\quad = (2\pi)^{1-s-t} \left\| \int_{\mathbb{R}^3} \frac{\left| \mathcal{F}_{y,z}\left(|\nabla_y|^{s+t-1} f \right)(\xi_y - l, \xi_z + l) \right|}{|l|^2}\, \mathrm{d}l \right\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)} \\ &\quad = 2^{1-s-t}\pi^{2-s-t} \left\| |y-z|^{-1} \mathcal{F}^{-1}_{y,z}\left(\left| \mathcal{F}_{y,z}\left(|\nabla_y|^{s+t-1} f \right) \right| \right) \right\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)}. \end{aligned}$$

As $0 \leqslant t \leqslant s$ and $t+s<3/2$, we have $t \leqslant 3/4$. Thus by Lemma 3.6,

$$\begin{aligned} \left\| |y-z|^{-1} \mathcal{F}^{-1}_{y,z}\left(\left| \mathcal{F}_{y,z}\left(|\nabla_y|^{s+t-1} f \right) \right| \right) \right\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)} &\leqslant 2c_1 \left\| |\nabla_y|^{1-t} |\nabla_z|^t \mathcal{F}^{-1}_{y,z}\left(\left| \mathcal{F}_{y,z}\left(|\nabla_y|^{s+t-1} f \right) \right| \right) \right\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)} \\ &= 4\pi c_1 \left\| |\xi_y|^{1-t} |\xi_z|^t \mathcal{F}_{y,z}\left(|\nabla_y|^{s+t-1} f \right) \right\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)} \\ &= 2c_1 \left\| |\nabla_y|^s |\nabla_z|^t f \right\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)}. \end{aligned}$$

Consequently, for $0 \leqslant t \leqslant s$ and $1 < s+t < 3/2$, we deduce

$$\left\| |\nabla_y|^{s+t-1} |y-z|^{-1} f \right\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)} \leqslant \left(\frac{2^{s+t}\pi^{s+t-2} b_{s+t} c_{s+t}}{b_{3-s-t}} + 2c_1 \right) \left\| |\nabla_y|^s |\nabla_z|^t f \right\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)}.$$

Thus $C'_{s,t} := \left(\frac{2^{s+t}\pi^{s+t-2} b_{s+t} c_{s+t}}{b_{3-s-t}} + 2c_1 \right)$ if $1 < s+t < 3/2$ and $0 < t \leqslant s$. This ends the proof.

4.2.2. Proof of Lemma 4.5

When $s = 0$, by Lemma 3.6, we have

$$\Big\| |\nabla_y|^{-1/2} |\nabla_z|^{-1/2} |y-z|^{-1} f \Big\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)} \leqslant 2c_1 \|f\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)}.$$

Thus, $C_{\mathrm{anti},0} := 2c_1$

Now, we assume $1 \leqslant s < 5/4$. By the formal identity

$$|\nabla_y|^{s-1/2} |\nabla_z|^{s-1/2} = |\nabla_y| |\nabla_y|^{s-3/2} |\nabla_z| |\nabla_z|^{s-3/2},$$

we have

$$\begin{aligned}
\Big\| |\nabla_y|^{s-1/2} |\nabla_z|^{s-1/2} |y-z|^{-1} f \Big\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)} &= \Big\| \nabla_y \otimes \nabla_z |\nabla_y|^{s-3/2} |\nabla_z|^{s-3/2} |y-z|^{-1} f \Big\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)} \\
&\leqslant \Big\| |\nabla_y|^{s-3/2} |\nabla_z|^{s-3/2} |y-z|^{-1} \nabla_y \otimes \nabla_z f \Big\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)} \\
&\quad + \Big\| |\nabla_y|^{s-3/2} |\nabla_z|^{s-3/2} |y-z|^{-3} (y-z) \otimes \nabla_z f \Big\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)} \\
&\quad + \Big\| |\nabla_y|^{s-3/2} |\nabla_z|^{s-3/2} |y-z|^{-3} (z-y) \otimes \nabla_y f \Big\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)} \\
&\quad + \Big\| |\nabla_y|^{s-3/2} |\nabla_z|^{s-3/2} \big(\nabla_y \otimes \nabla_z |y-z|^{-1} \big) f \Big\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)}. \qquad (4.13)
\end{aligned}$$

As $-1/2 \leqslant s - 3/2 < -1/4$, by Lemma 3.6, we have

$$\Big\| |\nabla_y|^{s-3/2} |\nabla_z|^{s-3/2} g \Big\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)} \leqslant 2\, c_{2s-3} \big\| |y-z|^{3-2s} g \big\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)}.$$

Besides, it is not difficult to see that

$$|\nabla_y \otimes \nabla_z |y-z|^{-1}| \leqslant 6\, |y-z|^{-3}.$$

Thus,

$$\begin{aligned}
&\Big\| |\nabla_y|^{s-1/2} |\nabla_z|^{s-1/2} |y-z|^{-1} f \Big\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)} \\
&\quad \leqslant 2c_{3-2s} \big\| |y-z|^{2-2s} \nabla_y \otimes \nabla_z f \big\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)} + 2c_{3-2s} \big\| |y-z|^{1-2s} \nabla_z f \big\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)} \\
&\qquad + 2c_{3-2s} \big\| |y-z|^{1-2s} \nabla_y f \big\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)} + 12 c_{3-2s} \big\| |y-z|^{-2s} f \big\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)}. \qquad (4.14)
\end{aligned}$$

By Lemma 3.6, we have

$$\big\| |y-z|^{2-2s} \nabla_y \otimes \nabla_z f \big\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)} \leqslant 2c_{2s-2} \big\| |\nabla_y|^s |\nabla_z|^s f \big\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)},$$

and, as $1 \leqslant 2s - 1 < 3/2$,

$$\begin{aligned}
\big\| |y-z|^{1-2s} \nabla_z f \big\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)} &\leqslant 2c_{2s-1} \big\| |\nabla_y|^s |\nabla_z|^{s-1} \nabla_z f \big\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)} \\
&= 2c_{2s-1} \big\| |\nabla_y|^s |\nabla_z|^s f \big\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)}.
\end{aligned}$$

Analogously, we have

$$\big\| |y-z|^{1-2s} \nabla_y f \big\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)} \leqslant 2c_{2s-1} \big\| |\nabla_y|^s |\nabla_z|^s f \big\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)}.$$

Finally, by Lemma 3.9 and Remark 3.10, we get

$$\big\||y-z|^{-2s}f\big\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)} \leqslant c_{2s}\||\nabla_y|^s|\nabla_z|^s f\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)}.$$

Thus, when $1 \leqslant s < 5/4$, we have

$$\Big\||\nabla_y|^{s-1/2}|\nabla_z|^{s-1/2}|y-z|^{-1}f\Big\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)} \leqslant C_{\mathrm{anti},s}\||\nabla_y|^s|\nabla_z|^s f\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)}$$

with $C_{\mathrm{anti},s} := 4c_{3-2s}c_{2s-2} + 4c_{3-2s}c_{2s-1} + 24c_{3-2s}c_{2s}$.

Finally, by using the interpolation theory between the cases $s = 0$ and $s = 1$, we immediately obtain the conclusion: for $0 < s < 1$,

$$\Big\||\nabla_y|^{s-1/2}|\nabla_z|^{s-1/2}|y-z|^{-1}f\Big\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)} \leqslant C_{\mathrm{anti},s}\||\nabla_y|^s|\nabla_z|^s f\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)},$$

where $C_{\mathrm{anti},s} = C_{\mathrm{anti},0}^{1-s}C_{\mathrm{anti},1}^{s}$. This ends the proof.

5. Application to mixed regularity of eigenfunctions

This section is devoted to the proof of Theorem 2.3.

Let $I \subset \{1, \cdots, N\}$. Imitating the proof in [18], we split the eigenfunction $u_* \in H_I^1((\mathbb{R}^3)^N)$ of (1.2) into the high-frequency part and the low-frequency part. Denote the projector P_Ω to the high-frequency part by

$$\mathcal{F}_{x_1,\cdots,x_N}(P_\Omega u)(\xi) := \mathbb{1}_{|\cdot|\geqslant\Omega}(\xi)\mathcal{F}_{x_1,\cdots,x_N}(u)(\xi), \quad u \in L_I^2\Big(\big(\mathbb{R}^3\big)^N\Big),\ \xi = (\xi_1, \cdots, \xi_N), \tag{5.1}$$

where Ω is a constant such that

$$\Omega \geqslant \frac{2}{\pi}C_{\mathrm{mix},\alpha,\beta}\sqrt{N}\max\{N, Z\}. \tag{5.2}$$

For any function $u \in L_I^2\Big(\big(\mathbb{R}^3\big)^N\Big)$, let

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

Given a functional space Y, the subspaces $P_\Omega Y$ and $(1-P_\Omega)Y$ are formally defined by

$$P_\Omega Y := \{u_H; u \in Y\} \quad \text{and} \quad (1-P_\Omega)Y := \{u_L; u \in Y\}.$$

Then, under Assumption 2.1 on α, β, the low-frequency part $u_L \in X_{I,\alpha,\beta}$ for any $u \in H_I^1((\mathbb{R}^3)^N)$. Hence $u_{*,L} := (1-P_\Omega)u_* \in X_{I,\alpha,\beta}$. Thus to prove $u_* \in X_{I,\alpha,\beta}$, it suffices to prove $u_{*,H} := P_\Omega u_* \in X_{I,\alpha,\beta}$.

To prove $u_{*,H} \in X_{I,\alpha,\beta}$, we consider the following variational problem in u for the eigenvalue problem (1.2):

$$\langle \mathcal{L}_{I,\alpha,\beta}Hu, \mathcal{L}_{I,\alpha,\beta}v_H\rangle - \lambda\langle \mathcal{L}_{I,\alpha,\beta}u, \mathcal{L}_{I,\alpha,\beta}v_H\rangle = 0 \quad \text{for any } \ v_H \in P_\Omega X_{I,\alpha,\beta}, \tag{5.3}$$

from which, using the fact that $u = u_H + u_L$, we deduce

$$\langle \mathcal{L}_{I,\alpha,\beta}(H-\lambda)u_H, \mathcal{L}_{I,\alpha,\beta}v_H\rangle = -\langle \mathcal{L}_{I,\alpha,\beta}(V_{ne}+V_{ee})u_L, \mathcal{L}_{I,\alpha,\beta}v_H\rangle \quad \text{for any } \ v_H \in P_\Omega X_{I,\alpha,\beta}. \tag{5.4}$$

Obviously, when $\alpha = \beta = 0$, $\mathcal{L}_{I,\alpha,\beta} = 1$ and $X_{I,\alpha,\beta} = H_I^1$. Thus for $\alpha = \beta = 0$, u_* solves (5.3), then $u_{*,H}$ solves (5.4) with $u_L = u_{*,L}$.

Before going further, we study the properties of the variational problem (5.4).

Lemma 5.1. *Under Assumption 2.1 on α, β, for any given $u_L \in (1-P_\Omega)X_{I,\alpha,\beta}$, the variational problem (5.4) admits a unique solution $\psi_{H,\alpha,\beta}(u_L) \in P_\Omega X_{I,\alpha,\beta}$.*

Proof. We will prove this lemma by using Lions–Lax–Milgram's Theorem (see *e.g.*, [15], Thm. 2.1, Chap. III.2). Thanks to Theorem 2.2 and (5.2), for any $u_H, v_H \in P_\Omega X_{I,\alpha,\beta}$, we have

$$|\langle \mathcal{L}_{I,\alpha,\beta}(V_{ne}+V_{ee})u_H, \mathcal{L}_{I,\alpha,\beta}v_H\rangle| \leqslant \frac{\pi\Omega}{2}\|u\|_{0,I,\alpha,\beta}\|v\|_{1,I,\alpha,\beta} \leqslant \frac{1}{4}\|u_H\|_{1,I,\alpha,\beta}\|v_H\|_{1,I,\alpha,\beta},$$

since $\|u_H\|_{L^2((\mathbb{R}^3)^N)} \leqslant (2\pi\Omega)^{-1}\|\nabla u_H\|_{L^2((\mathbb{R}^3)^N)}$. Then, according to Remark 1.1, $\lambda < 0$, and we have

$$\begin{aligned}|\langle \mathcal{L}_{I,\alpha,\beta}(H-\lambda)v_H, \mathcal{L}_{I,\alpha,\beta}v_H\rangle| &\geqslant \left\langle \left(-\frac{1}{2}\Delta - \lambda\right)\mathcal{L}_{I,\alpha,\beta}v_H, \mathcal{L}_{I,\alpha,\beta}v_H \right\rangle - \frac{1}{4}\|v_H\|^2_{1,I,\alpha,\beta} \geqslant \frac{1}{4}\|v_H\|^2_{1,I,\alpha,\beta}\\ &\geqslant \frac{1}{8}\|v_H\|^2_{I,\alpha,\beta}.\end{aligned}$$

Thus we get the weak coercivity: for $u_H, v_H \in P_\Omega X_{I,\alpha,\beta}$,

$$\inf_{\|v_H\|_{I,\alpha,\beta}=1}\ \sup_{\|u_H\|_{I,\alpha,\beta}\leqslant 1}|\langle \mathcal{L}_{I,\alpha,\beta}(H-\lambda)u_H, \mathcal{L}_{I,\alpha,\beta}v_H\rangle| \geqslant \inf_{\|v_H\|_{I,\alpha,\beta}=1}|\langle \mathcal{L}_{I,\alpha,\beta}(H-\lambda)v_H, \mathcal{L}_{I,\alpha,\beta}v_H\rangle| \geqslant \frac{1}{8}, \tag{5.5}$$

the continuity:

$$|\langle \mathcal{L}_{I,\alpha,\beta}(H-\lambda)u_H, \mathcal{L}_{I,\alpha,\beta}v_H\rangle| \leqslant \|u_H\|_{I,\alpha,\beta}\|v_H\|_{I,\alpha,\beta}; \tag{5.6}$$

and the continuity of the right-hand side term in (5.4):

$$|\langle \mathcal{L}_{I,\alpha,\beta}(V_{ne}+V_{ee})u_L, \mathcal{L}_{I,\alpha,\beta}v_H\rangle| \leqslant \|u_L\|_{I,\alpha,\beta}\|v_H\|_{I,\alpha,\beta}. \tag{5.7}$$

Thus by Lions–Lax–Milgram's Theorem, under Assumption 2.1 on α,β, for any given $u_L \in (1-P_\Omega)X_{I,\alpha,\beta}$, equation (5.4) admits a unique solution $\psi_{H,\alpha,\beta}(u_L) \in P_\Omega X_{I,\alpha,\beta}$. □

Theorem 2.3 can be immediately obtained by the following.

Lemma 5.2. *For any α,β satisfying Assumption 2.1 and for $u_L = u_{*,L}$, $\psi_{H,\alpha,\beta}(u_{*,L}) = u_{*,H}$ is the unique solution to the variational problem (5.4). Thus $u_{*,H} \in X_{I,\alpha,\beta}$.*

Proof of Lemma 5.2. Let $u_L = u_{*,L}$ in (5.4). When $\alpha = \beta = 0$, by Lemma 5.1, $\psi_{H,0,0}(u_{*,L})$ is the unique solution to (5.4). On the other hand, for $\alpha = \beta = 0$, $u_{*,H}$ solves equally (5.4) with $u_L = u_{*,L}$. Thus by the uniqueness of solution to (5.4), $\psi_{H,0,0}(u_{*,L}) = u_{*,H}$.

To end the proof, it suffices to prove $\psi_{H,\alpha,\beta}(u_{*,L}) = u_{*,H}$ for any α,β satisfying Assumption 2.1. As the operator $\mathcal{L}_{I,\alpha,\beta}$ is invertible, we denote the functional space $X_{I,-\alpha,-\beta}$ by

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

Thus for any $v_H \in P_\Omega X_{I,\alpha,\beta}$, we have $\mathcal{L}^2_{I,\alpha,\beta}v_H \in P_\Omega X_{I,-\alpha,-\beta}$. On the other hand, for any $\phi_H \in P_\Omega X_{I,-\alpha,-\beta}$, $\mathcal{L}^{-2}_{I,\alpha,\beta}\phi_H \in P_\Omega X_{I,\alpha,\beta}$. Let $v_H = \mathcal{L}^{-2}_{I,\alpha,\beta}\phi_H$, then (5.4) can be rewritten as

$$\langle (H-\lambda)u_H, \phi_H\rangle = -\langle (V_{ne}+V_{ee})u_L, \phi_H\rangle \quad \text{for any } \ \phi_H \in P_\Omega X_{I,-\alpha,-\beta}. \tag{5.8}$$

Now, for any α',β' satisfying Assumption 2.1, let $\psi_{H,\alpha',\beta'}(u_L) \in P_\Omega X_{I,\alpha',\beta'}$ be the unique solution to (5.4) for $\alpha = \alpha'$ and $\beta = \beta'$. Obviously, $H^1_I((\mathbb{R}^3)^N) \subset X_{I,-\alpha',-\beta'}$. Then $P_\Omega H^1_I((\mathbb{R}^3)^N) \subset P_\Omega X_{I,-\alpha',-\beta'}$. Thus thanks to (5.8), for any $\phi_H \in P_\Omega H^1_I((\mathbb{R}^3)^N)$, we have

$$\langle (H-\lambda)\psi_{H,\alpha',\beta'}(u_L), \phi_H\rangle = -\langle (V_{ne}+V_{ee})u_L, \phi_H\rangle,$$

which implies that $\psi_{H,\alpha',\beta'}(u_L)$ also solves (5.4) for $\alpha = \beta = 0$. Then, by Lemma 5.1, for any α',β' satisfying Assumption 2.1, $\psi_{H,\alpha',\beta'}(u_L) = \psi_{H,0,0}(u_L)$. As $\psi_{H,0,0}(u_{*,L}) = u_{*,H}$, we finally get $\psi_{H,\alpha',\beta'}(u_{*,L}) = u_{*,H}$. By Lemma 5.1, $u_{*,H} = \psi_{H,\alpha',\beta'}(u_{*,L}) \in X_{I,\alpha',\beta'}$. This ends the proof. □

6. Application to the hyperbolic cross space approximation

Finally, in this section, we study the hyperbolic cross space approximation and prove Theorem 2.5. We need to replace in Theorem 2.2 the operator $\mathcal{L}_{I,\alpha,\beta}$ by $\mathcal{L}_{I,\alpha,\beta,\tau}$ which is defined by

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

We consider equally the following norms

$$\|u\|_{0,I,\alpha,\beta,\tau} := \|\mathcal{L}_{I,\alpha,\beta,\tau}u\|_{L^2((\mathbb{R}^3)^N)}, \quad \|u\|_{1,I,\alpha,\beta,\tau} := \|\nabla\mathcal{L}_{I,\alpha,\beta,\tau}u\|_{L^2((\mathbb{R}^3)^N)}.$$

It is easy to see that for $\tau \geqslant 1$

$$\tau^{-\alpha N}\|u\|_{0,I,\alpha,\beta} \leqslant \|u\|_{0,I,\alpha,\beta,\tau} \leqslant \|u\|_{0,I,\alpha,\beta}, \quad \tau^{-\alpha N}\|u\|_{1,I,\alpha,\beta} \leqslant \|u\|_{1,I,\alpha,\beta,\tau} \leqslant \|u\|_{1,I,\alpha,\beta},$$

while for $0<\tau<1$

$$\|u\|_{0,I,\alpha,\beta} \leqslant \|u\|_{0,I,\alpha,\beta,\tau} \leqslant \tau^{-\alpha N}\|u\|_{0,I,\alpha,\beta}, \quad \|u\|_{1,I,\alpha,\beta} \leqslant \|u\|_{1,I,\alpha,\beta,\tau} \leqslant \tau^{-\alpha N}\|u\|_{1,I,\alpha,\beta}.$$

Before going further, we need the following.

Lemma 6.1. *Under Assumption 2.1 on α,β, we have for any $u,v\in X_{I,\alpha,\beta}$,*

$$|\langle\mathcal{L}_{I,\alpha,\beta,\tau}(V_{ne}+V_{ee})u,\mathcal{L}_{I,\alpha,\beta,\tau}v\rangle| \leqslant C_{\mathrm{mix},\alpha,\beta}\sqrt{N}\max\{Z,N\}\|u\|_{0,I,\alpha,\beta,\tau}\|v\|_{1,I,\alpha,\beta,\tau}, \tag{6.1}$$

where $C_{\mathrm{mix},\alpha,\beta}$ is defined in Theorem 2.2.

Proof. Let $u_\tau(x) := \tau^{-3N/2}u(\tau^{-1}x)$ and $v_\tau(x) := \tau^{-3N/2}v(\tau^{-1}x)$ where $x=(x_1,\cdots,x_N)\in(\mathbb{R}^3)^N$. Let

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

It is easy to see $u_\tau,v_\tau\in X_{I,\alpha,\beta}$ since $u,v\in X_{I,\alpha,\beta}$. Then, by Theorem 2.2, we have

$$|\langle\mathcal{L}_{I,\alpha,\beta}(V_{ne}^\tau+V_{ee})u_\tau,\mathcal{L}_{I,\alpha,\beta}v_\tau\rangle| \leqslant C_{\mathrm{mix},\alpha,\beta}\sqrt{N}\max\{Z,N\}\|u_\tau\|_{0,I,\alpha,\beta}\|v_\tau\|_{1,I,\alpha,\beta}. \tag{6.2}$$

The scaling definition yields

$$|\langle\mathcal{L}_{I,\alpha,\beta}(V_{ne}^\tau+V_{ee})u_\tau,\mathcal{L}_{I,\alpha,\beta}v_\tau\rangle| = \tau^{-1}|\langle\mathcal{L}_{I,\alpha,\beta,\tau}(V_{ne}+V_{ee})u,\mathcal{L}_{I,\alpha,\beta,\tau}v\rangle|. \tag{6.3}$$

On the other hand,

$$\|u_\tau\|_{0,I,\alpha,\beta} = \|\mathcal{L}_{I,\alpha,\beta}u_\tau\|_{L_I^2((\mathbb{R}^3)^N)} = \|\mathcal{L}_{I,\alpha,\beta,\tau}u\|_{L_I^2((\mathbb{R}^3)^N)} = \|u\|_{0,I,\alpha,\beta,\tau} \tag{6.4}$$

and

$$\|v_\tau\|_{1,I,\alpha,\beta} = \|\nabla\mathcal{L}_{I,\alpha,\beta}v_\tau\|_{L_I^2((\mathbb{R}^3)^N)} = \tau^{-1}\|\nabla\mathcal{L}_{I,\alpha,\beta,\tau}v\|_{L_I^2((\mathbb{R}^3)^N)} = \tau^{-1}\|v\|_{1,I,\alpha,\beta,\tau}. \tag{6.5}$$

Gathering together (6.2)–(6.5), equation (6.1) follows. ☐

Let $I \subset \{1, \cdots, N\}$. Let $u_* \in H^1_I(\mathbb{R}^3)^N$ be an eigenfunction of (1.2), and let $u_{*,H} = P_\Omega u_*$, $u_{*,L} = (1 - P_\Omega)u_*$ with P_Ω defined by (5.1). We consider the following variational problem: for any $v_H \in P_\Omega X_{I,\alpha,\beta}$,

$$\langle \mathcal{L}_{I,\alpha,\beta,\tau}(H - \lambda)u_H, \mathcal{L}_{I,\alpha,\beta,\tau}v_H\rangle = -\langle \mathcal{L}_{I,\alpha,\beta,\tau}(V_{ne} + V_{ee})u_{*,L}, \mathcal{L}_{I,\alpha,\beta,\tau}v_H\rangle. \tag{6.6}$$

Following the proof of Theorem 2.3 in Section 5 and under Assumption 2.1 on α, β, we know that $u_{*,H}$ is the unique solution to the variational problem (6.6).

Recall that $\Omega \geqslant \frac{2}{\pi} C_{\mathrm{mix},\alpha,\beta}\sqrt{N}\max\{N, Z\}$ and let $v_H = u_{*,H}$. Then we have

$$|\langle \mathcal{L}_{I,\alpha,\beta,\tau}(H - \lambda)u_{*,H}, \mathcal{L}_{I,\alpha,\beta,\tau}u_{*,H}\rangle| \geqslant \frac{1}{4}\, \|u_{*,H}\|^2_{1,I,\alpha,\beta,\tau} \tag{6.7}$$

and

$$|\langle \mathcal{L}_{I,\alpha,\beta,\tau}(V_{ne} + V_{ee})u_{*,L}, \mathcal{L}_{I,\alpha,\beta,\tau}u_{*,H}\rangle| \leqslant \frac{\pi\Omega}{2}\, \|u_{*,L}\|_{0,I,\alpha,\beta,\tau}\|u_{*,H}\|_{1,I,\alpha,\beta,\tau}. \tag{6.8}$$

By (6.7) and (6.8), we get

$$\frac{\pi\Omega}{2}\|u_{*,H}\|_{0,I,\alpha,\beta,\tau} \leqslant \frac{1}{4}\|u_{*,H}\|_{1,I,\alpha,\beta,\tau} \leqslant \frac{\pi\Omega}{2}\|u_{*,L}\|_{0,I,\alpha,\beta,\tau}. \tag{6.9}$$

It follows from (6.9) and the identity $\|u_*\|^2_{0,I,\alpha,\beta,\tau} = \|u_{*,L}\|^2_{0,I,\alpha,\beta,\tau} + \|u_{*,H}\|^2_{0,I,\alpha,\beta,\tau}$ that

$$\|u_{*,H}\|_{0,I,\alpha,\beta,\tau} \leqslant \sqrt{2}\|u_*\|_{0,I,\alpha,\beta,\tau}, \quad \|u_{*,H}\|_{1,I,\alpha,\beta,\tau} \leqslant 2\sqrt{2}\pi\Omega\|u_*\|_{0,I,\alpha,\beta,\tau}. \tag{6.10}$$

Lemma 6.2. *Let $\Omega \geqslant \frac{2}{\pi} C_{\mathrm{mix},\alpha,\beta}\sqrt{N}\max\{N, Z\}$ be large enough. Under Assumption 2.1 on α, β, we have*

$$\|u_*\|_{0,I,\alpha,\beta,2\pi\Omega} \leqslant \sqrt{2}\, e^{5/8}\, \|u_*\|_{L^2\left((\mathbb{R}^3)^N\right)}, \quad \|u_*\|_{1,I,\alpha,\beta,2\pi\Omega} \leqslant 2\sqrt{2}\,\pi e^{5/8}\,\Omega\, \|u_*\|_{L^2\left((\mathbb{R}^3)^N\right)}.$$

Proof. The proof is in the spirit of Theorem 9 from [18]. Under Assumption 2.1 on α, β, we have $0 \leqslant \beta \leqslant \alpha < 5/4$ and

$$\prod_{j\in I}\left(1 + \frac{|\xi_j|^2}{|\Omega|^2}\right)^\alpha \prod_{i\in I^c}\left(1 + \frac{|\xi_i|^2}{|\Omega|^2}\right)^\beta \leqslant \exp\left(\frac{5|\xi|^2}{4|\Omega|^2}\right),$$

where $\xi := (\xi_1, \cdots, \xi_N) \in (\mathbb{R}^3)^N$. Thus, by (5.1) and using the fact that $u_{*,L} = (1 - P_\Omega)u_*$, we have

$$\begin{aligned}\|u_{*,L}\|^2_{0,I,\alpha,\beta,2\pi\Omega} &= \int_{|\xi|<\Omega}\prod_{j\in I}\left(1 + \frac{|\xi_j|^2}{|\Omega|^2}\right)^\alpha \prod_{i\in I^c}\left(1 + \frac{|\xi_i|^2}{|\Omega|^2}\right)^\beta |\mathcal{F}_{x_1,\cdots,x_N}(u_*)(\xi)|^2\, \mathrm{d}\xi \\ &\leqslant \int_{|\xi|\leqslant\Omega}\exp\left(\frac{5|\xi|^2}{4|\Omega|^2}\right)|\mathcal{F}_{x_1,\cdots,x_N}(u_*)(\xi)|^2\, \mathrm{d}\xi \leqslant e^{5/4}\, \|u_*\|^2_{L^2\left((\mathbb{R}^3)^N\right)}.\end{aligned}$$

Let now $\tau = 2\pi\Omega$. Then equation (6.10) implies

$$\|u_*\|_{0,I,\alpha,\beta,2\pi\Omega} \leqslant \sqrt{2}e^{5/8}\|u_*\|_{L^2\left((\mathbb{R}^3)^N\right)}, \quad \|u_*\|_{1,I,\alpha,\beta,2\pi\Omega} \leqslant 2\sqrt{2}\pi e^{5/8}\Omega\|u_*\|_{L^2\left((\mathbb{R}^3)^N\right)}.$$

This ends the proof. □

Finally, we turn to the proof of Theorem 2.5.

Proof of Theorem 2.5. For any $\xi \in \mathcal{H}_{I,\alpha,\beta}(R,\Omega)^c$ where $\mathcal{H}_{I,\alpha,\beta}(R,\Omega)$ is defined by (2.9), we have

$$1 \leqslant \frac{1}{R^2}\prod_{i\in I}\left(1+\left|\frac{2\pi\xi_i}{2\pi\Omega}\right|^2\right)^{\alpha}\prod_{j\in I^c}\left(1+\left|\frac{2\pi\xi_i}{2\pi\Omega}\right|^2\right)^{\beta}.$$

Thus, by Lemma 6.2, it is easy to see that

$$\begin{aligned}\left\|\left(1-\mathcal{P}_{I,\alpha,\beta}^{R,\Omega}\right)u_*\right\|_{L^2\left((\mathbb{R}^3)^N\right)} &\leqslant \frac{1}{R}\left\|\left(1-\mathcal{P}_{I,\alpha,\beta}^{R,\Omega}\right)u_*\right\|_{0,I,\alpha,\beta,2\pi\Omega}\\ &\leqslant \frac{1}{R}\|u_*\|_{0,I,\alpha,\beta,2\pi\Omega} \leqslant \frac{\sqrt{2}e^{5/8}}{R}\|u_*\|_{L^2\left((\mathbb{R}^3)^N\right)}.\end{aligned}$$

Analogously,

$$\left\|\nabla\left(u_* - \mathcal{P}_{I,\alpha,\beta}^{R,\Omega}u_*\right)\right\|_{L^2\left((\mathbb{R}^3)^N\right)} \leqslant \frac{1}{R}\|u_*\|_{1,I,\alpha,\beta,2\pi\Omega} \leqslant \frac{2\sqrt{2}\pi e^{5/8}}{R}\Omega\|u_*\|_{L^2\left((\mathbb{R}^3)^N\right)}.$$

This ends the proof. □

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