A note about the mixed regularity of Schrödinger Coulomb system

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Abstract

We give a short and unified proof of mixed regularity of Coulomb system for several cases: antisymmetric case with order of derivatives smaller than 1.25 which is the best bound; mixture of antisymmetry and non-antisymmetry with order of derivatives $1+\beta$ and α respevtively for $0 \leqslant 0 < \alpha < 0.75$, $0.75 < \beta < 1.25$ and $\alpha + \beta < 1.5$ which is also the oprtimal bound; and purely non-antisymmetric case with order of derivatives up to 0.75. In addition to Hardy type inequality, it is based on the Herbst inequality. Such results are of particular importance for the study of sparse grid-like expansions of the wavefunctions. Moreover, we can get how fast the norm of these derivative can increase with the number of electrons.

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1 Introduction

In recent years, the mixed regularity about the Schrödinger Coulomb system Hamiltonian operator

$$H = -\frac{1}{2}\sum_{i=1}^{N} \triangle_i + V(x) \tag{1}$$

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with potential

$$V(x) = -\sum_{i=1}^{N}\sum_{\nu=1}^{K}\frac{Z_\nu}{|x_i - a_\nu|} + \frac{1}{2}\sum_{i,j=1,i\neq j}^{N}\frac{1}{|x_i - x_j|}$$

has been well studied, for the eigenvalues and eigenfunctions problem in [12–15]:

$$Hu = \lambda u;$$

and for the time-dependent case in [11],

$$\begin{cases} i\partial_t u(x,t) = H(t)u(x,t), & t \in [-T,T] \\ u(x,0) = u_0(x), \end{cases}$$

where $H(t)$ represents the same operator H but with the moving nuclei. In this note, we study the eigenvalues and eigenfunctions of equation (1) again, and give the other optimal case of the mixed regularity.

Assuming that we have q kinds of anti-symmetric particles and another kind of non-antisymmetric particles, with the index of particles in set $\mathcal{I}_q$ and $\{1, \cdots, N\}\backslash \bigcup_{i=1}^{q} \mathcal{I}_q$ respectively. Let $P_{i,j}$ is a permutation that exchange the position of variable x_i and x_j, we have

$$u(P_{i,j}x) = -u(x), \quad \text{if } \exists\ 1 \leqslant l \leqslant q, \text{ s.t. } i,j \in \mathcal{I}_l.$$

In [12], it is shown that

$$|||u|||_{\mathcal{I}}^2 = \int \left(1 + \sum_{i=1}^{N}|\omega_i|^2\right)\left(\sum_{l=1}^{q}\prod_{k\in\mathcal{I}_l}(1+|\omega_k|^2)\right)|\widehat{u}|^2\, d\omega < \infty$$

Later, [15] tells us that without anti-symmetry, the following integral

$$|||u|||_{\eta,\sigma}^2 = \int \left(1 + \sum_{i=1}^{N}|\omega_i|^2\right)^{\sigma}\left(\prod_{k=1}^{N}(1+|\omega_k|^2)\right)^{\eta}|\widehat{u}|^2\, d\omega$$

remains finite if $\sigma = 0, \eta = 1$ or $\sigma = 1, \eta < 3/4$.

The purpose if this paper is trifold

- We will give a new, much simpler proof of the mixed regularity which is more similar to the work [12]. While the method in [15] relied on rather involved relations between explicit correction factor, the present proof uses nothing more than Herbst inequalities.

- The orders of the derivatives of any cases are sharp, which is a new result can not be obtained by the method of [15].

- By this new proof, we can repeat the procedure of [13] to get the new rate of convergence.

Before presenting the precise statement of our results, we need the new norms describing the smoothness properties of the solution

$$|||u|||_{\mathcal{I},\alpha,1+\beta}^2 = \sum_{l=1}^{q}\int \left(1 + \sum_{i=1}^{N}|\omega_i|^2\right)\prod_{k\in\mathcal{I}_l}(1+|\omega_k|^{2+2\beta})\prod_{m\in\mathcal{I}\backslash\mathcal{I}_l}(1+|\omega_m|^{2\alpha})|\widehat{u}|^2\, d\omega.$$

And if $q = 0$,

$$|||u|||^2_{\mathcal{I},\alpha,1+\beta} = \int \left(1 + \sum_{i=1}^{N} |\omega_i|^2\right) \prod_{m=1}^{N} (1 + |\omega_m|^{2\alpha}) |\widehat{u}|^2 \, d\omega.$$

They are defined on the Hilbert spaces $H^{\alpha,1+\beta}_{\mathcal{I}}$. And let

$$\mathcal{I}^c = \{1, \cdots, N\} \backslash \bigcup_{i=1}^{q} \mathcal{I}_i.$$

Our result is:

Theorem 1.1. *Let u be the solution of the eigenvalue problems of operator 1, then we have the following results:*

1) if $\mathcal{I}^c = \varnothing$, then

$$u \in \bigcap_{1 \leqslant \beta < 1.25} H^{\beta,\beta}_{\mathcal{I}},$$

2) if $\mathcal{I}^c \neq \varnothing$ and $\mathcal{I}^c \neq \{1, \cdots, N\}$, then

$$u \in \bigcap_{\substack{0 \leqslant \alpha < 0.5, \\ 1 \leqslant \beta < 1.25, \\ \alpha + \beta < 1.5}} \bigcap_{\substack{0.5 \leqslant \alpha < 0.75, \\ 0.75 \leqslant \beta < 1, \\ \alpha + \beta < 1.5}} H^{\alpha,\beta}_{\mathcal{I}},$$

3) if $\mathcal{I}^c = \{1, \cdots, N\}$, then

$$u \in \bigcap_{0 \leqslant \alpha < 0.75} H^{\alpha,\alpha}_{\mathcal{I}}.$$

Let

$$\mathcal{H}(R) = \left\{ (\omega_1, \cdots, \omega_N) \in (\mathbb{R}^3)^N | \sum_{q} \prod_{k \in l_q} (1 + |\omega_k/\Omega|^{2\beta}) \prod_{m \in \mathcal{I} \backslash \mathcal{I}_l} (1 + |\omega_m/\Omega|^{2\alpha}) \leqslant R^2 \right\}$$

and we define the projector

$$(P_R u)(x) = \frac{1}{\sqrt{2\pi}}^{3N} \int \chi_R(\omega) \widehat{u}(\omega) \exp{(i\omega \cdot x)} d\omega$$

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

Then we have the following nrom convergence rate:

Theorem 1.2. *For all eigenfunctions $u \in H^1(\lambda)$, and $\Omega > 4\sqrt{2}C(N, \alpha, \beta, 1)(C_{\alpha,\beta,M,N,Z} + |\lambda|^{1/2}) + C(N, \alpha, \beta, 1)$ large enough, we have*

$$\|u - P_R u\|_{L^2} \leqslant \frac{\sqrt{2eq}}{R} \|u\|_0, \;\; \|\nabla(u - P_R u)\|_{L^2} \leqslant \frac{\sqrt{2eq} C(N, \alpha, \beta, 2)}{R} \Omega \|u\|_0,$$

where $C(N, \alpha, \beta, 1), C(N, \alpha, \beta, 2), C_{\alpha,\beta,M,N,Z}$ are constants only dependent on M, N, Z, α, β.

Remark 1.3. *The constants $C(N, \alpha, \beta, 1), C(N, \alpha, \beta, 2)$ are defined by inequality (11). And $C_{\alpha,\beta,M,N,Z}$ is given by inequality (10). More precisely, $C_{\alpha,\beta,M,N,Z} \sim (N + MZ)N^{1/2}$ and if $\min\{\alpha, \beta\} \leqslant 1$, $C(N, \alpha, \beta, 1) \sim \min\{N^{1/(2\alpha)-1/2}, N^{1/(2\beta)-1/2}\}$, $C(N, \alpha, \beta, 2) \sim 1$, if not $C(N, \alpha, \beta, 1) \sim 1$, $C(N, \alpha, \beta, 2) \sim \min\{N^{1/2-1/(2\alpha)}, N^{1/2-1/(2\beta)}\}$.*

2 Preliminary

At the beginning, recall the Herbst inequalities:

Theorem 2.1. *[5] Define the operator C_α on $\mathcal{S}(\mathbb{R}^N)$ by*

$$C_\alpha \equiv |x|^{-\alpha}|p|^{-\alpha}, \quad p = -i\nabla$$

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

$$c_{\alpha,p} = \|C_\alpha\|_{L^p\to L^p} = 2^{-\alpha}\frac{\Gamma(\frac{1}{2}(Np^{-1}-\alpha)\Gamma(\frac{1}{2}Nq^{-1}))}{\Gamma(\frac{1}{2}(Nq^{-1}+\alpha)\Gamma(\frac{1}{2}Np^{-1}))} \tag{2}$$

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

In this case, we only consider the case $N=3$ and $p=2$. Thus, we shorten $c_{\alpha,p}$ by c_α.

Considering the interation between electrons and electrons, we need to dispose of the term $\frac{1}{|x-y|}$:

Lemma 2.2. *Define the operator $C_{\alpha,\beta}$ on $\mathcal{S}(\mathbb{R}^{3\times 3})$ by*

$$C_\alpha \equiv |x-y|^{-\alpha-\beta}|p_x|^{-\alpha}|p_y|^{-\beta}, \quad p_x = -i\nabla_x, \ p_y = -i\nabla_y.$$

Suppose that $\alpha,\beta \geqslant 0$ and $3/(\alpha+\beta) > 2$. Then

$$\|C_{\alpha,\beta}\|_{L^2\to L^2} \leqslant 2c_{\alpha+\beta}.$$

Proof.

$$\begin{aligned}
&\||x-y|^{-\alpha-\beta}|p_x|^{-\alpha}|p_y|^{-\beta}\|_{L^2\to L^2}\\
&= \||p_x|^{-\alpha}|p_y|^{-\beta}|x-y|^{-\alpha-\beta}\|_{L^2\to L^2}\\
&\leqslant \||p_x|^{-\alpha-\beta}|x-y|^{-\alpha-\beta}\|_{L^2\to L^2} + \||p_y|^{-\alpha-\beta}|x-y|^{-\alpha-\beta}\|_{L^2\to L^2}\\
&= 2\||x-y|^{-\alpha-\beta}|p_x|^{-\alpha-\beta}\|_{L^2\to L^2}\\
&= 2c_{\alpha+\beta}
\end{aligned}$$

The inequality is based on $|x|^\alpha \leqslant |x|^{\alpha+\beta}+1$ and here $x = |p_x|/|p_y|$. □

Lemma 2.3. *[11] If $u \in C_0^\infty(\mathbb{R}^3\backslash\{0\})$, then*

$$\int_{\mathbb{R}^3}\frac{1}{|x|^{k-2}}\,|\nabla u(x)|^2\,dx \geqslant \frac{(k-3)^2}{4}\int_{\mathbb{R}^3}\frac{|u(x)|^2}{|x|^k}dx$$

for $k \in [2,3)\cup(3,5)$.

Corollary 2.4. *[11] If $u \in C_0^\infty((\mathbb{R}^3)^2)$ with $u(x,y) = -u(y,x)$ for $x,y \in \mathbb{R}^3$. Then we have the following inequality:*

$$\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\frac{1}{|x-y|^{k-4}}\,|\nabla_x\nabla_y u(x,y)|^2\,dxdy \geqslant \frac{(k-5)^2(k-3)^2}{16}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\frac{|u(x,y)|^2}{|x-y|^k}dxdy$$

for $k \in [4,5)$.

Combining the Lemma 2.2 and Corollary 2.4 together, we have

Corollary 2.5. *If $u \in C_0^\infty((\mathbb{R}^3)^2)$ with $u(x,y) = -u(y,x)$ for $x, y \in \mathbb{R}^3$. Then we have the following inequality:*

$$\left\| \frac{u}{|x-y|^k} \right\| \leqslant c_k \left\| |p_x|^{k/2} |p_y|^{k/2} u \right\|$$

with $c_k = \frac{8c_{k-4}}{(2k-5)(2k-3)}$ and $k \in [2, 2.5)$.

Lemma 2.6. *If $f(x,y) \in C_0^\infty((\mathbb{R}^3)^2)$ $0 \leqslant \alpha, \beta$ and $\alpha + \beta < 0.5$, we have*

$$\left\| |p_y|^\alpha |p_x|^\beta \frac{1}{|x-y|} f(x,y) \right\| \leqslant D_{\alpha,\beta} \left\| |p_x|^{\beta+0.5} |p_y|^{\alpha+0.5} f(x,y) \right\|$$

with

$$D_{\alpha,\beta} = 2\pi^{-1}((2\pi)^{\alpha+\beta} d_{1+\alpha+\beta} c_{1+\alpha+\beta} + (2\pi)^\alpha d_{1+\alpha} c_{1+\alpha} + (2\pi)^\beta d_{1+\beta} c_{1+\beta} + d_1 c_1)$$

and

$$d_x = \frac{\pi^{-x/2}\Gamma(x/2)}{\pi^{(3-x)/2}\Gamma((3-x)/2)}.$$

Proof. We change the variable at the beginning. Let $z = x - y$, then, $\widetilde{f}(z,y) = f(z + y, y)$.

As $\nabla_y f(x,y) = (\nabla_y - \nabla_z) f(z+y, y) = (\nabla_y - \nabla_z)\widetilde{f}(z,y)$, obviously,

$$\left\| |p_y|^\alpha |p_x|^\beta \frac{1}{|x-y|} f(x,y) \| = \| |p_y - p_z|^\alpha |p_z|^\beta \frac{1}{|z|} \widetilde{f}(z,y) \right\|$$

Let $\mathcal{F}(\widetilde{f})$ be the Fourier transform about z and y simultaneously. Then, we have

$$\begin{aligned}
&\left\| |p_y - p_z|^\alpha |p_z|^\beta \frac{1}{|z|} \widetilde{f}(x,y) \right\| \\
=&(2\pi)^{\alpha+\beta}\pi^{-1} \left\| |p_y - p_z|^\alpha |p_z|^\beta \int |p_z - p'_z|^{-2} \mathcal{F}(\widetilde{f})(p'_z, p_y) dp'_z \right\| \\
\leqslant&(2\pi)^{\alpha+\beta}\pi^{-1} \left\| \int |p_z - p'_z|^{\alpha+\beta-2} |\mathcal{F}(\widetilde{f})|(p'_z, p_y) dp'_z \right\| \\
&+ (2\pi)^{\alpha+\beta}\pi^{-1} \left\| \int |p_z - p'_z|^{\alpha-2} |p'_z|^\beta |\mathcal{F}(\widetilde{f})|(p'_z, p_y) dp'_z \right\| \\
&+ (2\pi)^{\alpha+\beta}\pi^{-1} \left\| \int |p_z - p'_z|^{\beta-2} |p_y - p'_z|^\alpha |\mathcal{F}(\widetilde{f})|(p'_z, p_y) dp'_z \right\| \\
&+ (2\pi)^{\alpha+\beta}\pi^{-1} \left\| \int |p_z - p'_z|^{-2} |p_y - p'_z|^\alpha |p'_z|^\beta |\mathcal{F}|(\widetilde{f})(p'_z, p_y) dp'_z \right\|
\end{aligned}$$

Then after applying the inverse Fourier transform, we have

$$\begin{aligned}
&\left\| \int |p_z - p_z'|^{\alpha+\beta-2} |\mathcal{F}(\widetilde{f})|(p_z', p_y) dp_z' \right\| \\
=& d_{1+\alpha+\beta} \left\| \frac{1}{|z|^{1+\alpha+\beta}} \mathcal{F}^{-1} |\mathcal{F}(\widetilde{f})|(z,y) \right\| \\
=& d_{1+\alpha+\beta} \left\| \frac{1}{|z|^{1+\alpha+\beta}} |p_z|^{-\beta-0.5} |p_y - p_z|^{-\alpha-0.5} |p_z|^{\beta+0.5} |p_y - p_z|^{\alpha+0.5} \mathcal{F}^{-1} |\mathcal{F}(\widetilde{f})|(z,y) \right\| \\
\leqslant& d_{1+\alpha+\beta} \left\| \frac{1}{|z|^{1+\alpha+\beta}} |p_z|^{-\alpha-\beta-1} |p_z|^{\beta+0.5} |p_y - p_z|^{\alpha+0.5} \mathcal{F}^{-1} |\mathcal{F}(\widetilde{f})|(z,y) \right\| \\
&+ d_{1+\alpha+\beta} \left\| \frac{1}{|z|^{1+\alpha+\beta}} + |p_y - p_z|^{-\alpha-\beta-1} |p_z|^{\beta+0.5} |p_y - p_z|^{\alpha+0.5} \mathcal{F}^{-1} |\mathcal{F}(\widetilde{f})|(z,y) \right\| \\
\leqslant& 2 d_{1+\alpha+\beta} c_{1+\alpha+\beta} \left\| |p_z|^{\beta+0.5} |p_y - p_z|^{\alpha+0.5} \mathcal{F}^{-1} |\mathcal{F}(\widetilde{f})|(z,y) \right\| \\
=& 2 (2\pi)^{\alpha+\beta+1} d_{1+\alpha+\beta} c_{1+\alpha+\beta} \left\| |p_z|^{\beta+0.5} |p_y - p_z|^{\alpha+0.5} \mathcal{F}(\widetilde{f})(p_z, p_y) \right\| \\
=& 2 d_{1+\alpha+\beta} c_{1+\alpha+\beta} \left\| |p_z|^{\beta+0.5} |p_y - p_z|^{\alpha+0.5} \widetilde{f}(z,y) \right\| \\
=& 2 d_{1+\alpha+\beta} c_{1+\alpha+\beta} \left\| |p_x|^{\beta+0.5} |p_y|^{\alpha+0.5} f(x,y) \right\|
\end{aligned}$$

For the second term, we have

$$\begin{aligned}
&\left\| \int |p_z - p_z'|^{\alpha-2} |p_z'|^{\beta} |\mathcal{F}(\widetilde{f})|(p_z', p_y) dp_z' \right\| \\
=& (2\pi)^{-\beta} d_{1+\alpha} \left\| \frac{1}{|z|^{1+\alpha}} |p_z|^{\beta} \mathcal{F}^{-1} |\mathcal{F}(\widetilde{f})|(z,y) \right\| \\
\leqslant& 2 (2\pi)^{-\beta} d_{1+\alpha} c_{1+\alpha} \left\| |p_z|^{\beta+0.5} |p_y - p_z|^{\alpha+0.5} \widetilde{f}(z,y) \right\| \\
=& 2 (2\pi)^{-\beta} d_{1+\alpha} c_{1+\alpha} \left\| |p_x|^{\alpha+0.5} |p_y|^{\alpha+0.5} f(x,y) \right\|
\end{aligned}$$

Similarly, for the other three terms, we have

$$\begin{aligned}
\left\| \int |p_z - p_z'|^{\alpha-2} |p_y - p_z'|^{\alpha} |\mathcal{F}(\widetilde{f})|(p_z', p_y) dp_z' \right\| &\leqslant 2(2\pi)^{-\alpha} d_{1+\beta} c_{1+\beta} \left\| |p_x|^{\beta+0.5} |p_y|^{\alpha+0.5} f(x,y) \right\| \\
\left\| \int |p_z - p_z'|^{-2} |p_y - p_z'|^{\alpha} |p_z'|^{\beta} |\mathcal{F}|(\widetilde{f})(p_z', p_y) dp_z' \right\| &\leqslant 2(2\pi)^{-\alpha+\beta} d_1 c_1 \left\| |p_x|^{\beta+0.5} |p_y|^{\alpha+0.5} f(x,y) \right\|.
\end{aligned}$$

Finally, we have

$$\left\| |p_y|^{\alpha} |p_x|^{\alpha} \frac{1}{|x-y|} f(x,y) \right\| \leqslant D_{\alpha,\beta} \left\| |p_x|^{\beta+0.5} |p_y|^{\alpha+0.5} f(x,y) \right\|,$$

with

$$D_{\alpha,\beta} = 2\pi^{-1}((2\pi)^{\alpha+\beta} d_{1+\alpha+\beta} c_{1+\alpha+\beta} + (2\pi)^{\alpha} d_{1+\alpha} c_{1+\alpha} + (2\pi)^{\beta} d_{1+\beta} c_{1+\beta} + d_1 c_1).$$

□

3 Analysis of the potential

In the proof of the mixed regularity, the analysis of the potential plays the core role. In this section, we study the regularity of the potential. At the beginning, we choose the test function in infinitely defferentiable function space $\mathcal{D}(\mathbb{R}^{3N})$, and then by the density of the space $\mathcal{D}$ in any Hilbert space we get conclusion.

3.1 Electron-nuclei interaction

Following the Theorem 1.1, we split it into two cases to accord with the cases 1),2) and 3). And let u, v be infinitely diffenrentiable functions in the variables $x_j \in \mathbb{R}^3$, and $p_j = -i\nabla_j$.

For the case $j \notin \mathcal{I}^c$, if $0 \leqslant \beta < 0.5$ we have

$$\begin{aligned}
&\left(|p_j|^{1+\beta}\frac{u}{|x_j - a_\nu|}, |p_j|^{1+\beta}v\right)\\
=&\left(\nabla_j\frac{u}{|x_j - a_\nu|}, |p_j|^{2\beta}\nabla_j v\right)\\
=&\left(\frac{\nabla_j u}{|x_j - a_\nu|}, |p_j|^{2\beta}\nabla_j v\right) + \left(\nabla_j\frac{1}{|x_j - a_\nu|}u, |p_j|^{2\beta}\nabla_j v\right)\\
\leqslant&\left\|\frac{\nabla_j u}{|x_j - a_\nu|^{\beta}}\right\|\left\|\frac{|p_j|^{2\beta}\nabla_j v}{|x_j - a_\nu|^{1-\beta}}\right\| + \left\|\frac{u}{|x_j - a_\nu|^{1+\beta}}\right\|\left\|\frac{|p_j|^{2\beta}\nabla_j v}{|x_j - a_\nu|^{1-\beta}}\right\|\\
\leqslant&c_{1-\beta}(c_\beta + c_{1+\beta})\left\||p|^{\beta}\nabla_j u\right\|\left\||p_j|^{2+\beta}v\right\|\\
=&c_{1-\beta}(c_\beta + c_{1+\beta})\left\||p_j|^{1+\beta}u\right\|\left\||p_j|^{2+\beta}v\right\|.
\end{aligned} \tag{3}$$

And for the case $j \in \mathcal{I}^c$, if $0 \leqslant \alpha < 0.75$ we have

$$\begin{aligned}
&\left(|p_j|^{\alpha}\frac{u}{|x_j - a_\nu|}, |p_j|^{\alpha}v\right)\\
=&\left(\frac{u}{|x_j - a_\nu|}, |p_j|^{2\alpha}v\right)\\
\leqslant&\left\|\frac{u}{|x_j - a_\nu|^{\alpha}}\right\|\left\|\frac{|p_j|^{2\alpha}v}{|x_j - a_\nu|^{1-\alpha}}\right\|\\
\leqslant&c_\alpha c_{1-\alpha}\left\||p_j|^{\alpha}u\right\|\left\||p_j|^{1+\alpha}v\right\|.
\end{aligned} \tag{4}$$

3.2 Electron-electron interaction

let u, v be infinitely diffenrentiable functions in the variables $x_j, x_k \in \mathbb{R}^3$, and let $p_j = -i\nabla_j$ and $p_k = -i\nabla_k$ for x_j, x_k respectively.

For the case $j, k \in \mathcal{I}_l$ with $1 \leqslant l \leqslant q$, we have

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

Then for $0 \leqslant \beta < 0.25$,

$$\begin{aligned}
&\left(|p_j|^{1+\beta}p_k|^{1+\beta}\frac{u}{|x_j-x_k|},|p_j|^{1+\beta}|p_k|^{1+\beta}v\right)\\
=&\left(\nabla_j\nabla_k\frac{u}{|x_j-x_k|},|p_j|^{2\beta}|p_k|^{2\beta}\nabla_j\nabla_k v\right)\\
=&\left(\frac{\nabla_j\nabla_k u}{|x_j-x_k|},|p_j|^{2\beta}|p_k|^{2\beta}\nabla_j\nabla_k v\right)+\left(\nabla_j\frac{1}{|x_j-x_k|}\nabla_k u,|p_j|^{2\beta}|p_k|^{2\beta}\nabla_j\nabla_k v\right)\\
&+\left(\nabla_k\frac{1}{|x_j-x_k|}\nabla_j u,|p_j|^{2\beta}|p_k|^{2\beta}\nabla_j\nabla_k v\right)+\left(\nabla_j\nabla_k\frac{1}{|x_j-x_k|}u,|p_j|^{2\beta}|p_k|^{2\beta}\nabla_j\nabla_k v\right)\\
\leqslant&\left\|\frac{\nabla_j\nabla_k u}{|x_j-x_k|^{2\beta}}\right\|\left\|\frac{|p_j|^{2\beta}|p_k|^{2\beta}\nabla_j\nabla_k v}{|x_j-x_k|^{1-2\beta}}\right\|+\left\|\frac{\nabla_j u}{|x_j-x_k|^{1+2\beta}}\right\|\left\|\frac{|p_j|^{2\beta}|p_k|^{2\beta}\nabla_j\nabla_k v}{|x_j-x_k|^{1-2\beta}}\right\|\\
&+\left\|\frac{\nabla_k u}{|x_j-x_k|^{1+2\beta}}\right\|\left\|\frac{|p_j|^{2\beta}|p_k|^{2\beta}\nabla_j\nabla_k v}{|x_j-x_k|^{1-2\beta}}\right\|+\left\|\frac{u}{|x_j-x_k|^{2+2\beta}}\right\|\left\|\frac{|p_j|^{2\beta}|p_k|^{2\beta}\nabla_j\nabla_k v}{|x_j-x_k|^{1-2\beta}}\right\|\\
\leqslant&4c_{1-2\beta}(c_{2\beta}+2c_{1+2\beta}+c_{2+2\beta})\left\||p_j|^{1+\beta}|p_k|^{1+\beta}u\right\|\left\||p_j|^{3/2+\beta}|p_k|^{3/2+\beta}v\right\|\\
\leqslant&2c_{1-2\beta}(c_{2\beta}+2c_{1+2\beta}+c_{2+2\beta})\left\||p_j|^{1+\beta}|p_k|^{1+\beta}u\right\|\left(\left\||p_j|^{1+\beta}|p_k|^{2+\beta}v\right\|+\left\||p_j|^{2+\beta}|p_k|^{1+\beta}v\right\|\right).
\end{aligned}\tag{5}$$

For the case $j \in \mathcal{I}_l$ and $k \notin \mathcal{I}_l$ with $1 \leqslant l \leqslant q$, if $0 \leqslant \alpha < 0.5, 0 \leqslant \beta < 0.25$ and $0 \leqslant \alpha+\beta < 0.5$ we have

$$\begin{aligned}
&\left(|p_j|^{1+\beta}|p_k|^{\alpha}\frac{u}{|x_j-x_k|},|p_j|^{1+\beta}|p_k|^{\alpha}v\right)\\
=&\left(\nabla_j\frac{u}{|x_j-x_k|},|p_j|^{2\beta}|p_k|^{2\alpha}\nabla_j v\right)\\
=&\left(\frac{\nabla_j u}{|x_j-x_k|},|p_j|^{2\beta}|p_k|^{2\alpha}\nabla_j v\right)+\left(\nabla_j\frac{1}{|x_j-x_k|}u,|p_j|^{2\beta}|p_k|^{2\alpha}\nabla_j v\right)\\
\leqslant&\left\|\frac{\nabla_j u}{|x_j-x_k|^{\beta+\alpha}}\right\|\left\|\frac{|p_j|^{2\beta}|p_k|^{2\alpha}\nabla_j v}{|x_j-x_k|^{1-\alpha-\beta}}\right\|+\left\|\frac{u}{|x_j-x_k|^{1+\alpha+\beta}}\right\|\left\|\frac{|p_j|^{2\beta}|p_k|^{2\alpha}\nabla_j v}{|x_j-x_k|^{1-\alpha-\beta}}\right\|\\
\leqslant&4c_{1-\alpha-\beta}(c_{\alpha+\beta}+c_{1+\alpha+\beta})\left\||p_j|^{1+\beta}|p_k|^{\alpha}u\right\|\left\||p_j|^{3/2+\beta}|p_k|^{1/2+\alpha}v\right\|\\
\leqslant&2c_{1-\alpha-\beta}(c_{\alpha+\beta}+c_{1+\alpha+\beta})\left\||p_j|^{1+\beta}|p_k|^{\alpha}u\right\|\left(\left\||p_j|^{1+\beta}|p_k|^{1+\alpha}v\right\|+\left\||p_j|^{2+\beta}|p_k|^{\alpha}v\right\|\right).
\end{aligned}\tag{6}$$

And if $0.5 \leqslant \alpha < 0.75, -0.25 \leqslant \beta < 0$ and $0 \leqslant \alpha+\beta < 0.5$, by lemma 2.6, we have

$$\begin{aligned}
&\left(|p_j|^{1+\beta}|p_k|^{\alpha}\frac{u}{|x_j-x_k|},|p_j|^{1+\beta}|p_k|^{\alpha}v\right)\\
=&\left(|p_j|^{0.5+\beta}|p_k|^{\alpha-0.5}\frac{u}{|x_j-x_k|},|p_j|^{1.5+\beta}|p_k|^{\alpha+0.5}v\right)\\
\leqslant&\left\||p_j|^{0.5+\beta}|p_k|^{\alpha-0.5}\frac{u}{|x_j-x_k|}\right\|(\||p_j|^{2.5+\beta}|p_k|^{\alpha}v\|+\||p_j|^{1+\beta}|p_k|^{\alpha+1}v\|)\\
\leqslant&1/2D_{\alpha-0.5,\beta+0.5}\||p_j|^{\beta+1}|p_k|^{\alpha}u\|(\||p_j|^{2.5+\beta}|p_k|^{\alpha}v\|+\||p_j|^{1+\beta}|p_k|^{\alpha+1}v\|).
\end{aligned}\tag{7}$$

Finally, for the case $j, k \in \mathcal{I}^c$, if $0 \leqslant \alpha \leqslant 0.5$ we have

$$
\begin{aligned}
&\left(|p_j|^\alpha |p_k|^\alpha \frac{u}{|x_j - x_k|}, |p_j|^\alpha |p_k|^\alpha v\right) \\
=&\left(\frac{u}{|x_j - x_k|}, |p_j|^{2\alpha} |p_k|^{2\alpha} v\right) \\
\leqslant&\left\|\frac{u}{|x_j - x_k|^{2\alpha}}\right\| \left\|\frac{|p_j|^{2\alpha}|p_k|^{2\alpha} v}{|x_j - x_k|^{1-2\alpha}}\right\| \\
\leqslant& 4c_{1-2\alpha} c_{2\alpha} \left\||p_j|^\alpha |p_k|^\alpha u\right\| \left\||p_j|^{1/2+\alpha}|p_k|^{1/2+\alpha} v\right\| \\
\leqslant& 2c_{1-2\alpha} c_{2\alpha} \left\||p_j|^\alpha |p_k|^\alpha u\right\| \left(\left\||p_j|^{1+\alpha}|p_k|^\alpha v\right\| + \left\||p_j|^\alpha |p_k|^{1+\alpha} v\right\|\right).
\end{aligned} \tag{8}
$$

And if $0.5 < \alpha < 0.75$, it is a bit different.

$$
\begin{aligned}
&\left(|p_j|^\alpha |p_k|^\alpha \frac{u}{|x_j - x_k|}, |p_j|^\alpha |p_k|^\alpha v\right) \\
=&\left(|p_j|^{\alpha-0.5} |p_k|^{\alpha-0.5} \frac{u}{|x_j - x_k|}, |p_j|^{\alpha+0.5} |p_k|^{\alpha+0.5} v\right) \\
\leqslant&\left\||p_j|^{\alpha-0.5} |p_k|^{\alpha-0.5} \frac{u}{|x_j - x_k|}\right\| \left\||p_j|^{\alpha+0.5}|p_k|^{\alpha+0.5} v\right\| \\
\leqslant& 1/2 D_{\alpha-0.5,\alpha-0.5} \left\||p_j|^\alpha |p_k|^\alpha u\right\| \left(\left\||p_j|^\alpha |p_k|^{\alpha+1} v\right\| + \left\||p_j|^{\alpha+1} |p_k|^\alpha v\right\|\right)
\end{aligned} \tag{9}
$$

3.3 Conclusion

According to this Fourier transform, we denote the operator $\mathcal{L}_{\mathcal{I}',\mathcal{I}'',\alpha,1+\beta}$ by

$$
\mathcal{L}_{\mathcal{I}',\mathcal{I}'',\alpha,1+\beta} = \prod_{k\in\mathcal{I}'} |\omega_k|^{1+\beta} \prod_{m\in\mathcal{I}''} |\omega_m|^\alpha,
$$

and

$$
\mathcal{L}_{\mathcal{I},\alpha,1+\beta} = \left(\sum_{l=1}^{q} \prod_{k\in\mathcal{I}_l} (1 + |\omega_k|^{2+2\beta}) \prod_{m\in\mathcal{I}\setminus\mathcal{I}_l} (1 + |\omega_m|^{2\alpha})\right)^{1/2}.
$$

Thus,

$$
\mathcal{L}^2_{\mathcal{I},\alpha,1+\beta} = \sum_{l=1}^{q} \sum_{\mathcal{I}'\subset\mathcal{I}_l} \sum_{\mathcal{I}''\subset\mathcal{I}\setminus\mathcal{I}_l} \mathcal{L}^2_{\mathcal{I}',\mathcal{I}'',\alpha,1+\beta},
$$

and

$$
|||u|||^2_{\mathcal{I},\alpha,1+\beta} = \sum_{l} \sum_{\mathcal{I}\subset\mathcal{I}_l} \sum_{\mathcal{I}''\subset\mathcal{I}\setminus\mathcal{I}_l} \|\mathcal{L}_{\mathcal{I}',\mathcal{I}'',\alpha,1+\beta} u\|^2_{H^1(\mathbb{R}^{3N})}.
$$

Now, we yield

$$
(\mathcal{L}_{\mathcal{I}',\mathcal{I}'',\alpha,1+\beta} V u, \mathcal{L}_{\mathcal{I}',\mathcal{I}'',\alpha,1+\beta} v) \leqslant C_{\alpha,\beta,M,N,Z} \|\mathcal{L}_{\mathcal{I}',\mathcal{I}'',\alpha,1+\beta} u\| \|\nabla \mathcal{L}_{\mathcal{I}',\mathcal{I}'',\alpha,1+\beta} v\|
$$

and

$$
(\mathcal{L}_{\mathcal{I},\alpha,1+\beta} V u, \mathcal{L}_{\mathcal{I},\alpha,1+\beta} v) \leqslant C_{\alpha,\beta,M,N,Z} \|\mathcal{L}_{\mathcal{I},\alpha,1+\beta} u\| \|\nabla \mathcal{L}_{\mathcal{I},\alpha,1+\beta} v\| \tag{10}
$$

with $\nabla = (\nabla_1, \cdots, \nabla_N)$ and $C_{\alpha,\beta,M,N,Z}$ a constant only dependent on α, β, M, N, Z. And the choices of α and β differ by the anti-symmetry:

1) if $\mathcal{I}^c = \varnothing$, then $\alpha = 0$ and $0 \leqslant \beta < 0.25$,

2) if $\mathcal{I}^c \neq \varnothing$ and $\mathcal{I}^c \neq \{1, \cdots, N\}$, then $0 \leqslant \alpha < 0.75$, $-0.25 \leqslant \beta < 0.25$ and $0 \leqslant \alpha + \beta < 0.5$, or $0.5 \leqslant \alpha < 0.75$, $-0.25 \leqslant \beta < 0$ and $0 \leqslant \alpha + \beta < 0.5$,

3) if $\mathcal{I}^c = \{1, \cdots, N\}$, then $0 \leqslant \alpha < 0.75$ and $\beta = -1$.

4 The Regularity of Solutions

Repeating the proof in [13], we split the eigenfunctions into a high-frequency part and a low frequency part and first to estimate the hign-frequency part by the low frequency part. Let P_Ω be the projector to the hign frequency part, with

$$\widehat{P_\Omega u}(\omega) = \mathbb{1}_{|\omega|_\gamma \geqslant \Omega} \widehat{u}.$$

with

$$|\omega|_\gamma^\gamma = \sum |\omega_i|^\gamma$$

where

$$\gamma = 2 \min\{\beta, \alpha\}.$$

By the equivalence of norm in finite dimension, we have

$$C(N, \alpha, \beta, 1)^{-1} |\omega|_\gamma \leqslant |\omega|_2 \leqslant C(N, \alpha, \beta, 2) |\omega|_\gamma. \tag{11}$$

And let

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

Thus,

$$\|u_H\| \leqslant C(N, \alpha, \beta, 1)/\Omega \|\nabla u_H\|.$$

Taking $v_H \in P_\Omega H_{\mathcal{I}}^{\alpha, 1+\beta}$, then for the mixed regularity we need to study

$$(\mathcal{L}_{\mathcal{I},\alpha,1+\beta} H u, \mathcal{L}_{\mathcal{I},\alpha,1+\beta} v_H) - \lambda (\mathcal{L}_{\mathcal{I},\alpha,1+\beta} u, \mathcal{L}_{\mathcal{I},\alpha,1+\beta} v_H) = 0$$

Decomposing u by u_H and u_L, we have

$$\begin{aligned}(\nabla \mathcal{L}_{\mathcal{I},\alpha,1+\beta} u_H, \nabla \mathcal{L}_{\mathcal{I},\alpha,1+\beta} v_H) + (\mathcal{L}_{\mathcal{I},\alpha,1+\beta} V u_H, \mathcal{L}_{\mathcal{I},\alpha,1+\beta} v_H) \\ - \lambda (\mathcal{L}_{\mathcal{I},\alpha,1+\beta} u_H, \mathcal{L}_{\mathcal{I},\alpha,1+\beta} v_H) = (\mathcal{L}_{\mathcal{I},\alpha,1+\beta} V u_L, \mathcal{L}_{\mathcal{I},\alpha,1+\beta} v_H)\end{aligned}$$

Let

$$\Omega \geqslant 4\sqrt{2} C(N, \alpha, \beta, 1)(C_{\alpha,\beta,M,N,Z} + |\lambda|^{1/2}) + C(N, \alpha, \beta, 1), \tag{12}$$

hence

$$\begin{aligned}&(\mathcal{L}_{\mathcal{I},\alpha,1+\beta} V u_H, \mathcal{L}_{\mathcal{I},\alpha,1+\beta} v_H) \leqslant 1/4 \|\nabla \mathcal{L}_{\mathcal{I},\alpha,1+\beta} u_H\| \|\nabla \mathcal{L}_{\mathcal{I},\alpha,1+\beta} v_H\|, \\ &\lambda (\mathcal{L}_{\mathcal{I},\alpha,1+\beta} u_H, \mathcal{L}_{\mathcal{I},\alpha,1+\beta} v_H) \leqslant 1/4 \|\nabla \mathcal{L}_{\mathcal{I},\alpha,1+\beta} u\| \|\nabla \mathcal{L}_{\mathcal{I},\alpha,1+\beta} v\|, \\ &\|\mathcal{L}_{\mathcal{I},\alpha,1+\beta} u_H\| \leqslant \|\nabla \mathcal{L}_{\mathcal{I},\alpha,1+\beta} u_H\|.\end{aligned}$$

Therefore, we have

$$\begin{aligned}(\nabla \mathcal{L}_{\mathcal{I},\alpha,1+\beta} u_H, \nabla \mathcal{L}_{\mathcal{I},\alpha,1+\beta} u_H) + (\mathcal{L}_{\mathcal{I},\alpha,1+\beta} V u_H, \mathcal{L}_{\mathcal{I},\alpha,1+\beta} u_H) \\ - \lambda (\mathcal{L}_{\mathcal{I},\alpha,1+\beta} u_H, \mathcal{L}_{\mathcal{I},\alpha,1+\beta} u_H) \geqslant 1/4 \|\mathcal{L}_{\mathcal{I},\alpha,1+\beta} u_H\|_{H^1}\end{aligned} \tag{13}$$

And now, we prove the regularity of the eigenfunctions.

Sketch of Proof of the Theorem 1.1. This proof is similar to the proof in [12,14]. So we just give the sketch of proof.

Step 1. For the frequency bounds Ω as in (12), the equation

$$\begin{aligned}&(\nabla\mathcal{L}_{\mathcal{I},\alpha,1+\beta}u_H,\nabla\mathcal{L}_{\mathcal{I},\alpha,1+\beta}v_H)+(\mathcal{L}_{\mathcal{I},\alpha,1+\beta}Vu_H,\mathcal{L}_{\mathcal{I},\alpha,1+\beta}v_H)\\ -&\lambda\left(\mathcal{L}_{\mathcal{I},\alpha,1+\beta}u_H,\mathcal{L}_{\mathcal{I},\alpha,1+\beta}v_H\right)=\left(\mathcal{L}_{\mathcal{I},\alpha,1+\beta}V\psi,\mathcal{L}_{\mathcal{I},\alpha,1+\beta}v_H\right),\ \forall v_H\in P_\Omega H_{\mathcal{I}}^{\alpha,\beta}\end{aligned}\tag{14}$$

processes a unique solution $u_H \in P_\Omega H_{\mathcal{I}}^{\alpha,\beta}$ for all given functions $\psi \in H_{\mathcal{I}}^{\alpha,\beta}$.

Using the Lax-Milgram theorem, and combining (13) and (10), we get conclusion.

Step 2. For the frequency bounds Ω as in (12), the equation

$$(\nabla u_H,\nabla\chi_H)+(Vu_H,\chi_H)-\lambda\left(u_H,\chi_H\right)=\left(V\psi,\chi_H\right),\ \forall\chi_H\in P_\Omega H^1\tag{15}$$

processes a unique solution $u_H \in P_\Omega H^1$ for all given functions $\psi \in H^1$.

Using the Lax-Milgram theorem agian, we can get conclusion. Indeed, it has been studied in [12–14].

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

By Fourier transform, we have

$$\left(\sum_{l=1}^{q}\prod_{k\in\mathcal{I}_l}(1+|\omega_k|^{2+2\beta-2\alpha})\prod_{m\in\mathcal{I}\setminus\mathcal{I}_l}(1+|\omega_m|^{2\alpha})\right)\widehat{v_H}(\omega)=\widehat{\chi_H}(\omega),$$

Thus get conclusion.

Step 4. The solution of (15) is contained in the space $H_{\mathcal{I}}^{\alpha,1+\beta}$.

We rewrite the equation (14) as

$$\begin{aligned}&\left(\nabla u_H,\nabla\mathcal{L}^2_{\mathcal{I},\alpha,1+\beta}v_H\right)+\left(Vu_H,\mathcal{L}^2_{\mathcal{I},\alpha,1+\beta}v_H\right)\\ -&\lambda\left(u_H,\mathcal{L}^2_{\mathcal{I},\alpha,1+\beta}v_H\right)=\left(V\psi,\mathcal{L}^2_{\mathcal{I},\alpha,1+\beta}v_H\right),\ \forall v_H\in P_\Omega H_{\mathcal{I}}^{\alpha,\beta}.\end{aligned}$$

And by the steps above, we know the solution of equation (14) satisfies the original equation (15) for all $\chi_H \in P_\Omega H^1$. Hence for all $\mathcal{L}_{\mathcal{I},\alpha,1+\beta}\psi \in L^2$, by the uniqueness of solution, we get conclusion.

Step 5. Since the low-frequency part u_L of the solution is contained in $\mathcal{D}$ hence in $H_{\mathcal{I}}^{\alpha,\beta}$, and $\mathcal{L}_{\mathcal{I},\alpha,1+\beta}u \in L^2$, we know the solution $u \in H_{\mathcal{I}}^{\alpha,\beta}$.

And combining the condition of α and β, we get the Theorem 1.1. □

5 Numerical analysis

In this part, we study the hyperbolic cross space approximation, which is almost same with [13]. So we just give the sketch.

Obviously, there is a $\Omega > 4\sqrt{2}C(N,\alpha,\beta,1)(C_{\alpha,\beta,M,N,Z} + |\lambda|^{1/2}) + C(N,\alpha,\beta,1)$ large engough, such that

$$\|\mathcal{L}_{\mathcal{I},\alpha,1+\beta}u_H\|_{L^2}\leqslant\sqrt{2}\|\mathcal{L}_{\mathcal{I},\alpha,1+\beta}u_L\|,\ \|u_H\|\leqslant\sqrt{2}\|u_L\|$$

and

$$\|\nabla\mathcal{L}_{\mathcal{I},\alpha,1+\beta}u_H\|_{L^2}\leqslant\sqrt{2}C(N,\alpha,\beta,2)\Omega\|\mathcal{L}_{\mathcal{I},\alpha,1+\beta}u_L\|,\ \|\nabla u_H\|\leqslant\sqrt{2}C(N,\alpha,\beta,2)\Omega\|u_L\|.$$

We take the following norm:

$$\||u\||^2_{\mathcal{I}_l,\alpha,\beta,1} = \int \left(\sum_{i=1}^{N} |\omega_i/\Omega|^2\right) \left(\prod_{k\in\mathcal{I}_l}(1+|\omega_k/\Omega|^{2\beta}) \prod_{m\in\mathcal{I}\setminus\mathcal{I}_l}(1+|\omega_m/\Omega|^{2\alpha})\right)|\widehat{u}|^2\, d\omega.$$

and

$$\||u\||^2_{\mathcal{I}_l,\alpha,\beta,0} = \int \left(\prod_{k\in\mathcal{I}_l}(1+|\omega_k/\Omega|^{2\beta}) \prod_{m\in\mathcal{I}\setminus\mathcal{I}_l}(1+|\omega_m/\Omega|^{2\alpha})\right)|\widehat{u}|^2\, d\omega.$$

Lemma 5.1. *For scaling parameters* $\Omega > 4\sqrt{2}C(N,\alpha,\beta,1)(C_{\alpha,\beta,M,N,Z}+|\lambda|^{1/2})+C(N,\alpha,\beta,1)$ *large enough, the eigenfunctions* $u \in H^{\alpha,\beta}_{\mathcal{I}}$ *satisfy the estimates*

$$\||u\||_{\mathcal{I}_l,\alpha,\beta,0} \leqslant \sqrt{2e}\|u\|,\ \||u\||_{\mathcal{I}_l,\alpha,\beta,1} \leqslant \sqrt{2e}C(N,\alpha,\beta,2)\|u\|.$$

Proof. The proof is similar with [13, Theorem 9]. As $|\omega_k/\Omega| \leqslant 1$, we have

$$|\omega_k/\Omega|^{2\alpha} \leqslant |\omega_k/\Omega|^{\gamma},\ |\omega_k/\Omega|^{2\beta} \leqslant |\omega_k/\Omega|^{\gamma}$$

Thus,

$$\prod_{k\in\mathcal{I}_l}(1+|\omega_k/\Omega|^{2\beta}) \prod_{m\in\mathcal{I}\setminus\mathcal{I}_l}(1+|\omega_m/\Omega|^{2\alpha}) \leqslant \exp\big(\sum_{\mathcal{I}_l}|\omega_k/\Omega|^{2\beta} + \sum_{\mathcal{I}\setminus\mathcal{I}_l}|\omega_m/\Omega|^{2\alpha}\big) \leqslant e.$$

And the case $\||u\||_{\mathcal{I}_l,\alpha,\beta,1} \leqslant \sqrt{2e}\|u\|$ is treated equally by using the inequality

$$|\omega/\Omega|_2 \leqslant C(N,\alpha,\beta,2).$$

□

Thus, Theorem 1.2 can be proved just by repeating the proof of [13].

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