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Long Meng

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THÈSE DE DOCTORAT
DE L'UNIVERSITÉ PSL

Préparée à Université Paris-Dauphine

Le problème à N corps en Chimie quantique: solution exacte et approximations

Soutenue par

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The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble. It therefore becomes desirable that approximate practical methods of applying quantum mechanics should be developed, which can lead to an explanation of the main features of complex atomic systems without too much computation

Paul Dirac

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Introduction

Cette thèse est consacrée à une étude rigoureuse du problème à N corps en interaction coulombienne et de certaines de ses approximations en Chimie quantique non relativiste et relativiste.

La physique des atomes et des molécules (et donc presque toute la chimie) est largement régie par le problème de la mécanique quantique à N corps dans lequel les électrons et les noyaux interagissent par les forces d'attraction et de répulsion de Coulomb. A travers l'approximation de Born-Oppenheimer, le coeur de cette procédure est d'étudier l'opérateur hamiltonien électronique suivant :

$$H = -\frac{1}{2} \sum_{i=1}^N \Delta_i + V(x), \quad (0.1)$$

ou pour le cas relativiste :

$$D = \sum_{i=1}^N -i(\boldsymbol{\alpha} \cdot \nabla_i + \beta) + \alpha V(x)$$

avec potentiel

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

Le problème principal rencontré en chimie quantique est la complexité des calculs qui, à première vue, croît exponentiellement avec le nombre N d'électrons (voir par exemple [38]). Ce phénomène est couramment appelé la malédiction de la dimension. Il existe des méthodes d'approximation non-linéaire : Hartree-Fock, qui est une approximation de champ moyen, suivie par les modèles *multiconfiguration* plus précis, qui tiennent compte de la corrélation électronique négligée par le modèle Hartree-Fock [40]. Si l'on limite le nombre de configurations, la complexité des calculs multiconfiguration croît polynomialement avec N . Mais si l'on veut améliorer l'approximation de Schrödinger par les modèles multiconfiguration, il faut augmenter le nombre de configurations. Pour comprendre le taux de croissance de la qualité de l'approximation avec le nombre de configurations et tenter de l'améliorer, il est fondamental d'avoir une meilleure compréhension des propriétés de régularité des solutions du modèle exact de Schrödinger à N corps, en tant que fonction de $3N$ variables.

Pour l'étude des atomes lourds (à partir du Fer), une difficulté supplémentaire apparaît: il faut tenir compte des effets relativistes. La théorie exacte est alors l'électrodynamique quantique, qui est mal comprise du point de vue mathématique. Cette théorie donne d'excellents résultats dans un cadre perturbatif, mais en chimie quantique son utilisation est beaucoup plus délicate. En effet la chimie quantique nécessite toujours un premier calcul non perturbatif. Le modèle le plus utilisé permettant un tel calcul est le modèle de Dirac-Fock qui est l'équivalent relativiste du modèle de Hartree-Fock.

Cette thèse porte à la fois sur des aspects non relativistes et relativistes du problème à N corps en chimie quantique. Elle est divisée en deux parties principales: la régularité dans les problèmes à N corps non-relativiste; l'existence de minimiseurs dans le modèle de Dirac-Fock pour les cristaux.

La première partie est consacrée aux régularités de modèle Born-Openheimer stationnaire ou dépendent du temps, et ses applications à l'analyse numérique. Les systèmes de particules quantiques sont divisés en deux familles : les bosons et les fermions. Les premières sont décrites par une fonction d'onde symétrique et les secondes par une fonction d'onde antisymétrique sous l'échange d'électrons de même spin à cause du principe d'exclusion de Pauli. Pour les fermions, la fonction d'onde s'annule là où ces électrons se rencontrent, ce qui contrebalance les singularités du potentiel d'interaction entre les électrons. Grâce à cette observation, H. Yserentant [59] introduit une régularité mixte des solutions pour les problèmes stationnaires. En combinant des estimations de Strichartz et une extension d'inégalité de Caldéron-Zygmund, nous prouvons l'existence et la régularité de solutions du problème d'évolution. Et grâce aux propriétés de régularisation du propagateur de l'opérateur de Schrödinger, nous proposons une approximation nouvelle et directe pour le problème d'évolution.

Pour le cas non-antisymétrique (par exemple bosons), les fonctions d'onde ne pourraient plus contrebalancer les singularités. Cependant, la singularité venant du potentiel coulombien est localement intégrable. Grâce à cela et l'inégalité de Herbst, nous obtenons des estimations dans des espaces de Sobolev fractionnaires pour les solutions du problème stationnaire, qui améliorent les résultat de Yserentant.

Dans la seconde partie, nous présentons l'étude en collaboration avec Isabelle Catto, Eric Paturol et Eric Séré d'un modèle de champ moyen en mécanique quantique relativiste, le modèle de Dirac-Fock pour les cristaux, issu de la limite thermodynamique. Comme le modèle Dirac-Fock pour les molécules ou les atomes, c'est un problème de min-max. Cependant, pour le modèle périodique; la solution peut être décomposée par la décomposition intégrale directe avec les fibres quasi-périodiques à travers la décomposition de Bloch. La décomposition fait perdre la compacité à la fonctionnelle. Grâce à la redéfinition de l'état fondamental et à une méthode nouvelle pour résoudre le problème quasi-périodique, nous montrons l'existence d'état fondamental qui est également la solution de l'équation auto-cohérente.

1 Notions de base en mécanique quantique à N corps

Dans cette section, nous présentons des connaissances fondamentales en mécanique quantique. C'est une théorie qui permet la description des systèmes quantiques, comme des molécules composées d'électrons et de noyaux.

1.1 Les particules quantiques

Un système de N particules quantiques se déplaçant dans l'espace euclidien à 3 dimensions est représenté par une fonction d'onde normalisée $\Psi \in L^2(\mathbb{R}^3)^{\otimes N}$, c'est-à-dire

$$\|\Psi\|_{L^2((\mathbb{R}^3)^N)}^2 = \int_{\mathbb{R}^{3N}} |\Psi(x_1, \dots, x_N)|^2 dx_1 \cdots dx_N = 1.$$

Ici $x_i \in \mathbb{R}^3$ est la coordonnée spatiale de la $i^{\text{ème}}$ particule.

En physique, pour les systèmes électroniques, ou les systèmes fermioniques plus généraux, la fonction d'onde Ψ devrait satisfaire au principe d'exclusion de Pauli, ce qui signifie qu'elle est antisymétrique sous le changement de coordonnées électroniques pour un état de spin [42]. Si une particule possède s degrés internes de liberté (c'est-à-dire s états de spin), alors nous les étiquetons par l'entier

$$\sigma \in \{1, 2, \dots, s\}.$$

Et pour un système de N particules, supposons que la $i^{\text{ème}}$ particule ait s_i états de spin. Alors, une fonction d'onde pour ces N particules peut alors être écrite comme

$$\Psi(x_1, \sigma_1, \dots, x_N, \sigma_N)$$

où $1 \leq \sigma_i \leq s_i$.

Pour le système à spin fixe σ , Ψ n'est qu'une fonction de x_1, \dots, x_N , alors elle peut être considérée comme

$$\Psi(x_1, \dots, x_N).$$

Soit

$$\mathcal{I}_l = \{i | \sigma_i = l\}, \quad l = 1, \dots, s,$$

et $P_{i,j}$ est une permutation qui échange simultanément la position des variables x_i, x_j et le spin σ_i, σ_j . Par le principe de Pauli, pour des fermions, nous savons que

$$\Psi(P_{i,j}X) = -\Psi(X), \quad \text{si } \exists 1 \leq l \leq s, \text{ t.q. } i, j \in \mathcal{I}_l. \quad (1.1)$$

où $X = (x_1, \dots, x_N)$. Donc, pour une permutation τ quelconque et les fermions indiscernables, nous savons que

$$\Psi(x_{\tau(1)}, \sigma_{\tau(1)}, \dots, x_{\tau(N)}, \sigma_{\tau(N)}) = \epsilon(\tau) \Psi(x_1, \sigma_1, \dots, x_N, \sigma_N),$$

où $\epsilon(\tau)$ désigne la signature de la permutation τ .

Un autre genre de particules appelées bosons satisfait à la statistique de Bose–Einstein. Ses fonctions d’onde ont également des états de spin comme les fermions. Contrairement aux fermions, pour une permutation τ quelconque et les bosons, nous savons que

$$\Psi(P_{i,j}X) = \Psi(X), \quad \text{if } \exists 1 \leq l \leq s, \text{ t.q. } i, j \in \mathcal{I}_l. \quad (1.2)$$

Et alors, pour les bosons indiscernables, on doit avoir

$$\Psi(x_{\tau(1)}, \sigma_{\tau(1)}, \dots, x_{\tau(N)}, \sigma_{\tau(N)}) = \Psi(x_1, \sigma_1, \dots, x_N, \sigma_N).$$

De manière générale, ces relations signifient que la densité $|\Psi|^2$ est invariante si l’on permute l’indexation des particules. Donc, pour σ fixe, la quantité qui est appelée *la fonction de la densité*

$$\rho_\Psi(x) := \sum_{i=1}^N \rho_\Psi^i(x) \quad (1.3)$$

où

$$\rho_\Psi^i(x) = \int_{(\mathbb{R}^3)^{N-1}} |\Psi(x_1, \dots, x_{i-1}, x, x_{i+1}, \dots, x_N)|^2 dx_1 \cdots \widehat{dx}_i \cdots dx_N,$$

s’interprète alors comme la densité de probabilité de présence de la particule dans l’espace. La notation \widehat{dx}_i signifie que l’intégration sur la $i^{\text{ème}}$ coordonnée est omise. Evidemment,

$$\int_{\mathbb{R}^3} \rho_\Psi dx = N.$$

La transformée de Fourier $\widehat{\Psi}(p)$ est également normalisée dans $L^2((\mathbb{R}^3)^N)$ et $|\widehat{\Psi}|^2(p)$ représente la densité de moment cinétique.

Comme les fonctions d’onde à N particules sont parfois difficiles à manipuler, on utilise souvent *l’opérateur de densité* à un corps, défini par son noyau

$$\begin{aligned} \gamma_\Psi(x, y) &= \sum_{i=1}^N \int_{(\mathbb{R}^3)^{N-1}} \Psi(x_1, \dots, x_{i-1}, x, x_{i+1}, \dots, x_N) \\ &\quad \times \overline{\Psi(x_1, \dots, x_{i-1}, y, x_{i+1}, \dots, x_N)} dx_1 \cdots \widehat{dx}_i \cdots dx_N, \end{aligned}$$

c’est-à-dire

$$(\gamma_\Psi \phi)(x) = \int_{\mathbb{R}^3} \gamma_\Psi(x, y) \phi(y) dy \quad (1.4)$$

qui vérifie par ailleurs $0 \leq \gamma_\Psi \leq 1$, $\text{Tr}(\gamma_\Psi) = N$ et $\rho_\Psi(x) = \gamma_\Psi(x, x)$.

1.2 Opérateur de Schrödinger et de Dirac

Quelle est la relation de dispersion pour l’onde de matière?

Un bon point de départ est l’interprétation d’Einstein de l’effet photoélectrique. Lorsque des plaques métalliques polies sont irradiées par une lumière de longueur d’onde suffisamment courte, elles peuvent émettre des électrons. L’explication d’Einstein, pour

laquelle il a reçu le prix Nobel, était que la lumière est constituée de quanta de lumière unique avec énergie et quantité de mouvement

$$E = \hbar\omega, \quad p = \hbar k$$

ne dépendant que de la fréquence ω et du vecteur d'onde k . Pour établir la connexion entre ω et k ou E et p , évidemment on utilise:

$$E = \sqrt{c^2 p^2 + m^2 c^4} \quad (1.5)$$

où m est la masse de l'électron, et c la vitesse de la lumière. Les remplacements $E \leftarrow i\hbar\partial_t$ et $p \leftarrow -i\hbar\nabla$ fournissent la relation de dispersion de l'équation de Klein-Gordon

$$-\frac{\partial^2}{\partial t^2}\Psi(t, x) = (-c^2\Delta + m^2 c^4)\Psi(t, x). \quad (1.6)$$

Cependant, cette équation n'a pas répondu à ses attentes et a conduit à des fausses prédictions, car elle décrit un autre type de particules (celles avec spin zéro), pas des électrons. Schrödinger revient donc à la physique classique et remplace par la relation énergie-momentum

$$E = \frac{1}{2m}|p|^2$$

de la mécanique Newtonienne. Par conséquent, il a obtenu l'équation non-relativiste, à savoir l'équation de Schrödinger:

$$i\hbar\frac{\partial}{\partial t}\Psi = -\frac{\hbar^2}{2m}\Delta\Psi.$$

Et pour le cas relativiste, l'équation (1.6) est du second ordre. Donc elle ne décrit pas correctement l'évolution d'un système quantique qui doit être du premier ordre par rapport à t . Il faut donc chercher un opérateur auto-adjoint H vérifiant

$$H^2 = -c^2\Delta + m^2 c^4 \quad (1.7)$$

pour l'étude de l'équation

$$i\hbar\frac{\partial}{\partial t}\Psi(t, x) = H \cdot \Psi(t, x).$$

Le cas le plus simple sera

$$H = \sqrt{-c^2\Delta + m^2 c^4}.$$

Ici $\sqrt{-c^2\Delta + m^2 c^4}$ est l'opérateur pseudo-différentiel du symbole $\sqrt{c^2|p|^2 + m^2 c^4}$. Cependant, cet opérateur est non-local, ce qui contredit le principe de causalité en mécanique relativiste. Donc, Dirac reformula l'opérateur par

$$D_0^{m,c} = -ic \sum_{j=1}^3 \alpha_j \partial_j + \beta mc^2 = -ic\boldsymbol{\alpha} \cdot \nabla + \beta mc^2$$

où $\alpha = (\alpha_1, \alpha_2, \alpha_3)$ et β doivent être déterminés en imposant (1.7). Il est très aisé de voir que les α_i et β doivent être des matrices de dimension 4 qui sont appelées matrices de Pauli:

$$\beta = \begin{pmatrix} \mathbb{1}_2 & 0 \\ 0 & \mathbb{1}_2 \end{pmatrix}, \quad \alpha_k = \begin{pmatrix} 0 & \sigma_k \\ \sigma_k & 0 \end{pmatrix},$$

où

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

Ici, on choisit un système d'unités tel que la masse d'un électron, la vitesse de la lumière ainsi que la constante de Plank valent 1:

$$m = c = 1 = \hbar; D_0 = -i\alpha \cdot \nabla + \beta.$$

L'opérateur de Dirac agit donc sur des spineurs:

$$\Psi = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix} \in L^2(\mathbb{R}^4; \mathbb{C}^4).$$

Evidemment, l'opérateur de Schrödinger (resp. l'opérateur de Dirac) est auto-adjoint sur $L^2(\mathbb{R}^3, \mathbb{C})$ (resp. $L^2(\mathbb{R}^3; \mathbb{C}^4)$), de domaines $H^2(\mathbb{R}^3, \mathbb{C})$ (resp. $H^1(\mathbb{R}^3, \mathbb{C})$). Les spectres sont purement continus:

$$\sigma(-\Delta) = [0, +\infty); \quad \sigma(D_0) = (-\infty, -1] \cup [1, +\infty).$$

Notons que $\Lambda_0^- = \mathbb{1}_{\mathbb{R}^-}(D_0)$ et $\Lambda_0^+ = \mathbb{1}_{\mathbb{R}^+}(D_0)$ sont les projecteurs sur les espaces respectivement associés au spectre négatif et positif de D_0 .

1.3 Potentiel coulombien

En chimie quantique, les molécules sont composées d'électrons (charges négatives) et de noyaux (charges positives) interagissant via la force coulombienne. Le potentiel entre deux particules de charge Z et Z' qui se trouvent dans x et x' en \mathbb{R}^3 est:

$$\frac{ZZ'}{|x - x'|}.$$

Normalement, un système de molécules comporte beaucoup de noyaux et d'électrons. Alors, pour un système de M noyaux de charges Z_i qui se trouvent en a_i pour le $i^{\text{ème}}$ atome et N électrons, le potentiel est

$$-\sum_{j=1}^N \sum_{\mu=1}^M \frac{Z_\nu}{|x_j - a_\nu|} + \sum_{k < j}^N \frac{1}{|x_j - x_k|} + \sum_{k < j}^M \frac{Z_j Z_k}{|a_j - a_k|}$$

Il agit sur les fonctions avec les variables x_1, \dots, x_N dans \mathbb{R}^3 , coordonnées des électrons donnés.

Il y a deux difficultés qui surviennent pour le système électronique, [24]. La première est la singularité de $1/|x|$ en 0: il est nécessaire d'expliquer à l'aide du principe d'incertitude pourquoi une particule ne se précipitera pas vers une particule de charge opposée.

Une version plus puissante du principe d'incertitude est l'inégalité de type Hardy:

- *Hardy*: (le cas non-relativiste) pour toutes $v \in H^1(\mathbb{R}^3)$

$$\| |x|^{-1}v \|_{L^2(\mathbb{R}^3)} \leq 2 \|\nabla v\|_{L^2(\mathbb{R}^3)} \leq 2 \|\sqrt{-\Delta + 1}v\|_{L^2(\mathbb{R}^3)},$$

- *Kato, Herbst*: (le cas relativiste) pour toutes $v \in H^{1/2}(\mathbb{R}^3)$

$$\langle v, |x|^{-1}v \rangle \leq \frac{\pi}{2} \langle v, \sqrt{-\Delta}v \rangle \leq \frac{\pi}{2} \langle v, \sqrt{-\Delta + 1}v \rangle.$$

Plus généralement, on a le théorème suivant:

Théorème 1.1. [25] Définissons l'opérateur C_α dans $\mathcal{S}(\mathbb{R}^N)$ par

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

et laissons $p^{-1} + q^{-1} = 1$. Supposons $\alpha > 0$ et $N\alpha^{-1} > p > 1$. Alors C_α s'étend en un opérateur borné sur $L^p(\mathbb{R}^N)$ avec

$$c_{\alpha,p} = \|C_\alpha\|_{L^p \rightarrow L^p} = 2^{-\alpha} \frac{\Gamma(\frac{1}{2}(Np^{-1} - \alpha)) \Gamma(\frac{1}{2}Nq^{-1})}{\Gamma(\frac{1}{2}(Nq^{-1} + \alpha)) \Gamma(\frac{1}{2}Np^{-1})} \quad (1.8)$$

Si $p \geq N\alpha^{-1}$ ou $p = 1$, alors C_α est illimité.

Le deuxième problème concerne le fait que le potentiel coulombien est à longue portée, c'est-à-dire qu'il ne diminue pas plus rapidement que r^{-d} où r est la distance et d est la dimensionnalité du système. Il est en effet nécessaire d'expliquer comment un très grand nombre d'électrons et de noyaux peuvent rester liés ensemble pour former des systèmes macroscopiques, bien que chaque particule interagisse avec beaucoup d'autres particules chargées en raison de la longue portée du potentiel d'interaction de Coulomb. C'est le Théorème de Stabilité de la Matière, qui fut d'abord prouvé par Dyson et Lenard, [39, 11], et puis, par une autre méthode par Lieb et Thirring (voir par exemple l'article [42]) et les références qu'il contient.

Ce problème est également lié à *la limite thermodynamique* pour des modèles d'approximation du système à N corps, par exemple, le modèle de Thomas-Fermi(-von-Weizsäcker) et le modèle de Hartree-Fock, [43, 9, 7, 8]. Grosso modo, la limite thermodynamique est la limite mathématique conjointe où

- le nombre de particules $M = N$ du système considéré tend vers l'infini;

- le volume occupé par la molécule considéré tend vers l'infini;
- la densité de particules $\rho = N/V$ du système considéré reste constante.

Par rapport à la limite thermodynamique, on obtient les modèles périodiques pour les cristaux, et le potentiel coulombien devient périodique. Le potentiel G coulombien périodique dans $Q := [-1/2, 1/2]^3$ est défini par

$$-\Delta G = 4\pi(-1 + \sum_{y \in \mathbb{Z}^3} \delta(\cdot - y)),$$

et

$$\int_Q G = 0.$$

G est en fait la fonction de Green de l'opérateur périodique sur Q . La série de Fourier de G est

$$G(x) = \frac{1}{\pi} \sum_{\substack{p \in \mathbb{Z}^3 \\ p \neq 0}} \frac{e^{2i\pi p \cdot x}}{|p|^2}.$$

G est borné sur Q sauf une singularité en $x = 0$, et

$$M = \lim_{x \rightarrow 0} G(x) - \frac{1}{|x|}$$

existe.

2 Régularité des solutions pour un système électronique et leurs applications à l'analyse numérique

En combinant l'opérateur de Schrödinger avec le système de potentiel coulombien, nous pouvons obtenir le modèle à N corps quantiques non-relativistes. Comme les noyaux sont plus lourds que les électrons, les électrons suivent presque instantanément leur mouvement. Par conséquent, il est habituel en chimie quantique et dans les domaines connexes de séparer le mouvement des noyaux de celui des électrons. Donc, nous avons l'opérateur hamiltonien de l'approximation de Born-Oppenheimer:

$$H = \sum_{i=1}^N \left(-\frac{1}{2} \Delta_i - V(x_i) \right) + \sum_{i < j}^N \frac{1}{|x_i - x_j|} \quad (2.1)$$

avec le potentiel

$$V(x_i) = \sum_{\nu=1}^K \frac{Z_\nu}{|x_i - a_\nu|}.$$

En physique et chimie quantique, deux problèmes sont intéressants. Le premier est l'étude des valeurs propres et les fonctions propres de cet opérateur

$$Hu = \lambda u. \quad (2.2)$$

En particulier, la fonction propre associée à la première valeur propre est l'état fondamental

$$\mathcal{E}(\Psi) = \inf \{ \langle \Psi, H\Psi \rangle ; \Psi \in \mathcal{W}_N \}; \quad (2.3)$$

avec

$$\mathcal{W}_N = \left\{ \Psi \in L^2((\mathbb{R}^3)^N; \mathbb{C}), \int_{\mathbb{R}^{3N}} |\Psi|^2 = 1, \int_{\mathbb{R}^{3N}} |\nabla \Psi|^2 < \infty \right\}.$$

Et le deuxième est le problème d'évolution par rapport au temps (le problème de Cauchy), surtout si les noyaux sont mobiles et dépendants du temps:

$$\begin{cases} i\partial_t u = H(t)u, & t \in [-a, a] = I_a, x = (x_1, \dots, x_N) \in (\mathbb{R}^3)^N \\ u(0, x) = u_0(x). \end{cases} \quad (2.4)$$

Ici,

$$H(t) = \sum_{j=1}^N -\Delta_j - \sum_{j=1}^N V(x_j, t) + \sum_{k < j}^N W(x_j, x_k).$$

où

$$V(x_j, t) = \sum_{\mu=1}^M \frac{Z_\mu}{|x_j - a_\mu(t)|} \quad (2.5)$$

et

$$W(x_k, x_j) = \frac{1}{|x_k - x_j|}. \quad (2.6)$$

Cependant, les avantages de la modélisation d'une molécule avec le modèle de Schrödinger s'évanouissent lorsqu'il s'agit d'effectuer des calculs réels à cause de sa grande dimensionnalité. En effet, pour un système à N électrons, on doit travailler dans $L^2(\mathbb{R}^{3N}; \mathbb{C})$. Donc, pour simuler des systèmes un peu plus grands, on utilise des modèles approchés.

En chimie quantique, pour les fermions indiscernables, les approximations du problème (2.3) sont schématiquement classées en deux catégories [37]:

La méthode de la fonction d'onde est utilisée de préférence par les chimistes, sur des petits systèmes, lorsque la précision est l'objectif principal et que le temps de calcul est un problème secondaire. Le plus connu est *le modèle de Hartree-Fock* et ses nombreuses variantes, extensions et successeurs. Le modèle Hartree-Fock est obtenu en restreignant l'énergie (2.3) aux fonctions qui sont égales à un unique déterminant de Slater

$$\Psi = \psi_1 \wedge \dots \wedge \psi_N, \quad \langle \psi_i, \psi_j \rangle = \delta_{ij},$$

où les ψ_1, \dots, ψ_N sont appelées *orbitales*. Alors, on a

$$\begin{aligned} \langle \Psi, H\Psi \rangle &= \sum_{i=1}^N \left\langle \left(-\frac{\Delta}{2} - V(x_i) \right) \psi_i, \psi_i \right\rangle + \frac{1}{2} \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{\rho_\Psi(x)\rho_\Psi(y)}{|x-y|} dx dy \\ &\quad - \frac{1}{2} \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{|\gamma_\Psi(x, y)|^2}{|x-y|} dx dy \\ &= \text{Tr}\left(\left(-\frac{\Delta}{2} - V(x_i)\right)\gamma_\Psi\right) + \frac{1}{2} \text{Tr}(W_\Psi \gamma_\Psi) \end{aligned} \quad (2.7)$$

où

$$W_{\Psi}\phi(x) = \rho_{\Psi} * \frac{1}{|x|} - \int_{\mathbb{R}^3} \frac{\gamma_{\Psi}(x, y)\phi(y)}{|x - y|} dy,$$

avec

$$\gamma_{\Psi}(x, y) = \sum_{i=1}^N \psi_i(x)\psi_i(y)^*; \quad \rho_{\Psi}(x) = \gamma_{\Psi}(x, x) = \sum_{i=1}^N |\psi_i(x)|^2.$$

La deuxième égalité de la formule (2.7) est l'expression de l'opérateur de densité. Et le terme dernier $\iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{|\gamma_{\Psi}(x, y)|^2}{|x - y|} dx dy$ est appelé *le terme d'échange*. Et le modèle sans terme d'échange est appelé *Hartree-Fock réduit*.

D'autre part, *la méthode de la théorie de la fonctionnelle de la densité* (DFT) est utilisé de préférence pour les grands systèmes (et au-delà pour la science des matériaux), lorsque le temps de calcul est important et que les méthodes de fonctions d'onde sont trop coûteuses. Ils consistent à reformuler le problème (2.3) en termes de densité électronique (1.3).

La contribution révolutionnaire qui a rendue la DFT un outil utile pour effectuer des calculs, est due à Kohn et Sham[35], qui ont introduit le modèle Kohn-Sham à la DFT. Il est similaire au modèle de Hartree-Fock où le terme d'échange est remplacé par une fonctionnelle d'échange-corrélation $E_{xc}(\rho_{\Psi})$, qui est obtenue à l'aide de données expérimentales [1].

Et pour le problème (2.4), la difficulté est renforcée par la prise en compte de la variable du temps: Les échelles de temps sont très différentes l'un l'autre. Par rapport à l'échelle de temps, les approximations sont classées en deux catégories principales: *la simulation adiabatique* et *la simulation non-adiabatique* [4]. Et l'approximation adiabatique consiste à supposer que pour chaque temps t , les fermions sont dans l'état fondamental. Sinon, c'est l'approximation non-adiabatique. Comme dans le problème (2.3), l'approximation non-adiabatique consiste en *le modèle de Hartree-Fock dépendant du temps* et *la théorie de la fonctionnelle dépendant du temps* (TDDFT).

A partir de 2004, H. Yserentant [59, 60, 61, 62, 63, 36] consiste à reconnaître (2.3) comme une équation différentielle partielle de grande dimension, et appliquer des techniques de produits tensoriels clairsemés pour approximer le problème (2.2). C'est la base de nos travaux dans cette partie. Donc, pour bien l'expliquer, on commence par décrire les travaux d'Yserentant.

2.1 Les travaux d'Yserentant

Rappelons que

$$\mathcal{I}_l = \{i | \sigma_i = l\}, \quad l = 1, \dots, s.$$

Par rapport à l'équation (1.1) pour les fermions, on observe que s'il existe un $l = 1, \dots, s$, $i, j \in \mathcal{I}_l$,

$$u(x_1, \dots, x_{i-1}, x_i, x_{i+1}, \dots, x_{j-1}, x_i, x_{j+1}, \dots, x_N) = 0.$$

Donc le principe de Pauli contrebalance les singularités de potentiel d'interaction entre électrons. Alors, Yserentant propose un opérateur relié au spin:

$$\mathcal{L}_{\mathcal{I}_l} = \prod_{i \in \mathcal{I}_k} (1 - \Delta_i)^{1/2}, \quad l = 1, \dots, s, \quad (2.8)$$

où Δ_i est l'opérateur aplacien du $i^{\text{ème}}$ fermion.

D'autre part, on a

Lemme 2.1. [59] *Pour toutes les fonctions lisses $v(x) \in C_0^\infty(\mathbb{R}^3)$ qui s'annulent à l'origine,*

$$\int \frac{|v|^2}{|x|^4} dx \leq 4 \int \frac{|\nabla v|^2}{|x|^2} dx.$$

Donc, combinant l'inégalité de Hardy avec le Théorème de Fubini, pour une fonction $u \in C_0^\infty(\mathbb{R}^3 \times \mathbb{R}^3)$, telle que $u(x, y) = -u(y, x)$, on a

$$\int_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{|u|^2}{|x - y|^4} dx dy \leq 16 \int_{\mathbb{R}^3 \times \mathbb{R}^3} |\nabla_x \otimes \nabla_y u|^2 dx dy.$$

Donc, on a

$$\left| \left(\mathcal{L}_{\mathcal{I}_l} \frac{u}{|x_i - a_\nu|}, \mathcal{L}_{\mathcal{I}_l} v \right) \right| \leq C \|\mathcal{L}_{\mathcal{I}_l} u\|_{L^2} \|\mathcal{L}_{\mathcal{I}_l} v\|_{\dot{H}^1},$$

et

$$\left| \left(\mathcal{L}_{\mathcal{I}_l} \frac{u}{|x_i - x_j|}, \mathcal{L}_{\mathcal{I}_l} v \right) \right| \leq C \|\mathcal{L}_{\mathcal{I}_l} u\|_{L^2} \|\mathcal{L}_{\mathcal{I}_l} v\|_{\dot{H}^1},$$

où

$$\|u\|_{\dot{H}^1}^2 = \|\nabla_i u\|_{L^2}^2 + \|\nabla_j u\|_{L^2}^2.$$

Le lien entre le potentiel coulombien et l'opérateur $\mathcal{L}_{\mathcal{I}_l}$ a été établi.

Donc, au lieu d'analyser le problème (2.2), on étudie l'équation

$$\mathcal{L}_{\mathcal{I}_l} H u = \lambda \mathcal{L}_{\mathcal{I}_l} u. \quad (2.9)$$

L'idée d'Yserentant est de diviser les fonctions propres en une partie de fréquence haute et une partie de fréquence basse et d'abord d'estimer la partie de fréquence haute par la partie de fréquence basse. Soit

$$\hat{u}_L = \mathbb{1}_{|\omega| \leq \Omega}(\hat{u})(\omega), \quad \hat{u}_H = \hat{u} - \hat{u}_L.$$

Evidemment $u_L \in C^\infty((\mathbb{R}^3)^N)$. Donc,

$$\mathbb{1}_{|\omega| \leq \Omega}(\mathcal{L}_{\mathcal{I}_l}(H - \lambda)u_H) = -\mathbb{1}_{|\omega| \leq \Omega} \left(\mathcal{L}_{\mathcal{I}_l} \left(\sum_{i=1}^N V(x_i) + \sum_{i < j}^N \frac{1}{|x_i - x_j|} \right) u_L \right),$$

et dans le cadre variationnel:

$$\langle \mathcal{L}_{\mathcal{I}_l}(H - \lambda)u_H, \mathcal{L}_{\mathcal{I}_l}v_H \rangle = - \left\langle \mathcal{L}_{\mathcal{I}_l} \left(\sum_{i=1}^N V(x_i) + \sum_{i < j}^N \frac{1}{|x_i - x_j|} \right) u_L, \mathcal{L}_{\mathcal{I}_l}v_H \right\rangle, \quad v_H \in X_{\mathcal{I}, H}^1, \quad (2.10)$$

où

$$X_{\mathcal{I}, H}^1 = \{v_H; \mathcal{L}_{\mathcal{I}_l}v_H \in H^1, \mathbb{1}_{|\omega| \leq \Omega}(v_H) = 0\}.$$

Soit $\theta(N, Z) = \sqrt{N} \max\{N, Z\}$ avec $Z = \sum_\nu Z_\nu$. Donc, on a

Théorème 2.2. [61] Si $\Omega > 4C\theta(N, Z)$ et $u_L \in \{v_L \in L^2; \mathbb{1}_{|\omega| \leq \Omega}(v_L) = v_L\}$, la solution $u_H \in H^1$ avec l'état de spin σ de l'équation (2.10) est contenue dans l'espace $X_{\mathcal{I}, H}^1$, et satisfait

$$\|\mathcal{L}_{\mathcal{I}_l} u_H\|_{L^2} \leq \sqrt{2} \|\mathcal{L}_{\mathcal{I}_l} u_L\|_{L^2}, \quad \|\nabla \mathcal{L}_{\mathcal{I}_l} u_H\|_{L^2} \leq \sqrt{2\Omega} \|\mathcal{L}_{\mathcal{I}_l} u_L\|_{L^2},$$

où $\nabla = (\nabla_1, \dots, \nabla_N)$ est le gradient pour tous les électrons.

Maintenant, soit

$$\mathcal{H}_1(R) = \left\{ (\omega_1, \dots, \omega_N) \in (\mathbb{R}^3)^N; \sum_{l=1}^s \prod_{i \in \mathcal{I}_l} \left(1 + \left| \frac{\omega_i}{\Omega} \right|^2 \right) \leq R^2 \right\}.$$

Et on introduit le projecteur

$$(P_{1,R}u)(x) = \int \mathbb{1}_{\mathcal{H}_1(R)}(\omega) \hat{u}(\omega) \exp(2\pi i \omega \cdot x) d\omega$$

avec $\mathbb{1}_{\mathcal{H}_1(R)}$ la fonction d'indicatrices du domaine $\mathcal{H}_1(R)$. On a ensuite les estimations d'erreur pour la norme L^2 et la semi-norme \dot{H}^1 .

Théorème 2.3. [61] Pour toutes les fonctions propres de valeurs propres négatives $u \in H^1$ avec l'état de spin σ ,

$$\|u - P_{1,R}u\|_{L^2} \leq \frac{\sqrt{es}}{R} \|u\|_{L^2}, \quad \|\nabla u - \nabla P_{1,R}u\|_{L^2} \leq \frac{\sqrt{es}}{R} \Omega \|u\|_{L^2}.$$

De plus, Yserentant a montré dans [62] que les régularités mixtes des fonctions d'onde décroissent de façon exponentielle dans le sens L^2 . En utilisant ces propriétés, on peut estimer [62] le taux de convergence de développement du type "sparse grid" de la fonction d'onde en produits tensoriels antisymétrisés d'une base de fonctions tridimensionnelles. Le résultat est surprenant compte tenu de la grande dimensionnalité de l'équation. Le taux de convergence de ces expansions est essentiellement le même pour N particules que le cas des s particules (s est le nombre d'état de spin).

Maintenant, le but ultime est d'avoir la même complexité que le cas d'une particule. Inspiré par [17, 27], Yserentant a montré que l'on peut atteindre presque la même complexité que dans le cas d'un électron en ajoutant un facteur simple de régularisation qui dépend explicitement des distances interélectroniques. Ces méthodes sont désignées comme *r12-méthodes* en chimie quantique. Par le facteur de régularisation et l'interpolation de Sobolev, Kreuzler et Yserentant [36] ont prouvé que pour les fonctions d'onde sans spin u , on a

$$\|\mathcal{L}_{\mathcal{I}_l}^\alpha u\|_{H^1} < \infty, \quad \forall 0 \leq \alpha < 3/4.$$

Ici, $\mathcal{I}_l = \{1, \dots, N\}$.

2.2 Les régularités mixtes optimales de système coulombien stationnaire

Dans cette partie, on améliore les travaux d'Yserentant, et on donne les régularités mixtes optimales pour tous les cas (fermions et bosons) à travers les inégalités de Herbst et de Hardy. Nous décrivons ici nos résultats [46] présentés au Chapitre 1.

Les états de spin de fermions peuvent être divisés en trois cas qui peuvent fournir des régularités différentes:

- (A) Chacune des deux particules a un état de spin différent: pour chaque $l \in \{1, \dots, s\}$, $|\mathcal{I}_l| \leq 1$, c'est-à-dire, $s = N$.
- (B) Certaines particules ont les mêmes états de spin tandis que d'autres ne les ont pas: il y a un $l \in \{1, \dots, s\}$, tel que $1 < |\mathcal{I}_l| < N$, c'est-à-dire, $1 < s < N$.
- (C) Les particules sont identiques: il existe un $l \in \{1, \dots, s\}$, tel que $\mathcal{I}_l = \{1, \dots, N\}$ et si $k \neq l$, $\mathcal{I}_k = \emptyset$, c'est-à-dire, $s = 1$.

En fait, le cas (A) indique que la fonction d'onde u est totalement non-antisymétrique; et le cas (B) indique que la fonction d'onde u possède une sorte de propriété antisymétrique; le cas (C) indique que la fonction d'onde u est totalement antisymétrique. En particulier, les bosons peuvent être vus mathématiquement comme un cas spécial de (A) car ils sont totalement non-antisymétriques.

Comme dans [59], on considère les fonctions tests sur l'espace des fonctions différentiables $\mathcal{D}_{\mathcal{I}}$

$$u : (\mathbb{R}^3)^N \rightarrow \mathbb{C} : (x_1, \dots, x_N) \rightarrow u(x_1, \dots, x_N)$$

à support compact avec les états de spin σ pris en considération. Et sa complétion sur L^2, H^1 est désignée par $L_{\mathcal{I}}^2, H_{\mathcal{I}}^1$ respectivement.

Pour le cas (B), on définit l'opérateur $\mathcal{L}_{\mathcal{I}, \alpha, \beta}$ par

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

Pour le cas (A) ou le cas (C), on définit un autre opérateur $\mathcal{L}_{\mathcal{I}, \alpha}$ par

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

Il peut être considéré comme un cas particulier d'opérateur $\mathcal{L}_{\mathcal{I}, \alpha, \beta}$: $s = 1, \mathcal{I}_l = \emptyset$ pour le cas (A); et pour le cas (C), $s = 1, \mathcal{I}_l = \{1, \dots, N\}$.

Maintenant, on introduit les espaces fonctionnels suivants $X_{\mathcal{I}, \alpha, \beta}$ et $X_{\mathcal{I}, \alpha}$ qui sont définis par

$$X_{\mathcal{I}, \alpha, \beta} := \{u, \mathcal{L}_{\mathcal{I}, \alpha, \beta} u \in H_{\mathcal{I}}^1\},$$

et

$$X_{\mathcal{I},\alpha} := \{u, \mathcal{L}_{\mathcal{I},\alpha}u \in H_{\mathcal{I}}^1\},$$

avec la norme

$$\|u\|_{\mathcal{I},\alpha,\beta} := \|\mathcal{L}_{\mathcal{I},\alpha,\beta}u\|_{H_{\mathcal{I}}^1},$$

et

$$\|u\|_{\mathcal{I},\alpha} := \|\mathcal{L}_{\mathcal{I},\alpha}u\|_{H_{\mathcal{I}}^1}.$$

Théorème 2.4. *Soit u la solution de problème (2.2) sous l'état de spin fixe σ , alors on a les résultats suivants:*

- Pour le cas (A),

$$u \in \bigcap_{0 \leq \beta < 0.75} X_{\mathcal{I},\beta}.$$

- Pour le cas (B),

$$u \in \bigcap_{\substack{0 \leq \alpha < 1.25, \\ 0 < \beta < 0.75, \\ \alpha + \beta < 1.5}} X_{\mathcal{I},\alpha,\beta}.$$

- Pour le cas (C),

$$u \in \bigcap_{0 \leq \alpha < 1.25} X_{\mathcal{I},\alpha}.$$

Maintenant, on étudie l'approximation correspondante.

Définition 2.5. • Pour le cas (A), si $0 \leq \beta < 0.75$, soit

$$\mathcal{H}_{\alpha,\beta}(R) := \left\{ (\omega_1, \dots, \omega_N) \in (\mathbb{R}^3)^N \mid \prod_{i=1}^N \left(1 + \left|\frac{\omega_i}{\Omega}\right|^2\right)^\beta \leq R^2 \right\}.$$

- Pour le cas (B), si $1 \leq \alpha < 1.25$ (ou $0 < \alpha < 0.75$), $0 < \beta < 0.75$ et $\alpha + \beta < 1.5$, soit

$$\mathcal{H}_{\alpha,\beta}(R) := \left\{ (\omega_1, \dots, \omega_N) \in (\mathbb{R}^3)^N \mid \sum_{l=1}^s \left(\prod_{i \in \mathcal{I}_l} \left(1 + \left|\frac{\omega_i}{\Omega}\right|^2\right)^\alpha \right) \left(\prod_{j \in \mathcal{I} \setminus \mathcal{I}_l} \left(1 + \left|\frac{\omega_j}{\Omega}\right|^2\right)^\beta \right) \leq R^2 \right\}.$$

- Pour le cas (C), si $1 \leq \alpha < 1.25$ (ou $0 \leq \alpha < 0.75$), soit

$$\mathcal{H}_{\alpha,\beta}(R) := \left\{ (\omega_1, \dots, \omega_N) \in (\mathbb{R}^3)^N \mid \prod_{i=1}^N \left(1 + \left|\frac{\omega_i}{\Omega}\right|^2\right)^\alpha \leq R^2 \right\}.$$

On définit le projecteur

$$(P_{\alpha,\beta,R}u)(x) = \int \mathbb{1}_{\mathcal{H}_{\alpha,\beta}(R)}(\xi) \hat{u}(\xi) \exp(2\pi i \xi \cdot x) d\xi$$

avec $\mathbb{1}_{\mathcal{H}_{\alpha,\beta}(R)}$ la fonction d'indicatrice du domaine $\mathcal{H}_{\alpha,\beta}(R)$.

Alors on a les estimations d'erreur suivantes pour la norme L^2 et la semi-norme \dot{H}^1 :

Théorème 2.6. *Sous la Définition 2.5, pour toutes les fonctions propres $u \in H^1$ avec l'état de spin fixe σ et la valeur propre λ négative ou nulle, il y a un Ω assez grand tel que*

$$\|u - P_{\alpha,\beta,R}u\|_{L^2((\mathbb{R}^3)^N)} \leq \frac{\sqrt{2s}}{R} e^{0.625} \|u\|_{L^2((\mathbb{R}^3)^N)},$$

et

$$\|\nabla(u - P_{\alpha,\beta,R}u)\|_{L^2((\mathbb{R}^3)^N)} \leq \frac{\sqrt{2s}}{R} e^{0.625} \Omega \|u\|_{L^2((\mathbb{R}^3)^N)}.$$

2.3 Les régularités mixtes de système coulombien dépendant du temps

Dans cette section nous continuons nos travaux sur les régularités mixtes des solutions d'un système à N corps. Maintenant, nous traitons le problème (2.4) avec les résultats obtenus dans le Chapitre 2. Et nous nous intéressons à son approximation.

Tout d'abord, au lieu d'analyser les potentiels V et W dans les équations (2.5) et (2.6), on considère un cas plus général:

Hypothèse 2.7. $V(x, t) \in \mathbb{R}^3 \times \mathbb{R}$ satisfait

$$V \in L_{t,\text{loc}}^{\alpha_q}(L^{q/(q-2)}(\mathbb{R}^3)) + L_{t,\text{loc}}^{\beta_q}(L^\infty(\mathbb{R}^3))$$

et $W(x_j, x_k, t) = w(x_i - x_k, t)$ avec $w \in \mathbb{R}^3 \times \mathbb{R}$ tel que

$$w \in L_t^{\alpha_p}(L^{p/(p-2)}(\mathbb{R}^3)) + L_t^{\beta_p}(L^\infty(\mathbb{R}^3)).$$

pour certaines p et q , tels que

$$2 \leq p, q < 6$$

et

$$\theta_{\alpha,\beta} > 0$$

avec

$$1/\theta_{\alpha,\beta} = \min\{3/p - 1/2 - 1/\alpha_p, 3/q - 1/2 - 1/\alpha_q, 1 - 1/\beta_p, 1 - 1/\beta_q\}. \quad (2.11)$$

Evidemment, les fonctions V et W données par les équations (2.5) et (2.6) satisfont cette hypothèse, avec par exemple $p = q = 4$ et $\alpha_p = \alpha_q = \beta_p = \beta_q = \infty$.

La première difficulté pour ce système est la complexité de l'espace fonctionnel. Soit

$$r_{i,j} = x_i - x_j, \quad D_{i,j} = x_i + x_j,$$

et

$$\mathcal{R}_{i,j}u(r_{i,j}, D_{i,j}, x_1, \dots, x_{i-1}, x_{i+1}, \dots, x_{j-1}, x_{j+1}, \dots, x_N) = u(x_1, \dots, x_N). \quad (2.12)$$

Alors, on définit l'espace fonctionnel $L_{x_i}^{p,2}$ par

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

avec la norme

$$\|u\|_{L_{x_i}^{p,2}}^p = \int_{\mathbb{R}_{x_i}^3} \left(\int_{(\mathbb{R}^3)^{N-1}} |u|^2 dx_1 \cdots \widehat{dx}_i \cdots dx_N \right)^{p/2} dx_i.$$

On l'abrège par $L_i^{p,2}$. Et on définit

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

avec la norme

$$\|u\|_{L_{i,j}^{p,2}}^p = \int_{\mathbb{R}_{r_{i,j}}^3} \left(\int_{(\mathbb{R}^3)^{N-1}} |\mathcal{R}_{i,j}u|^2 dD_{i,j} dx_1 \cdots \widehat{dx}_i \cdots \widehat{dx}_j \cdots dx_N \right)^{p/2} dr_{i,j}.$$

Evidemment, $\|u\|_{L_{i,j}^{p,2}} = \|\mathcal{R}_{i,j}u\|_{L_{i,j}^{p,2}}$.

Maintenant, on peut construire l'espace fonctionnel suivant:

$$X(T) = L_t^\infty([0, T], L^2) \bigcap_{i < j} L_t^{\theta_p}([0, T], L_{i,j}^{p,2}) \bigcap_k L_t^{\theta_q}([0, T], L_k^{q,2})$$

avec la norme

$$\|u\|_{X(T)} = \max_{\substack{1 \leq i < j \leq N \\ 1 \leq k \leq N}} \left\{ \|u\|_{L_t^\infty(L^2)}, \|u\|_{L_t^{\theta_p}(L_{i,j}^{p,2})}, \|u\|_{L_t^{\theta_q}(L_k^{q,2})} \right\},$$

où $2/\theta_p = 3(1/2 - 1/p)$ et $2/\theta_q = 3(1/2 - 1/q)$. Si $p, q = 2$, alors $\theta_p, \theta_q = +\infty$. Ici nous utilisons la notation abrégée $X = X(T)$ sans risque de confusion.

Donc, nous avons le premier résultat:

Théorème 2.8. *Sous l'hypothèse 2.7, l'équation (2.4) a une solution unique $u \in X(a)$, pour chaque $u_0 \in L^2((\mathbb{R}^3)^N)$.*

Et il y a une constante C ne dépendant que de p, q, V, W avec $1/\theta_{\alpha,\beta} > 0$, telle que pour T vérifiant la condition $CT^{1/\theta_{\alpha,\beta}} N(N+1) < 1/2$, on a

$$\|u\|_X \lesssim_{p,q} \|u_0\|_{L^2}.$$

Maintenant, définir l'opérateur

$$\mathcal{L}_{\mathcal{I}_l} = \bigotimes_{i \in \mathcal{I}_l} \nabla_i, \quad l = 1, \dots, s.$$

Et soit

$$1/\theta = \min\{3/(2p) + 3/(2\tilde{p}) - 1/2, 3/(2q) + 3/(2\tilde{q}) - 1/2\}.$$

Nous pouvons donc énoncer le résultat principal de la régularité:

Théorème 2.9. *Si u_0 possède l'état de spin fixe σ , $\mathcal{L}_{\mathcal{I}_l}u_0 \in L^2((\mathbb{R}^3)^N)$, $l = 1, \dots, s$, et $0 < \alpha < 1/2$, $\frac{6}{3-2\alpha} < p, q \leq 6$, la solution de l'équation (2.4) a une solution unique u avec le même état de spin que σ , et $\mathcal{L}_{\mathcal{I}_l}u \in X(a)$.*

Et il y a une constante C_1 ne dépendant que de $\alpha, \tilde{p}, p, \tilde{q}$ et q avec $\frac{6}{1+2\alpha} < \tilde{p}, \tilde{q} \leq 6$ et $1/\theta > 0$, telle que pour T vérifiant la condition $C_1(\sum_\mu Z_\mu + N)NT^{1/\theta} < 1/2$, on a

$$\|\mathcal{L}_{\mathcal{I}_l}u\|_{L_t^\infty(L^2)} \leq \|\mathcal{L}_{\mathcal{I}_l}u\|_X \lesssim_{p,q} \|\mathcal{L}_{\mathcal{I}_l}u_0\|_{L^2}.$$

Pour obtenir une approximation comme dans le Théorème 2.3, nous introduisons l'opérateur suivant

$$\mathcal{K}_{\mathcal{I}_l} = \prod_{j \in \mathcal{I}_l} (1 - \Delta_j)^{1/2}.$$

Maintenant, il nous faut prouver la régularité des solutions associée à l'opérateur $\mathcal{K}_{\mathcal{I}_l}$ au lieu de l'opérateur $\mathcal{L}_{\mathcal{I}_l}$. Cependant, à cause de la complexité de l'espace fonctionnel X , on a besoin des estimations pour l'opérateur $\mathcal{K}_{\mathcal{I}_l}$. En généralisant l'inégalité de Calderón-Zygmund dans l'annexe de Chapitre 2, on a le théorème suivant:

Théorème 2.10. *Si $1 < p < \infty$, alors les inégalités suivantes sont vrais:*

$$\|\nabla_i u\|_{L_i^{p,2}} \lesssim_p \|(1 - \Delta_i)^{1/2} u\|_{L_i^{p,2}}, \quad i = 1, \dots, N \quad (2.13a)$$

$$\|u\|_{L_i^{p,2}} \lesssim_p \|(1 - \Delta_i)^{1/2} u\|_{L_i^{p,2}}, \quad i = 1, \dots, N \quad (2.13b)$$

$$\|(1 - \nabla_i)u\|_{L_i^{p,2}} \lesssim_p \|(1 - \Delta_i)^{1/2} u\|_{L_i^{p,2}}, \quad i = 1, \dots, N \quad (2.13c)$$

$$\|\nabla_{i,j} u\|_{L_{i,j}^{p,2}} \lesssim_p \|(1 - \Delta_i)^{1/2} u\|_{L_{i,j}^{p,2}}, \quad i, j = 1, \dots, N \quad (2.13d)$$

$$\|u\|_{L_{i,j}^{p,2}} \lesssim_p \|(1 - \Delta_i)^{1/2} u\|_{L_{i,j}^{p,2}}, \quad i, j = 1, \dots, N \quad (2.13e)$$

$$\|(1 - \nabla_i)u\|_{L_{i,j}^{p,2}} \lesssim_p \|(1 - \Delta_i)^{1/2} u\|_{L_{i,j}^{p,2}}, \quad i = 1, \dots, N. \quad (2.13f)$$

En conséquence,

Théorème 2.11. *Si u_0 possède l'état de spin fixe σ , $\mathcal{K}_{\mathcal{I}_l} u_0 \in L^2((\mathbb{R}^3)^N)$, $l = 1, \dots, s$, et $0 < \alpha < 1/2$, $\frac{6}{3-2\alpha} < p, q \leq 6$, la solution de l'équation (2.4) a une solution unique u avec le même état de spin que σ , et $\mathcal{L}_{\mathcal{I}_l} u \in X(a)$.*

Et il y a une constante C_2 ($C_2 > C_1$) ne dépendant que de α , \tilde{p} , p , \tilde{q} et q avec $\frac{6}{1+2\alpha} < \tilde{p}, \tilde{q} \leq 6$ et $1/\theta > 0$, telle que pour T vérifiant la condition $C_2(\sum_{\mu} Z_{\mu} + N)NT^{1/\theta} < 1/2$, on a

$$\|\mathcal{K}_{\mathcal{I}_l} u\|_{L_i^{\infty}(L^2)} \leq \|\mathcal{K}_{\mathcal{I}_l} u\|_X \lesssim_{p,q} \|\mathcal{K}_{\mathcal{I}_l} u_0\|_{L^2}.$$

De façon analogue à Yserentant [61], on construit l'opérateur $P_{\chi,R}$ par

$$(P_{\chi,R}u)(x) = \left(\frac{1}{\sqrt{2\pi}}\right)^{3N} \int_{\omega \in (\mathbb{R}^3)^N} \chi_R(\omega) \hat{u}(\omega) \exp(i\omega \cdot x) d\omega.$$

où $\chi : (\mathbb{R}^3)^N \rightarrow [0, 1]$ est une fonction avec la valeur $\chi_R(\omega) = 1$ pour $\omega \in \mathcal{H}_3(R)$, et

$$\mathcal{H}_3(R) = \left\{ (\omega_1, \dots, \omega_N) \in (\mathbb{R}^3)^N \mid \sum_{1 \leq l \leq s} \prod_{i \in \mathcal{I}_l} (1 + |\omega_i|^2)^{1/2} \leq R \right\}.$$

Le plus simple cas de l'opérateur $P_{\chi,R}$ est le projecteur $\mathbb{1}_{\mathcal{H}_3(R)}(\omega)$.

Comme dans le Théorème 2.3, on a

Lemme 2.12. *Sous l'hypothèse de Théorème 2.11, on a*

$$\|u - P_{\chi,R}u\|_X \lesssim_{p,q} 1/R \sum_{1 \leq l \leq s} \|\mathcal{K}_{\mathcal{I}_l} u_0\|_{L^2}.$$

Etonnamment, nous avons directement une approximation pour le problème (2.4):

$$\begin{cases} i\partial_t u_R = H_R(u_R), & t \in [-a, a] = I_a, \quad x = (x_1, \dots, x_N) \in (\mathbb{R}^3)^N \\ u_R(0, x) = P_{\chi, R}(u_0)(x) \end{cases} \quad (2.14)$$

avec

$$H_R(u) = \sum_{j=1}^N -\Delta_j u - \sum_{j=1}^N \sum_{\mu=1}^M P_{\chi, R}(V(x_j, t)u) + \sum_{k < j}^N P_{\chi, R}(W(x_j, x_k)u).$$

Théorème 2.13. *Si u_0 possède l'état de spin fixe σ , $\mathcal{K}_{\mathcal{I}_l} u_0 \in L^2((\mathbb{R}^3)^N)$, $l = 1, \dots, s$, et $0 < \alpha < 1/2$, $\frac{6}{3-2\alpha} < p, q < 6$, alors la solution d'équation (2.14) a une solution unique u_R .*

Et il y a une constante C_3 ($C_3 > C_2$) ne dépendant que de α , \tilde{p} , p , \tilde{q} et q avec $\frac{6}{1+2\alpha} < \tilde{p}, \tilde{q} < 6$ et $1/\theta > 0$, telle que pour T vérifiant la condition $C_3(\sum_{\mu} Z_{\mu} + N)NT^{1/\theta} < 1/2$, on a

$$\|u - u_R\|_{L_t^\infty(L^2)} \leq \|u - u_R\|_X \lesssim_{p,q} 1/R \sum_{l=1}^s \|\mathcal{K}_{\mathcal{I}_l} u_0\|_{L^2}, \quad (2.15)$$

où u est la solution d'équation (2.4).

C'est un résultat surprenant, d'abord parce que le volume de $\mathcal{H}_3(R)$ est beaucoup plus petit que celui de $\mathcal{H}_1(R)$ pour le système stationnaire, mais aussi parce que l'on peut fournir directement une approximation.

Remarque 2.14. Comme l'opérateur $P_{\chi, R}$ est similaire au projecteur $P_{1, R}$ pour le système stationnaire, les méthodes numériques pour le problème (1.4) (voir par exemple [60, 22]) peuvent être appliquées au problème (2.14).

3 L'existence pour le modèle de Dirac-Fock dans les cristaux

En chimie quantique relativiste, la théorie exacte est l'électrodynamique quantique, mais il s'agit d'une théorie très complexe et des approximations sont nécessaires si l'on veut pouvoir faire des calculs. Le modèle de Dirac-Fock est une de ces approximations: voir [48] pour une justification physique, et [3, 2] pour une étude mathématique de cette justification.

Donc, au lieu d'analyser les régularités mixtes de problèmes relativistes, on étudie le problème Dirac-Fock. L'énergie de Dirac-Fock peut aussi s'obtenir directement à partir de celle du modèle de Hartree-Fock non-relativiste, en remplaçant l'opérateur de Schrödinger par l'opérateur de Dirac. Cela donne

$$\begin{aligned} \mathcal{E}(\Psi) &= \sum_{i=1}^N \langle (D_0 - V(x_i)) \psi_i, \psi_i \rangle + \frac{\alpha}{2} \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{\rho_{\Psi}(x) \rho_{\Psi}(y)}{|x - y|} dx dy \\ &\quad - \frac{\alpha}{2} \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{\text{Tr}_4(\gamma_{\Psi}(x, y) \gamma_{\Psi}(y, x))}{|x - y|} dx dy \\ &= \text{Tr}((D_0 - V(x_i)) \gamma_{\Psi}) + \frac{\alpha}{2} \text{Tr}(W_{\Psi} \gamma_{\Psi}) \end{aligned} \quad (3.1)$$

$$W_{\Psi}\phi(x) = \rho_{\Psi} * \frac{1}{|x|} - \int_{\mathbb{R}^3} \frac{\gamma_{\Psi}(x, y)\phi(y)}{|x - y|} dy,$$

avec

$$\gamma_{\Psi}(x, y) = \sum_{i=1}^N (\psi_i(x), \psi_i(y)); \quad \rho_{\Psi}(x) = \gamma_{\Psi}(x, x) = \sum_{i=1}^N \psi_i(x) \otimes \psi_i^*(y).$$

et

$$\int_{\mathbb{R}^3} \psi_i^* \psi_j = \delta_{i,j}.$$

Notons que $\psi \in H^{1/2}(\mathbb{R}^3, \mathbb{C}^4)$, et que Tr_4 est la trace de la matrice 4×4 .

Son équation d'Euler-Lagrange est

$$H_{\Psi}\psi_k := D_0 - V(x)\psi_k + \alpha W_{\Psi}\psi_k = \lambda_k \psi_k, \quad k = 1, \dots, N, \quad (3.2)$$

et

$$\Psi = (\psi_1, \dots, \psi_N).$$

où $\lambda_k, k = 1, \dots, N$ sont des multiplicateurs de Lagrange associés à ces contraintes. Et pour simplifier le modèle, on prend

$$V(x) = \frac{\alpha Z}{|x|}.$$

Comme $\sigma(D_0) = (-\infty, -1] \cup [+1, +\infty)$, la borne inférieure de la fonctionnelle (3.1) est $-\infty$. En physique, le problème intéressant est la recherche de valeurs propres positives. Donc, nous nous intéressons à la théorie des points critiques pour résoudre l'équation (3.2) avec les valeurs propres dans $[0, 1)$. Pour le problème (3.2), l'existence d'une infinité de solutions avec les valeurs propres dans $[0, 1)$ a été étudiée par MJ. Esteban et E. Séré [14], et sous des hypothèse plus générales par E. Patrel [49]. Dans [13], MJ. Esteban et E. Séré ont prouvé que la première solution de l'équation (3.2) converge vers le minimiseur de Hartree-Fock dans la limite $\alpha \rightarrow 0$ avec N, Z fixe. En conséquence, il est naturel de définir l'état fondamental du modèle de Dirac-Fock par la formule:

$$E = \min_{\substack{0 \leq \gamma \leq P_{\gamma}^+ \\ \text{Tr}_{L^2}(\gamma) = N}} \mathcal{E}(\gamma). \quad (3.3)$$

Autrement dit, l'état fondamental de Dirac-Fock minimise l'énergie de Dirac-Fock parmi les états qui se trouvent dans le sous-ensemble de spectre positif. Par le point fixe, M. Huber et H. Siedentop [29] ont obtenu un résultat pour le problème (3.3). Finalement, E. Séré [53] a proposé une rétraction nouvelle, et a analysé directement le problème (3.3).

Maintenant, grâce au travail [53], on étudie l'existence de solutions pour le modèle de Dirac-Fock pour les cristaux. Cependant, il nous faut d'abord mentionner le modèle de Hartree-Fock pour les cristaux.

3.1 Le modèle de Hartree-Fock pour les cristaux

Dans le réduction de la limite thermodynamique aux modèles de Hartree-Fock, I. Catto, C. Le Bris et P.L. Lions [7] ont proposé un modèle de Hartree-Fock pour les cristaux.

Ici on considère le modèle sur la cellule élémentaire $Q_l = [-\frac{l}{2}, \frac{l}{2}]^3$. Pour les modèles de cristaux, notamment les modèles périodiques, il nous faut considérer la décomposition de Bloch, qui indique que les états propres d'énergie pour un électron peuvent être écrits comme des ondes de Bloch. Donc, par la décomposition de Floquet on a la cellule duale du réseau $Q_l^* = [-\frac{\pi}{l}, \frac{\pi}{l}]^3$, et $L^2(Q_l) = \frac{l^3}{(2\pi)^3} \int_{Q_l^*}^{\oplus} L_{\xi}^2(Q_l) d\xi$, où pour chaque $\xi \in Q_l^*$,

$$L_{\xi}^2(Q_l) = \{u \in L_{\text{loc}}^2(\mathbb{R}^3); e^{-i\xi \cdot x} u \text{ est } Q_l\text{-périodique}\}.$$

On a besoin de la définition suivante:

Définition 3.1 (Définition de \mathcal{K}). Considérons les familles d'opérateurs auto-adjoints γ_{ξ} sur $L_{\xi}^2(Q_l)$ satisfaisant les propriétés suivantes, pour presque chaque $\xi \in Q_l^*$:

$$(H2') \quad 0 \leq \gamma_{\xi} \leq \mathbb{1}_{L_{\xi}^2(Q_l)};$$

$$(H3) \quad \text{l'opérateur } \gamma_{\xi} \text{ possède une trace finie et satisfait } \frac{l^3}{(2\pi)^3} \int_{Q_l^*} \text{Tr}_{L_{\xi}^2(Q_l)} \gamma_{\xi} d\xi < \infty;$$

$$(H4) \quad \text{Tr}_{L_{\xi}^2(Q_l)}(-\Delta_{\xi} \gamma_{\xi}) < +\infty \text{ et } \frac{l^3}{(2\pi)^3} \int_{Q_l^*} \text{Tr}_{L_{\xi}^2(Q_l)}(-\Delta_{\xi} \gamma_{\xi}) d\xi < +\infty.$$

Une telle famille des opérateurs est associée, d'une manière unique, à un opérateur auto-adjoint γ dans $L^2(\mathbb{R}^3)$, défini par $\gamma := \frac{l^3}{(2\pi)^3} \int_{Q_l^*}^{\oplus} \gamma_{\xi} d\xi$, tel que

$$(H1) \quad \gamma \text{ commute avec les translations de } l\mathbb{Z}^3;$$

$$(H2) \quad 0 \leq \gamma \leq \mathbb{1}_{L^2}.$$

On note par \mathcal{K} l'ensemble d'opérateurs $\gamma = \frac{l^3}{(2\pi)^3} \int_{Q_l^*}^{\oplus} \gamma_{\xi} d\xi$ qui satisfont les conditions (H2'),(H3) et (H4), et nous appellerons γ un opérateur de densité Q_l -périodique.

Définition 3.2. Soit γ appartenant à \mathcal{K} . Alors on peut définir d'une manière unique une densité Q_l -périodique ρ_{γ} associée à γ par

$$\rho_{\gamma}(x) = \frac{l^3}{(2\pi)^3} \int_{Q_l^*} \gamma_{\xi}(x, x) d\xi. \quad (3.4)$$

L'état fondamental de la modèle de Hartree-Fock pour les cristaux est

$$I^{HF} = \inf\{\mathcal{E}^{HF}(\gamma); \gamma \in \mathcal{K}, \text{Tr } \gamma = Z\}, \quad (3.5)$$

de plus

$$\begin{aligned} & \mathcal{E}^{HF}(\gamma) \\ &= \frac{l^3}{(2\pi)^3} \int_{Q_l^*} \text{Tr}_{L_{\xi}^2}(-\Delta_{\xi} \gamma_{\xi}) d\xi - \alpha Z \int_{Q_l} G_l(x) \rho_{\gamma}(x) dx + \frac{\alpha}{2} \iint_{Q_l^2} \rho_{\gamma}(x) G_l(x-y) \rho_{\gamma}(y) dx dy \\ & \quad - \frac{\alpha}{2} \frac{l^6}{(2\pi)^6} \iint_{(Q_l^*)^2} d\xi d\xi' \iint_{Q_l^2} [\gamma_{\xi}(x, y) \gamma_{\xi'}(y, x)] W_l^{\infty}(\xi - \xi', x - y) dx dy, \end{aligned} \quad (3.6)$$

où

$$G_l(x) = \frac{1}{\pi l} \sum_{\substack{p \in \mathbb{Z}^3 \\ p \neq 0}} \frac{e^{\frac{2i\pi}{l} p \cdot x}}{|p|^2},$$

et pour le terme d'échange

$$W_l^\infty(\eta, x) := \frac{4\pi}{l^3} \sum_{k \in \mathbb{Z}^3} \frac{1}{\left| \frac{2\pi k}{l} - \eta \right|} e^{i\left(\frac{2\pi k}{l} - \eta\right) \cdot x} = \lambda W_{\lambda l}^\infty\left(\frac{\eta}{\lambda}, \lambda x\right), \quad x, \eta \in \mathbb{R}^3.$$

Remarque 3.3. $\gamma(\cdot, \cdot)$ appartient à $L^2(Q_l \times \mathbb{R}^3)$ et pour le terme d'échange on a également

$$\begin{aligned} & \frac{l^6}{(2\pi)^6} \iint_{(Q_l^*)^2} d\xi d\xi' \iint_{Q_l^2} [\gamma_\xi(x, y) \gamma_{\xi'}(y, x)] W_l^\infty(\xi - \xi', x - y) dx dy \\ &= \int_{Q_l} \int_{\mathbb{R}^3} \frac{(\gamma(x, y) \gamma(y, x))}{|x - y|} dy. \end{aligned}$$

Théorème 3.4. [7] *Le problème de minimisation (3.5) admet un minimum.*

De plus,

Théorème 3.5. [20] *Supposons que $Z > 0$ et $N = Z$ et soit γ le minimiseur de (3.5). Alors γ résout l'équation nonlinéaire suivante:*

$$\begin{cases} \gamma = \mathbb{1}_{(-\infty, \nu)}(H_\gamma) + \epsilon \mathbb{1}_{\{\nu\}}(H_\gamma), \\ (H_\gamma)_\xi = -\Delta_\xi - ZG_l + \rho_\gamma * G_l - \frac{l^3}{(2\pi)^3} \int_{Q_l^*} W_l^\infty(\xi' - \xi, x - y) \gamma_{\xi'}(x, y) d\xi', \end{cases}$$

où $\epsilon \in \{0, 1\}$ et $\nu \in \mathbb{R}$ est un multiplicateur de Lagrange associé à la contrainte de charge $\int_{Q_l} \rho_\gamma = Z$.

3.2 Le modèle de Dirac-Fock pour les cristaux

Maintenant, on présente les résultats pour le modèle de Dirac-Fock pour les cristaux du Chapitre 3 qui ont été obtenus en collaboration avec I. Catto, E. Paturel et E. Séré.

En s'inspirant de la relation entre le modèle de Dirac-Fock et le modèle de Hartree-Fock, on construit le modèle Dirac-Fock pour les cristaux de la même manière. C'est-à-dire que l'on remplace l'opérateur $-\Delta_\xi$ par D_ξ dans le modèle de Hartree-Fock pour les cristaux. Donc, l'énergie de la fonctionnelle de Dirac-Fock périodique est

$$\begin{aligned} & \mathcal{E}^{DF}(\gamma) \\ &= \frac{l^3}{(2\pi)^3} \int_{Q_l^*} \text{Tr}_{L_\xi^2}(D_\xi \gamma_\xi) d\xi - \alpha Z \int_{Q_l} G_l(x) \rho_\gamma(x) dx + \frac{\alpha}{2} \iint_{Q_l^2} \rho_\gamma(x) G_l(x - y) \rho_\gamma(y) dx dy \\ & \quad - \frac{\alpha}{2} \frac{l^6}{(2\pi)^6} \iint_{(Q_l^*)^2} d\xi d\xi' \iint_{Q_l^2} \text{Tr}_4[\gamma_\xi(x, y) \gamma_{\xi'}(y, x)] W_l^\infty(\xi - \xi', x - y) dx dy. \end{aligned} \tag{3.7}$$

De plus, l'opérateur de Dirac-Fock périodique est

$$D_{\gamma,\xi} := D_\xi - \alpha Z G_l + V_{\gamma,\xi}$$

avec

$$V_{\gamma,\xi} = \alpha \rho_\gamma * G_l(x) - \alpha W_{\gamma,\xi}$$

où

$$\rho_\gamma * G_l(x) = \int_{Q_l} G_l(y-x) \rho_\gamma(y) dy = \text{Tr}_{L^2(Q_l)}(G_l(\cdot-x)\gamma)$$

et

$$W_{\gamma,\xi} \psi_\xi(x) = \frac{l^3}{(2\pi)^3} \int_{Q^*} d\xi' \int_Q W_l^\infty(\xi' - \xi, x-y) \gamma_{\xi'}(x,y) \psi_\xi(y) dy.$$

Par la Définition 3.1, on a :

Définition 3.6 (Définition de \mathcal{T}). Considérons les familles d'opérateurs auto-adjoints γ_ξ sur $L_\xi^2(Q_l)$ satisfaisant les propriétés suivantes, pour presque chaque $\xi \in Q_l^*$:

(H6') $0 \leq \gamma_\xi \leq \mathbb{1}_{L_\xi^2(Q_l)}$;

(H7) l'opérateur γ_ξ possède une trace finie et satisfait $\frac{l^3}{(2\pi)^3} \int_{Q_l^*} \text{Tr}_{L_\xi^2(Q_l)} \gamma_\xi d\xi < \infty$;

(H8) $\text{Tr}_{L_\xi^2(Q_l)}(|D_\xi| \gamma_\xi) < +\infty$ et $\frac{l^3}{(2\pi)^3} \int_{Q_l^*} \text{Tr}_{L_\xi^2(Q_l)}(|D_\xi| \gamma_\xi) d\xi < +\infty$.

Une telle famille d'opérateurs est associée, d'une manière unique, à un opérateur auto-adjoint γ dans $L^2(\mathbb{R}^3)$, défini par $\gamma := \frac{l^3}{(2\pi)^3} \int_{Q_l^*}^\oplus \gamma_\xi d\xi$, tel que

(H5) γ commute avec les translations de $l\mathbb{Z}^3$;

(H6) $0 \leq \gamma \leq \mathbb{1}_{L^2}$.

On note par \mathcal{T} l'ensemble d'opérateurs $\gamma = \frac{l^3}{(2\pi)^3} \int_{Q_l^*}^\oplus \gamma_\xi d\xi$ qui satisfont les conditions (H6'),(H7) et (H8), et nous appellerons γ un opérateur de densité Q_l -périodique.

Correspondant à cette définition, on a l'espace fonctionnel suivant pour les opérateurs de densité Q_l -périodique:

•

$$\sigma_1(\xi) = \left\{ \gamma_\xi \in \mathcal{B}(L_\xi^2(Q_l^*)); \text{Tr}_{L_\xi^2}(|\gamma_\xi|) < \infty \right\}$$

avec la norme

$$\|\gamma_\xi\|_{\sigma_1(\xi)} = \text{Tr}_{L_\xi^2}(|\gamma_\xi|),$$

•

$$\sigma_{1,1} = \left\{ \gamma; \gamma = \frac{l^3}{(2\pi)^3} \int_{Q_l^*}^\oplus \gamma_\xi d\xi, (\gamma_\xi)_{\xi \in Q_l^*} \in \mathcal{T}, \int_{Q_l^*} \|\gamma_\xi\|_{\sigma_1(\xi)} d\xi < \infty \right\}$$

avec la norme

$$\|\gamma\|_{\sigma_{1,1}} = \frac{l^3}{(2\pi)^3} \int_{Q_l^*} \|\gamma_\xi\|_{\sigma_1(\xi)} d\xi,$$

•

$$X = \left\{ \gamma; \gamma = \frac{l^3}{(2\pi)^3} \int_{Q_l^*}^{\oplus} \gamma_\xi d\xi, (\gamma_\xi)_{\xi \in Q_l^*} \in \mathcal{T}, \int_{Q_l^*} \| |D_\xi|^{1/2} \gamma_\xi |D_\xi|^{1/2} \|_{\sigma_1(\xi)} d\xi < \infty \right\},$$

avec la norme

$$\|\gamma\|_X = \frac{l^3}{(2\pi)^3} \int_{Q_l^*} \| |D_\xi|^{1/2} \gamma_\xi |D_\xi|^{1/2} \|_{\sigma_1(\xi)} d\xi.$$

Enfin, soit

$$P_{\gamma, \xi}^\pm := \mathbb{1}_{\mathbb{R}_\pm}(D_{\gamma, \xi}), \quad P_\gamma^\pm = \frac{l^3}{(2\pi)^3} \int_{Q_l^*}^{\oplus} P_{\gamma, \xi}^\pm d\xi,$$

et

$$P_\gamma^\pm \gamma' = \int_{Q_l^*}^{\oplus} P_{\gamma, \xi}^\pm \gamma'_\xi d\xi.$$

Maintenant, on définit

$$\Gamma_N := \left\{ \gamma \in \mathcal{T}; \int_{Q_l} \rho_\gamma(x) dx = N \right\},$$

et

$$\Gamma_N^+ := \{ \gamma \in \Gamma_N; P_\gamma^- \gamma = 0 \}.$$

Par [13] et [53], l'état fondamental de Dirac-Fock de cristaux est

$$I := \inf \{ \mathcal{E}^{DF}(\gamma); \gamma \in \Gamma_N^+ \}.$$

Pour le potentiel G_l on a les inégalités suivantes:

Lemme 3.7. *Il existe de constantes $C_H > 0$, $C'_H > 0$ et C_G , telles que, pour chaque $\xi \in Q_l^*$ et chaque $\psi_\xi \in H_\xi^{1/2}(Q_l; \mathbb{C}^4)$, on a:*

$$(\psi_\xi, G_l \psi_\xi)_{L^2(Q_l)} \leq C_H (\psi_\xi, |D_\xi| \psi_\xi)_{Q_l}, \quad (3.8a)$$

$$(\psi_\xi, |G_l| \psi_\xi)_{L^2(Q_l)} \leq C'_H (\psi_\xi, |D_\xi| \psi_\xi)_{Q_l}, \quad (3.8b)$$

De plus, il existe de constante $C_G \geq C'_H > 0$, telle que, pour chaque $\xi \in Q_l^$ et chaque $\phi_\xi \in H_\xi^1(Q_l; \mathbb{C}^4)$, on a:*

$$\|G_l \phi_\xi\|_{L^2(Q_l)} \leq C_G \| |D_\xi| \phi_\xi \|_{L_\xi^2(Q_l)}. \quad (3.8c)$$

Pour le potentiel W_l^∞ , on a

Lemme 3.8. *Il existe de constantes C_W, C'_W, C''_W , telles que, pour chaque $\xi \in Q_l^*$ et chaque $\psi_\xi \in H_\xi^{1/2}(Q_l; \mathbb{C}^4)$, on a:*

• soit $\gamma \in X$,

$$\|W_{\gamma, \xi} \psi_\xi\|_{L_\xi^2} \leq C_W \max\{\|\gamma\|_X, 1\} \|\psi_\xi\|_{L_\xi^2}. \quad (3.9)$$

• soit $\gamma \in \sigma_{1,1}$,

$$\|W_{\gamma, \xi} \psi_\xi\|_{L_\xi^2} \leq C'_W \max\{\|\gamma\|_{\sigma_{1,1}}, 1\} \| |D_\xi| \psi_\xi \|_{L_\xi^2} \quad (3.10)$$

On a besoin de quelques conditions pour obtenir leur existence:

Hypothèse 3.9. Soit $N^+ := \max\{N, 1\}$, $\kappa := \alpha((C'_H(Z + N) + C'_W N^+))$, $C_{EE} := C'_H + C'_W$, $A > 1/4\alpha(1 - \kappa)^{-2}(1 + \kappa)C_{EE}$, et

$$c^*(k) := \sup_{\xi \in Q_i^*} \inf_{\substack{\dim V = k \\ V \subset \Lambda_\xi^+ H_\xi^{1/2}}} \sup_{u_\xi^+ \in V} \frac{\| |D_\xi|^{1/2} u_\xi^+ \|_{L_\xi^2}}{\| u_\xi^+ \|_{L_\xi^2}}$$

on suppose que

1. $\kappa < 1 - 1/2\alpha C_{EE} N^+$,
2. $\kappa' := \alpha(C'_G(Z + N) + C'_W N^+) < 1$,
3. $A \sqrt{\max\{(1 - \kappa - 1/2\alpha C_{EE} N^+)^{-1}(1 - \kappa)^{-1} c^*(N + 1)N, 1\}} N^+ < 1$.

Théorème 3.10. *Sous l'Hypothèse 3.9, il existe un minimiseur $\gamma_* \in \Gamma_N^+$ tel que*

$$\mathcal{E}^{DF}(\gamma_*) = I := \min_{\gamma \in \Gamma_N^+} \mathcal{E}^{DF}(\gamma). \quad (3.11)$$

En outre, γ_* résout l'équation auto-cohérente suivante:

$$\begin{cases} \gamma = \mathbb{1}_{[0, \nu)}(D_\gamma) + \delta \\ D_\gamma = \frac{l^3}{(2\pi)} \int_{Q_i^*}^\oplus d\xi D_{\gamma, \xi}, \end{cases} \quad (3.12)$$

où $0 \leq \delta \leq \mathbb{1}_{\{\nu\}}(D_\gamma)$ et $0 \leq \nu \leq c^*(N + 1)(1 - \kappa)^{-1}$.

Remarque 3.11. En physique du solide, la longueur de la cellule unitaire est d'environ quelques Angströms. Et dans le système d'unités, $\hbar = m = c = 1$, on a $\alpha \approx \frac{1}{137}$ et $l \approx 1000$. Sous la condition $Z = N$ pour la neutralité électronique, on trouve que l'Hypothèse 3.9 est satisfaite pour $N \leq 4$.

Part I

The mixed regularity for Coulomb potential

Chapter 1

A note about the mixed regularity of Schrödinger Coulomb system

In this note, by extending the Herbst's inequality we prove some inequalities for Coulomb-type potential which can be used in the proof of the optimal mixed regularity of Schrödinger Coulomb system directly even in consideration of Pauli exclusion principle. And by analogy with [61], we deduced the estimates of the errors for L^2 -norm and H^1 -semi-norm.

1 Introduction and results

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

$$H = -\frac{1}{2} \sum_{i=1}^N \Delta_i - V_{ne} + V_{ee} \quad (1.1)$$

with

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

and

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

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

Mathematically, the electronic ground state or excited state problem can be expressed by the Euler-Lagrange equation which is indeed the eigenvalues problems of the

operator (1.1):

$$Hu = \lambda u. \quad (1.2)$$

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

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

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

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

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

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

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

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

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

Problem (1.2) is well-explored mathematically (see for example [30], and about the regularity properties of the eigenfunction of problem (1.2) [31, 28, 16, 27, 17, 26, 18]). However, the advantage of this model vanishes when it comes to performing real calculation because of its large dimensionality. Thus models such as Hartree-Fock and Kohn-Sham are proposed, see for example [38]. However they are no true, unbiased discretizations of the Schrödinger equation in the sense of numerical analysis.

Decades ago, H. Yserentant [59, 61, 63, 36] proposed a mixed regularity about the eigenfunctions of problem (1.2), and this result can help to break the complexity barriers in computational quantum mechanics. For fixed spin state σ , he split the particles into the subset q parts with the same spin states

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

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

$$u(P_{i,j}x, \sigma) = -u(x, \sigma). \quad (1.3)$$

herein $P_{i,j}$ is a permutation which only exchange the space coordinate x_i and x_j . If $x_i = x_j$, $u(x) = 0$. Thus the eigenfunctions can counterbalance the singularity of the

interaction potential between electrons. Based on this observation, H. Yserentant proved in [59, 61] that the eigenfunction u of problem (1.2) under spin state σ satisfies

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

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

Later, by using $r12$ -methods and interpolation of Sobolev space, H.C. Kreuzler and H. Yserentant [63, 36] proved that the eigenfunction u of problem (1.2) without the spin state satisfies

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

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

But what is the optimal mixed regularities in consideration of the spin states? And could we provide an error estimate for its approximation based on this regularity? In this note, we are trying to answer these questions.

The spin state can be divided into three cases which can provide different regularities:

- (A) Any two particles have different spin states: for any $l \in \{1, \dots, q\}$, $|\mathcal{I}_l| \leq 1$, i.e., $q = N$.
- (B) Some particles have the same spin states while the others do not: there exists a $l \in \{1, \dots, q\}$, such that $1 < |\mathcal{I}_l| < N$, i.e., $1 < q < N$.
- (C) The particles are identical: there exists a $l \in \{1, \dots, q\}$, such that $\mathcal{I}_l = \{1, \dots, N\}$ and if $k \neq l$, $\mathcal{I}_k = \emptyset$, i.e., $q = 1$.

Indeed, the case (A) means that the eigenfunction u is totally non-anti-symmetric (for any $i, j \in \{1, \dots, N\}$, the equation (1.3) does not hold); and the case (B) means the eigenfunction u has some kind of anti-symmetric property (for some $l \in \{1, \dots, q\}$ and any $i, j \in \mathcal{I}_l$, the equation (1.3) holds); and the case (C) means that the eigenfunction u is totally anti-symmetric (for any $i, j \in \{1, \dots, N\}$, the equation (1.3) holds);

Similar to [59], we consider the test functions in $\mathcal{D}_{\mathcal{I}}$ which is the space of the infinite differentiable functions

$$u : (\mathbb{R}^3)^N \rightarrow \mathbb{C} : (x_1, \dots, x_N) \rightarrow u(x_1, \dots, x_N)$$

having a bounded support with spin states taken into consideration. And its completion in L^2, H^1 is denoted by $L_{\mathcal{I}}^2, H_{\mathcal{I}}^1$ respectively.

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

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

where ∇_i is the gradient for the coordinate x_i . This operator is defined by the Fourier transform, for details see Section 2. And the higher derivative parts is because of the anti-symmetry of eigenfunction u .

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

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

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

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

$$X_{\mathcal{I},\alpha,\beta} := \{u, \mathcal{L}_{\mathcal{I},\alpha,\beta}u \in H_{\mathcal{I}}^1\},$$

and

$$X_{\mathcal{I},\alpha} := \{u, \mathcal{L}_{\mathcal{I},\alpha}u \in H_{\mathcal{I}}^1\},$$

endowed with the norm

$$\|u\|_{\mathcal{I},\alpha,\beta} := \|\mathcal{L}_{\mathcal{I},\alpha,\beta}u\|_{H_{\mathcal{I}}^1},$$

and

$$\|u\|_{\mathcal{I},\alpha} := \|\mathcal{L}_{\mathcal{I},\alpha}u\|_{H_{\mathcal{I}}^1}.$$

Theorem 1.1. *Let u be the solution of the eigenvalue problems of operator 1.2 under the fixed spin state σ , then we have the following results:*

- For the case (A),

$$u \in \bigcap_{0 \leq \beta < 0.75} X_{\mathcal{I},\beta}.$$

- For case (B),

$$u \in \bigcap_{\substack{0 \leq \alpha < 1.25, \\ 0 < \beta < 0.75, \\ \alpha + \beta < 1.5}} X_{\mathcal{I},\alpha,\beta}.$$

- For case (C),

$$u \in \bigcap_{0 \leq \alpha < 1.25} X_{\mathcal{I},\alpha}.$$

Definition 1.2. • For the case (A), if $0 \leq \beta < 0.75$, let

$$\mathcal{H}_{\alpha,\beta}(R) := \left\{ (\omega_1, \dots, \omega_N) \in (\mathbb{R}^3)^N \mid \prod_{i=1}^N \left(1 + \left|\frac{\omega_i}{\Omega}\right|^2\right)^\beta \leq R^2 \right\}.$$

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

$$\mathcal{H}_{\alpha,\beta}(R) := \left\{ (\omega_1, \dots, \omega_N) \in (\mathbb{R}^3)^N \mid \sum_{l=1}^q \left(\prod_{i \in \mathcal{I}_l} \left(1 + \left|\frac{\omega_i}{\Omega}\right|^2\right)^\alpha \right) \left(\prod_{j \in \mathcal{I} \setminus \mathcal{I}_l} \left(1 + \left|\frac{\omega_j}{\Omega}\right|^2\right)^\beta \right) \leq R^2 \right\}.$$

- For the case (C), if $1 \leq \alpha < 1.25$ (or $0 \leq \alpha < 0.75$), let

$$\mathcal{H}_{\alpha,\beta}(R) := \left\{ (\omega_1, \dots, \omega_N) \in (\mathbb{R}^3)^N \mid \prod_{i=1}^N \left(1 + \left| \frac{\omega_i}{\Omega} \right|^2 \right)^\alpha \leq R^2 \right\}.$$

Now we define the projector

$$(P_{\alpha,\beta,R}u)(x) = \int \chi_R(\xi) \hat{u}(\xi) \exp(2\pi i \xi \cdot x) \, d\xi$$

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

Then we have the following norm convergence rate:

Theorem 1.3. *Under the Definition 1.2, for all eigenfunctions $u \in H^1$ with fixed spin state σ and λ non-positive, and for Ω large enough, we have*

$$\|u - P_{\alpha,\beta,R}u\|_{L^2((\mathbb{R}^3)^N)} \leq \frac{\sqrt{2q}}{R} e^{0.625} \|u\|_{L^2((\mathbb{R}^3)^N)},$$

and

$$\|\nabla(u - P_{\alpha,\beta,R}u)\|_{L^2((\mathbb{R}^3)^N)} \leq \frac{\sqrt{2q}}{R} e^{0.625} \Omega \|u\|_{L^2((\mathbb{R}^3)^N)}.$$

2 Fractional Laplacian and related inequalities

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

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

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

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

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

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

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

If we apply the Fourier transform to solve the Poisson equation

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

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

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

In principle, we need the restriction $0 < \alpha < d$ because when $\alpha \geq d$ the multiplier $|k|^{-\alpha}$ does not define a tempered distribution (for more details, see for example [55]).

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

$$b_\alpha \mathcal{F}(|\cdot|^{-\alpha})(\xi) = b_{d-\alpha} |\xi|^{-d+\alpha}, \quad b_\alpha = \pi^{-\alpha/2} \Gamma(\alpha/2), \quad (2.1)$$

(see for example [41]). Hence, if $0 < \alpha < d$, the operator $|\nabla|^\alpha$ can be represented by

$$|\nabla|^{-\alpha} u(x) = \frac{b_{d-\alpha}}{(2\pi)^\alpha b_\alpha} \int_{\mathbb{R}^d} |x-y|^{-d+\alpha} u(y) dy. \quad (2.2)$$

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

$$|\nabla|^\alpha |x|^{-\beta} = \frac{(2\pi)^\alpha b_{\alpha+\beta} b_{d-\beta}}{b_{d-\alpha-\beta} b_\beta} |x|^{-\alpha-\beta}. \quad (2.3)$$

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

$$|\nabla|^{-\alpha} |x|^{-\beta} = \frac{b_{\beta-\alpha} b_{d-\beta}}{(2\pi)^\alpha b_{d+\alpha-\beta} b_\beta} |x|^{\alpha-\beta}. \quad (2.4)$$

However, in this note, we need to deal with the term $|\nabla|^{\pm\alpha}(|x|^{-\beta}u)$. The first and most important result about it is the famous Herbst's inequality which is based on the Formula (2.2):

Theorem 2.1. [25] Define the operator C_α on $\mathcal{S}(\mathbb{R}^d)$ by

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

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

$$\|C_\alpha\|_{\mathcal{B}(L^p(\mathbb{R}^d))} = 2^{-\alpha} \frac{\Gamma(\frac{1}{2}(dp^{-1} - \alpha)) \Gamma(\frac{1}{2}dq^{-1})}{\Gamma(\frac{1}{2}(dq^{-1} + \alpha)) \Gamma(\frac{1}{2}dp^{-1})} \quad (2.5)$$

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

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

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

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

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

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

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

and

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

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

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

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

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

namely

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

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

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

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

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

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

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

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

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

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

Proof. Notice that

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

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

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

Herein $\xi := (\xi_x, \xi_y)$, and ξ_x, ξ_y are the frequency with respect to x and y respectively.

As $|t|^\alpha \leq |t|^{\alpha+\beta} + 1$ for $t \in \mathbb{R}$, and let $t = |\xi_x|/|\xi_y|$, we yield

$$|\xi_x|^{-\alpha} |\xi_y|^{-\beta} \leq |\xi_x|^{-\alpha-\beta} + |\xi_y|^{-\alpha-\beta}. \quad (2.6)$$

Thus,

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

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

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

Thus,

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

Analogously,

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

Consequently, we deduce that

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

namely,

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

□

If $u \in C_0^\infty(\mathbb{R}^3 \setminus \{0\})$, for $\alpha > d/2$, we have the following Hardy's type inequality which is the generalization of [59, Lemma 2] with a similar proof:

Lemma 2.6. [47] *If $u \in C_0^\infty(\mathbb{R}^3 \setminus \{0\})$, then*

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

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

And the the potential of the interaction between electrons:

Corollary 2.7. [47] *If $u \in C_0^\infty(\mathbb{R}^{3\times 3})$ with $u(x,y) = -u(y,x)$ for $x,y \in \mathbb{R}^3$. Then we have the following inequality:*

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

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

Combining the Lemma 2.5 with the Corollary 2.7, we have

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

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

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

3 Properties of the interaction potentials

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

3.1 Nucleus-electron interaction potential

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

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

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

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

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

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

Now we get the conclusion. □

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

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

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

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

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

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

Then,

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

And

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

Now we get

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

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

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

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

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

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

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

Thus,

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

□

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

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

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

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

Thus,

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

By Lemma 3.2, we get

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

and

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

Consequently,

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

□

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

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

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

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

Now, the main estimate in this subsection is

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

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

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

$$\begin{aligned} & \left\langle (1 + |\nabla|^2)^{\alpha/2} \frac{u}{|x - a_\nu|}, (1 + |\nabla|^2)^{\alpha/2} v \right\rangle \\ & = \left\langle \mathcal{K} \frac{u}{|x - a_\nu|}, (1 + |\nabla|^2)^{\alpha/2} v \right\rangle + \left\langle |\nabla|^\alpha \mathcal{K} \frac{u}{|x - a_\nu|}, (1 + |\nabla|^2)^{\alpha/2} v \right\rangle. \end{aligned} \quad (3.1)$$

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

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

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

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

And as

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

by Lemma 3.1, we know that

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

For the other part, obviously

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

Thus,

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

For the second term in the right-hand side of equation (3.1), by Hölder's inequality again

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

And we have that

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

By Corollary 3.4,

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

Consequently,

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

□

3.2 Electron-electron interaction potential

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

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

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

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

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

where $c_1 = 4$. By virtue of Formula (2.1) and as $\mathcal{F}(f(\cdot + z))(\xi) = e^{2\pi i z \cdot \xi} \mathcal{F}(f)(\xi)$, we obtain that for $0 < t < 3$,

$$\mathcal{F} \left(\frac{u(x, y)}{|x-y|^t} \right) (\xi_x, \xi_y) = \frac{b_{3-t}}{b_t} \int_{\mathbb{R}^3} \frac{\mathcal{F}(u)(\xi_x - l, \xi_y + l)}{|l|^{3-t}} dl. \quad (3.2)$$

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

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

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

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

Using the Formula (3.2) again, for the first term, we get

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

By Lemma 2.5, we obtain

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

For the second term, similarly

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

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

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

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

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

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

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

□

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

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

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

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

with

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

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

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

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

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

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

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

Now,

$$\begin{aligned} & \left\langle (1 + |\nabla_x|^2)^{\alpha/2} (1 + |\nabla_y|^2)^{\beta/2} |x - y|^{-1} u, (1 + |\nabla_x|^2)^{\alpha/2} (1 + |\nabla_y|^2)^{\beta/2} v \right\rangle \\ &= \left\langle (1 + |\nabla_x|^\alpha) (1 + |\nabla_y|^\beta) \mathcal{K}_{\alpha,x} \mathcal{K}_{\beta,y} |x - y|^{-1} u, (1 + |\nabla_x|^2)^{\alpha/2} (1 + |\nabla_y|^2)^{\beta/2} v \right\rangle \\ &= \left\langle \mathcal{K}_{\alpha,x} \mathcal{K}_{\beta,y} |x - y|^{-1} u, (1 + |\nabla_x|^2)^{\alpha/2} (1 + |\nabla_y|^2)^{\beta/2} v \right\rangle \\ & \quad + \left\langle (|\nabla_x|^\alpha + |\nabla_y|^\beta) \mathcal{K}_{\alpha,x} \mathcal{K}_{\beta,y} |x - y|^{-1} u, (1 + |\nabla_x|^2)^{\alpha/2} (1 + |\nabla_y|^2)^{\beta/2} v \right\rangle \\ & \quad + \left\langle |\nabla_x|^\alpha |\nabla_y|^\beta \mathcal{K}_{\alpha,x} \mathcal{K}_{\beta,y} |x - y|^{-1} u, (1 + |\nabla_x|^2)^{\alpha/2} (1 + |\nabla_y|^2)^{\beta/2} v \right\rangle \end{aligned} \quad (3.3)$$

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

Steps 1. *For the first term.*

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

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

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

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

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

Steps 2. *For the second term.*

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

We have that

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

By Lemma 3.1,

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

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

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

Thus,

$$\|\nabla_x^{|\alpha-1|} |x-y|^{-1} u\|_{L^2(\mathbb{R}^{3 \times 3})} \leq C_{\alpha-1} \|\nabla_x^\alpha u\|_{L^2(\mathbb{R}^{3 \times 3})}.$$

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

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

Consequently,

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

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

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

Thus,

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

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

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

We have that

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

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

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

thus

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

Now, we yield

$$\begin{aligned} & \left| \left\langle |\nabla_x|^\alpha |\nabla_y|^\beta \mathcal{K}_{\alpha,x} \mathcal{K}_{\beta,y} |x-y|^{-1} u, (1+|\nabla_x|^2)^{\alpha/2} (1+|\nabla_y|^2)^{\beta/2} v \right\rangle \right| \\ & \leq \left\| |\nabla_x|^{\alpha+\beta-1} |x-y|^{-1} u \right\|_{L^2(\mathbb{R}^{3 \times 3})} (\|\nabla_x v\|_{\alpha,\beta} + \|\nabla_y v\|_{\alpha,\beta}). \end{aligned} \tag{3.4}$$

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

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

And by Lemma 2.5,

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

If $\alpha + \beta \geq 1$, then by Lemma 3.6 we get

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

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

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

Steps 4. For the last term with anti-symmetry.

For $\alpha = 1$, it has been proved in [59], with

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

Thus,

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

If $\alpha > 1$, we have that

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

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

$$\begin{aligned} & \left| \left\langle |\nabla_x|^\alpha |\nabla_y|^\alpha \mathcal{K}_{\alpha,x} \mathcal{K}_{\alpha,y} |x-y|^{-1} u, (1 + |\nabla_x|^2)^{\alpha/2} (1 + |\nabla_y|^2)^{\alpha/2} v \right\rangle \right| \\ & \leq 1/2 \left\| |\nabla_x|^{\alpha-1/2} |\nabla_y|^{\alpha-1/2} |x-y|^{-1} u \right\|_{L^2(\mathbb{R}^{3 \times 3})} (\| |\nabla_x v \|_{\alpha,\alpha} + \| |\nabla_y v \|_{\alpha,\alpha}). \end{aligned} \tag{3.5}$$

Notice that

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

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

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

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

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

Thus,

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

For the second term,

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

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

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

Hence,

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

And,

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

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

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

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

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

Consequently, if $\alpha > 1$,

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

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

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

Steps 5. Conclusion.

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

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

with

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

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

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

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

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

□

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

Proof. By estimate (3.4), we only need

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

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

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

As $u \in C_0^\infty(\mathbb{R}^{3 \times 3})$, by cusp analysis, $u(r_1, r_2) \sim \mathcal{O}(r_1/|r_1|)$ and $|r_1|^{-1}u \sim \mathcal{O}(|r_1|^{-1})$ when $|r_1| \rightarrow 0$. And $|\nabla_x|^{\alpha+\beta-1} = |\nabla_1 + \nabla_2|^{\alpha+\beta-1} \sim |\nabla_1|^{\alpha+\beta-1}$ as $|r_1| \rightarrow 0$. Consequently, in a neighborhood of $|r_1| = 0$ small enough, by Formula (2.3)

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

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

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

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

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

Thus, if $\alpha \geq 1.25$,

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

□

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

3.3 For the Coulomb system

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

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

Obviously,

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

And recall that

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

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

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

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

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

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

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

Consequently,

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

Now, we need to consider the different cases: (A)-(C). For case (B), if $i, j \in \mathcal{I}_l$, u satisfies the equation (1.3). And for $1 \leq \alpha < 1.25$ (or $0 < \alpha < 0.75$), by Lemma 3.7,

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

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

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

And if $i, j \notin \mathcal{I}_l$, for $0 < \beta < 0.75$,

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

Finally, we yield

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

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

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

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

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

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

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

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

Now we conclude:

Lemma 3.10. • For case (A), if $0 < \beta < 0.75$,

$$\begin{aligned} & |\langle \mathcal{L}_{\mathcal{I},\beta} (V_{ne} + V_{ee}) u, \mathcal{L}_{\mathcal{I},\beta} v \rangle| \\ & \leq (C'_{\beta,\beta} Z + D'_{\beta,\beta} N) N^{1/2} \|\mathcal{L}_{\mathcal{I},\beta} u\|_{L^2((\mathbb{R}^3)^N)} \|\nabla \mathcal{L}_{\mathcal{I},\beta} v\|_{L^2((\mathbb{R}^3)^N)}. \end{aligned} \tag{3.6}$$

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

$$\begin{aligned} & |\langle \mathcal{L}_{\mathcal{I},\alpha,\beta}(V_{ne} + V_{ee})u, \mathcal{L}_{\mathcal{I},\alpha,\beta}v \rangle| \\ & \leq (C'_{\alpha,\beta}Z + D'_{\alpha,\beta}N)N^{1/2} \|\mathcal{L}_{\mathcal{I},\alpha,\beta}u\|_{L^2((\mathbb{R}^3)^N)} \|\nabla \mathcal{L}_{\mathcal{I},\alpha,\beta}v\|_{L^2((\mathbb{R}^3)^N)}. \end{aligned} \quad (3.7)$$

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

$$\begin{aligned} & |\langle \mathcal{L}_{\mathcal{I},\alpha}(V_{ne} + V_{ee})u, \mathcal{L}_{\mathcal{I},\alpha}v \rangle| \\ & \leq (C'_{\alpha,\alpha}Z + D'_{\alpha,\alpha}N)N^{1/2} \|\mathcal{L}_{\mathcal{I},\alpha}u\|_{L^2((\mathbb{R}^3)^N)} \|\nabla \mathcal{L}_{\mathcal{I},\alpha}v\|_{L^2((\mathbb{R}^3)^N)}. \end{aligned} \quad (3.8)$$

4 The Regularity of Solutions

Repeating the proof in [61], we split the eigenfunctions into the high-frequency part and the low frequency part and then we will show that the high-frequency part can be dominated by the low frequency part. Let P_Ω be the projector to the high frequency part, with

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

where

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

And let

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

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

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

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

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

Decomposing u into u_H and u_L , we have

$$\begin{aligned} & \langle \mathcal{L}_{\mathcal{I},\alpha,\beta}(H - \lambda)u_H, \mathcal{L}_{\mathcal{I},\alpha,\beta}v_H \rangle \\ & = 1/2 \langle \nabla \mathcal{L}_{\mathcal{I},\alpha,\beta}u_H, \nabla \mathcal{L}_{\mathcal{I},\alpha,\beta}v_H \rangle + \langle \mathcal{L}_{\mathcal{I},\alpha,\beta}(V_{ne} + V_{ee})u_H, \mathcal{L}_{\mathcal{I},\alpha,\beta}v_H \rangle \\ & \quad - \lambda \langle \mathcal{L}_{\mathcal{I},\alpha,\beta}u_H, \mathcal{L}_{\mathcal{I},\alpha,\beta}v_H \rangle \\ & = \langle \mathcal{L}_{\mathcal{I},\alpha,\beta}(V_{ne} + V_{ee})u_L, \mathcal{L}_{\mathcal{I},\alpha,\beta}v_H \rangle. \end{aligned} \quad (4.1)$$

Let

$$\Omega \geq (2\pi)^{-1} (C'_{\alpha,\beta}Z + D'_{\alpha,\alpha}N)N^{1/2} \geq 1, \quad (4.2)$$

then

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

As the eigenvalues of problem 1.2 are negatives, therefore we have the coercivity

$$\langle \mathcal{L}_{\mathcal{I},\alpha,\beta}(H - \lambda)u_H, \mathcal{L}_{\mathcal{I},\alpha,\beta}u_H \rangle \geq 1/8 \|u_H\|_{\mathcal{I},\alpha,\beta}^2, \quad (4.3)$$

the continuity

$$|\langle \mathcal{L}_{\mathcal{I},\alpha,\beta}(H - \lambda)u_H, \mathcal{L}_{\mathcal{I},\alpha,\beta}v_H \rangle| \leq \|u_H\|_{\mathcal{I},\alpha,\beta} \|v_H\|_{\mathcal{I},\alpha,\beta}, \quad (4.4)$$

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

$$|\langle \mathcal{L}_{\mathcal{I},\alpha,\beta}(V_{ne} + V_{ee})\psi, \mathcal{L}_{\mathcal{I},\alpha,\beta}v_H \rangle| \leq (C'_{\alpha,\beta}Z + D'_{\alpha,\beta}N)N^{1/2} \|\mathcal{L}_{\mathcal{I},\alpha,\beta}\psi\|_{L^2((\mathbb{R}^3)^N)} \|v_H\|_{\mathcal{I},\alpha,\beta}, \quad (4.5)$$

And now, we prove the regularity of the eigenfunctions.

Sketch Proof of the Theorem 1.1. This proof is similar to the proof in [59, 63]. So we just give the sketch of proof, and only consider the case (B), the proof of other cases is same. Now, we prove the theorem under the condition on α and β in Lemma 3.10, and then by Sobolev's interpolation, we get the conclusion.

Step 1. For the frequency bounds Ω as in (4.2), the equation

$$\langle \mathcal{L}_{\mathcal{I},\alpha,\beta}(H - \lambda)u_H, \mathcal{L}_{\mathcal{I},\alpha,\beta}v_H \rangle = \langle \mathcal{L}_{\mathcal{I},\alpha,\beta}(V_{ne} + V_{ee})\psi, \mathcal{L}_{\mathcal{I},\alpha,\beta}v_H \rangle, \quad \forall v_H \in P_\Omega X_{\mathcal{I},\alpha,\beta} \quad (4.6)$$

possesses a unique solution $u_H \in P_\Omega X_{\mathcal{I},\alpha,\beta}$ for all given functions $\psi \in X_{\mathcal{I},\alpha,\beta}$ by using the Lax-Milgram theorem, and by the estimate (4.3) and the estimate (3.7) for ψ .

Step 2. For the frequency bounds Ω as in (4.2), the equation

$$\langle (H - \lambda)u_H, \chi_H \rangle = \langle (V_{ne} + V_{ee})\psi, \chi_H \rangle, \quad \forall \chi_H \in P_\Omega H^1 \quad (4.7)$$

possesses a unique solution $u_H \in P_\Omega X_{\mathcal{I},\alpha,\beta}$ for all given functions $\psi \in H^1$, see [59, 61].

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

By Fourier transform, we have

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

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

Step 4. We rewrite the equation (4.6) as

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

And by the step 3, we know the solution of equation (4.6) satisfies the original equation (4.7) for all $\chi_H \in P_\Omega H^1$. Hence for all $\mathcal{L}_{\mathcal{I},\alpha,\beta}\psi \in L^2$, by the uniqueness of solution, we yield that the solution of problem (4.7) $u_H \in X_{\mathcal{I},\alpha,\beta}$.

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

5 Numerical analysis

In this part, we study the hyperbolic cross space approximation. Without loss of generality, we only consider the case (B). We need to modify the operator $\mathcal{I}_{\mathcal{I},\alpha,\beta}$ by operator $\mathcal{I}_{\mathcal{I},\alpha,\beta,\tau}$ defined below and give some estimates based on the new operator.

Define operator $\mathcal{L}_{\mathcal{I},\alpha,\beta,\tau}$ by

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

Before explaining the main ingredient in this section, we need the following estimate:

Lemma 5.1. *For case (B), if $1 \leq \alpha < 1.25$ (or $0 < \alpha < 0.75$), $0 < \beta < 0.75$ and $\alpha + \beta < 1.5$,*

$$\begin{aligned} & |\langle \mathcal{L}_{\mathcal{I},\alpha,\beta,\tau}(V_{ne} + V_{ee})u, \mathcal{L}_{\mathcal{I},\alpha,\beta,\tau}v \rangle| \\ & \leq (C'_{\alpha,\beta}Z + D'_{\alpha,\beta}N)N^{1/2} \|\mathcal{L}_{\mathcal{I},\alpha,\beta,\tau}u\|_{L^2((\mathbb{R}^3)^N)} \|\nabla \mathcal{L}_{\mathcal{I},\alpha,\beta,\tau}v\|_{L^2((\mathbb{R}^3)^N)}. \end{aligned} \quad (5.1)$$

Proof. Let $u_\tau(x) := \tau^{-3N/2}u(\tau^{-1}x)$, $v_\tau(x) := \tau^{-3N/2}v(\tau^{-1}x)$. And let

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

By inequality (3.7), we know that

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

As $(V_{ne}^\tau u_\tau)(x) = \tau^{-3N/2-1}(V_{ne}u)(\tau^{-1}x)$ and $(V_{ee}u_\tau)(x) = \tau^{-3N/2-1}(V_{ee}u)(\tau^{-1}x)$, by the property of scaling, we yield that

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

On the other hand,

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

We get conclusion. \square

Analogously to (4.1), we consider the variational problem:

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

Mimicking the proof of estimates (4.3) and (4.5), for $\Omega \geq (2\pi)^{-1}(C'_{\alpha,\beta}Z + D'_{\alpha,\alpha}N)N^{1/2}$, we have that

$$\langle \mathcal{L}_{\mathcal{I},\alpha,\beta,\tau}(H - \lambda)u_H, \mathcal{L}_{\mathcal{I},\alpha,\beta,\tau}u_H \rangle \geq 1/8 \|\mathcal{L}_{\mathcal{I},\alpha,\beta,\tau}u_H\|_{H^1_{\mathcal{I}}((\mathbb{R}^3)^N)},$$

and

$$\begin{aligned} & |\langle \mathcal{L}_{\mathcal{I},\alpha,\beta,\tau}(V_{ne} + V_{ee})u_L, \mathcal{L}_{\mathcal{I},\alpha,\beta,\tau}v_H \rangle| \\ & \leq (C'_{\alpha,\beta}Z + D'_{\alpha,\alpha}N)N^{1/2} \|\mathcal{L}_{\mathcal{I},\alpha,\beta,\tau}u_L\|_{L^2((\mathbb{R}^3)^N)} \|\mathcal{L}_{\mathcal{I},\alpha,\beta,\tau}v_H\|_{H^1_{\mathcal{I}}((\mathbb{R}^3)^N)}, \end{aligned}$$

Now we get

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

Thus,

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

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

$$\|\mathcal{L}_{\mathcal{I},\alpha,\beta,\tau}u_H\|_{L^2((\mathbb{R}^3)^N)} \leq \sqrt{2} \|\mathcal{L}_{\mathcal{I},\alpha,\beta,\tau}u_L\|_{L^2((\mathbb{R}^3)^N)}, \quad (5.2)$$

and

$$\|\nabla \mathcal{L}_{\mathcal{I},\alpha,\beta,\tau}u_H\|_{L^2} \leq \sqrt{2}\Omega \|\mathcal{L}_{\mathcal{I},\alpha,\beta,\tau}u_L\|_{L^2}. \quad (5.3)$$

We take the following norm:

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

and

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

Lemma 5.2. *For scaling parameters $\Omega \geq 2\pi^{-1}(C'_{\alpha,\beta}Z + D'_{\alpha,\alpha}N)N^{1/2}$ large enough, the eigenfunction $u \in X_{\mathcal{I},\alpha,\beta}$ satisfies the estimates*

$$\|u\|_{\mathcal{I},\alpha,\beta,0} \leq \sqrt{2qe^{0.625}} \|u\|_{L^2((\mathbb{R}^3)^N)}, \quad \|u\|_{\mathcal{I},\alpha,\beta,1} \leq \sqrt{2qe^{0.625}} \|u\|_{L^2((\mathbb{R}^3)^N)}.$$

Proof. The proof is similar with [61, Theorem 9]. By estimate (5.2) and let $\tau = 2\pi\Omega$, then

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

with

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

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

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

Thus,

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

Finally,

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

The other case can be repeated equally. \square

Proof of Theorem 2.6. Thus, we know that

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

And for the other term,

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

\square

Chapter 2

Regularity of many body evolution Schrodinger equation and its application to numerical analysis

A decade ago, the mixed regularity of stationary many-body Schrödinger equation has been studied by Harry Yserentant through the Pauli Principle and the Hardy inequality (Uncertainty Principle). In this article, we prove that the many-body evolution Schrödinger equation has a similar mixed regularity if the initial data u_0 satisfies the Pauli Principle. By generalization of the Strichartz estimates, our method also applies to the numerical approximation of this problem: based on these mixed derivatives, we design a new approximation which can hugely improve the computing capability especially in quantum chemistry.

1 Introduction

In this article, we study the existence, mixed regularity and its application to numerical analysis of the following evolution Schrödinger equation:

$$\begin{cases} i\partial_t u = H(t)u, & t \in [-a, a] = I_a, x = (x_1, \dots, x_N) \in (\mathbb{R}^3)^N \\ u(0, x) = u_0(x) \end{cases} \quad (1.1)$$

with

$$H(t) = \sum_{j=1}^N -\Delta_j - \sum_{j=1}^N \sum_{\mu=1}^M V(x_j, t) + \sum_{k < j}^N W(x_j, x_k).$$

where

$$V(x_j, t) = \sum_{\mu=1}^M \frac{Z_\mu}{|x_j - a_\mu(t)|} \quad (1.2)$$

and

$$W(x_i, x_j) = \frac{1}{|x_i - x_j|}. \quad (1.3)$$

In physics and chemistry, this equation is used to describe the quantum mechanical many-body problem in which the electrons and nuclei interact by Coulomb attraction and repulsion forces. It acts on the functions with variables $x_1, \dots, x_N \in \mathbb{R}^3$, the coordinates of given N electrons. The atom μ is positioned at $a_\mu(t) \in \mathbb{R}^3$ dependently on time with the charge Z_μ .

1.1 The Existence of Solution

At the beginning, instead of studying these given potentials V and W , we consider a more general case:

Assumption 1.1. $V(x, t) \in \mathbb{R}^3 \times \mathbb{R}$ satisfies

$$V \in L_{t,\text{loc}}^{\alpha_q}(L^{q/(q-2)}(\mathbb{R}^3)) + L_{t,\text{loc}}^{\beta_q}(L^\infty(\mathbb{R}^3))$$

and $W(x_j, x_k, t) = w(x_i - x_k, t)$ with $w \in \mathbb{R}^3 \times \mathbb{R}$ satisfies

$$w \in L_t^{\alpha_p}(L^{p/(p-2)}(\mathbb{R}^3)) + L_t^{\beta_p}(L^\infty(\mathbb{R}^3)).$$

for some p and q , such that

$$2 \leq p, q < 6$$

and

$$\theta_{\alpha,\beta} > 0$$

with

$$1/\theta_{\alpha,\beta} = \min\{3/p - 1/2 - 1/\alpha_p, 3/q - 1/2 - 1/\alpha_q, 1 - 1/\beta_p, 1 - 1/\beta_q\}. \quad (1.4)$$

Obviously, the case V and W in Equation (1.2) satisfies this Assumption, with $p = q = 4$ and $\alpha_p = \alpha_q = \beta_p = \beta_q = \infty$.

In the last century, for the one particle case which means $N = 1$ and $W = 0$, the evolution Schrödinger equation $i\partial_t u = H(t)u$ was well developed, see [51, 54]. In the case when $H(t) = H_0$ is independent of t and selfadjoint, the Stone theorem guarantees the existence and uniqueness of the unitary group $U_0(t, s) = \exp(-i(t - s)H_0)$ such that $U_0 H^2(\mathbb{R}^N) \subset H^2(\mathbb{R}^N)$. In 1987, Yajima [56] proved the time-dependent case by Duhamel formula and Strichartz estimate, and then the Schrödinger equation with magnetic field [57]. And it is until this century that the existence of one kind of many-body Schrödinger equation was proved, also by Yajima, see [58]. Inspired by his works, we find out another way to prove the existence of the many-body Schrödinger evolution equation, which is in fact equivalent to the method of Yajima, but much easier to deal with the regularity of the Coulombic potential.

Let

$$r_{i,j} = x_i - x_j, \quad D_{i,j} = x_i + x_j,$$

and

$$\mathcal{R}_{i,j}u(r_{i,j}, D_{i,j}, x_1, \dots, x_{i-1}, x_{i+1}, \dots, x_{j-1}, x_{j+1}, \dots, x_N) = u(x_1, \dots, x_N). \quad (1.5)$$

Then, define the functional space

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

with the norm

$$\|u\|_{L_{x_i}^{p,2}}^p = \int_{\mathbb{R}_{x_i}^3} \left(\int_{(\mathbb{R}^3)^{N-1}} |u|^2 dx_1 \cdots \widehat{dx_i} \cdots dx_N \right)^{p/2} dx_i.$$

We shorten it by $\|u\|_{L_i^{p,2}}$, and define

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

with the norm

$$\|u\|_{L_{i,j}^{p,2}}^p = \int_{\mathbb{R}_{d_{i,j}}^3} \left(\int_{(\mathbb{R}^3)^{N-1}} |\mathcal{R}_{i,j}u|^2 dD_{i,j} dx_1 \cdots \widehat{dx_i} \cdots \widehat{dx_j} \cdots dx_N \right)^{p/2} dr_{i,j}.$$

The notation $\widehat{dx_i}$ means that the integration over the i^{th} coordinate is omitted. Obviously, $\|u\|_{L_{i,j}^{p,2}} = \|\mathcal{R}_{i,j}u\|_{L_{d_{i,j}}^{p,2}}$.

Then we introduce the following functional space:

$$X(T) = L_t^\infty([0, T], L^2) \bigcap_{i < j} L_t^{\theta_p}([0, T], L_{i,j}^{p,2}) \bigcap_k L_t^{\theta_q}([0, T], L_k^{q,2})$$

with the norm

$$\|u\|_{X(T)} = \max_{\substack{1 \leq i < j \leq N \\ 1 \leq k \leq N}} \left\{ \|u\|_{L_t^\infty(L^2)}, \|u\|_{L_t^{\theta_p}(L_{i,j}^{p,2})}, \|u\|_{L_t^{\theta_q}(L_k^{q,2})} \right\},$$

where $2/\theta_p = 3(1/2 - 1/p)$ and $2/\theta_q = 3(1/2 - 1/q)$. And if $p, q = 2$, then $\theta_p, \theta_q = +\infty$. Herein we use the shorthand notation $X = X(T)$ without confusion.

And we use the notation

$$L_t^{\theta_q}(L_D^{q,2}) \quad (1.6)$$

to represent the separate functional spaces. If $q = 2$, then

$$L_t^{\theta_q}(L_D^{q,2}) := L_t^\infty(L^2).$$

If $D = \{k\}$, then

$$L_t^{\theta_q}(L_D^{q,2}) := L_t^{\theta_q}(L_k^{q,2}).$$

If $D = \{i, j\}$, then

$$L_t^{\theta_q}(L_D^{q,2}) := L_t^{\theta_q}(L_{i,j}^{q,2}).$$

Taking $U_0(t)$ the free propagator $\exp(it \sum_{j=1}^N \Delta_j)$, we have our first theorem:

Theorem 1.2. *Under the Assumption 1.1, the Equation (1.1) has a unique solution $u \in X(a)$, for every $u_0 \in L^2((\mathbb{R}^3)^N)$ and $s \in I_a$.*

And there is a constant C only dependent on p, q, V, W with $1/\theta_{\alpha, \beta} > 0$, if T small enough such that $CT^{1/\theta_{\alpha, \beta}}N(N+1) < 1/2$, we have

$$\|u\|_X \lesssim_{p,q} \|u_0\|_{L^2}$$

where $\theta_{\alpha, \beta}$ is defined by Equation (1.4).

Remark 1.3. Indeed, the constant C satisfies the Inequality (3.1).

Remark 1.4. For some kinds of potentials V and W , for example the Coulombic potentials V and W which satisfy the Equation (1.2) and (1.3) respectively, the case $p, q = 6$ is also correct. We can use the strategy of proof of Theorem 1.5, regard the potentials V and W as $|V|^\alpha|V|^{1-\alpha}$ and $|W|^\alpha|W|^{1-\alpha}$ with $0 \leq \alpha \leq 1$ and introduce other factor \tilde{p} and \tilde{q} . Then we get the case $p, q = 6$.

1.2 The Regularity under the Fixed Spin States

Nowadays, we return back to electronic evolution equation with V and W satisfying the Equation (1.2) and (1.3).

In physics, for electronic systems, or more general fermionic systems, the initial datum u_0 should satisfy the Pauli Exclusion Principle, which means it is of anti-symmetry under the change of electron coordinates for one spin state [42, 59]. If a particle has s spin states, then we label them by the integer

$$\sigma \in \{1, 2, \dots, s\}.$$

Suppose there are N particles and the i^{th} particle has s_i spin states. Then a wave function for these N particles can then be written as

$$u(x_1, \sigma_1, \dots, x_N, \sigma_N)$$

where $1 \leq \sigma_i \leq s_i$. For the fixed spin σ systems, u is only a function of x_1, \dots, x_N , then it can be regarded as

$$u(x_1, \dots, x_N).$$

Let

$$\mathcal{I}_s = \{i | \sigma_i = s\}, \quad s = 1, \dots, N,$$

and $P_{i,j}$ is one permutation that exchange the position of variable x_i, x_j and the spin σ_i, σ_j simultaneously. By the Pauli Principle, we know

$$u(P_{i,j}x) = -u(x), \quad \text{if } \exists 1 \leq l \leq s, \text{ s.t. } i, j \in \mathcal{I}_l. \quad (1.7)$$

In fact, in many-body quantum mechanics, fruitful results derive from the anti-symmetry. In the past three decades, the stability of Coulomb systems has been studied

extensively (see [42] for a textbook presentation). For all normalized, anti-symmetric wave function ψ with s spin state,

$$(\psi, H(0)\psi) \geq -0.231s^{2/3}N(1 + 2.16 \max_j Z_j(M/N)^{1/3})^2,$$

through the Lieb-Thirring inequalities which are one of the most important consequence of Pauli Exclusion Principle. And recently, new methods for the Lieb-Thirring inequality has been developed by lots of mathematicians [19, 45, 44].

For one smooth function u with s spin states, for the fixed σ , the Equation (1.7) holds, thus we know $|u(x)| \sim |x_i - x_j|^\alpha$ for some $\alpha \geq 1$ when $|x_i - x_j| \rightarrow 0$. Based on this observation, Yserentant [59, 61] found out the new mixed regularity and applied it to the numerical analysis.

Denote

$$\mathcal{L}_{\mathcal{I}_i} = \bigotimes_{i \in \mathcal{I}_i} \nabla_i$$

with ∇_i the gradient to the i th electron, and \otimes the tensor product.

Provided that $\Omega > C(N + \sum_\mu Z_\mu)N^{1/2} + \max\{\lambda, 0\}$, Yserentant [59, 61] tells us that if λ is the eigenvalue of the operator H , then for the eigenvalue equation

$$Hu = \lambda u,$$

there exists one anti-symmetric solution u , and

$$\|\mathcal{L}_{\mathcal{I}_i} u_H\|_{L^2} \leq \|\mathcal{L}_{\mathcal{I}_i} u_L\|_{L^2}, \quad \|\nabla \mathcal{L}_{\mathcal{I}_i} u_H\|_{L^2} \leq \Omega \|\nabla \mathcal{L}_{\mathcal{I}_i} u_L\|_{L^2} \quad (1.8)$$

with

$$\hat{u}_L = \hat{u} \mathbb{1}_{|\omega| < \Omega}, \quad u_H = u - u_L.$$

with \hat{u} is the Fourier Transform of u .

If $H(t) = H$ is independent of t , obviously it is selfadjoint with the domain $H^1((\mathbb{R}^3)^N)$. Hence there is for each Borel set $A \subset \mathbb{R}$, a projection, $E_A(H)$, so that $H = \int \lambda dE_\lambda$ and $\exp(itH) = \int \exp(it\lambda) dE_\lambda$. It is natural to consider the similar question: if u_0 anti-symmetric, and $\|\mathcal{L}_{\mathcal{I}_i} u_0\|_{L^2} < \infty$, does $\|\mathcal{L}_{\mathcal{I}_i} u\|_{L^2} < \infty$ hold?

There are fruitful works about the regularity of the eigenfunctions of the Hamiltonian operator H . Beginning from the work of Kato [31], in which he derived the famous cusp conditions that establish a connection between the function values and certain first order directional derivatives at the points where two particles meet and the corresponding interaction potential becomes singular, Fournais and others directed attention primarily to the local behaviour of the eigenfunctions near the singular points of the interaction potentials, rather than like Yserentant showing that the eigenfunctions possess global, square-integrable weak derivatives of partly very high order, see [16, 17, 18, 28, 27]. Now, we do the similar work of Yserentant, showing that the solutions of the electronic evolution Schrödinger equation has similar mixed high order derivative regularity.

To simplify the notation, we denote

$$1/\theta = \min\{3/(2p) + 3/(2\tilde{p}) - 1/2, 3/(2q) + 3/(2\tilde{q}) - 1/2\}. \quad (1.9)$$

Our main result is Theorem 1.5, 1.8 and 1.10:

Theorem 1.5. *If u_0 has the fixed spin states σ , $\mathcal{L}_{\mathcal{I}_l}u_0 \in L^2((\mathbb{R}^3)^N)$, $l = 1, \dots, s$, and $0 < \alpha < 1/2$, $\frac{6}{3-2\alpha} < p, q \leq 6$, the solution of Equation (1.1) has a unique solution u with the same spin states σ , and $\mathcal{L}_{\mathcal{I}_l}u \in X(s)$ for $s \in I_a$.*

And there is a constant C_1 only dependent on α , \tilde{p} , p , \tilde{q} and q with $\frac{6}{1+2\alpha} < \tilde{p}, \tilde{q} \leq 6$ and $1/\theta > 0$, if T small enough such that $C_1(\sum_{\mu} Z_{\mu} + N)NT^{1/\theta} < 1/2$, we have

$$\|\mathcal{L}_{\mathcal{I}_l}u\|_{L_t^{\infty}(L^2)} \leq \|\mathcal{L}_{\mathcal{I}_l}u\|_X \lesssim_{p,q} \|\mathcal{L}_{\mathcal{I}_l}u_0\|_{L^2},$$

where θ satisfies the Equation (1.9).

Remark 1.6. Indeed, the constant C_1 is such that the Inequality (4.4) holds.

If u_0 has N spins states, and for every $1 \leq l \leq N$, $|\mathcal{I}_l| = 1$, then it can be regarded as the case without spin states. So $\mathcal{L}_{\mathcal{I}_l} = \nabla_l$. Thus we have the following corollary:

Corollary 1.7. *If $\nabla_l u_0 \in L^2((\mathbb{R}^3)^N)$, $l = 1, \dots, N$, and $0 < \alpha < 1/2$, $\frac{6}{3-2\alpha} < p, q \leq 6$, the solution of Equation (1.1) has a unique solution u , and $\mathcal{L}_{\mathcal{I}_l}u \in X(s)$ for $s \in I_a$.*

And if $C_1(\sum_{\mu} Z_{\mu} + N)NT^{1/\theta} < 1/2$, we have

$$\|\nabla_l u\|_{L_t^{\infty}(L^2)} \leq \|\nabla_l u\|_X \lesssim_{p,q} \|\nabla_l u_0\|_{L^2},$$

where θ satisfies the Equation (1.9).

In Yserentant's works, the author also introduced another type of operator

$$\mathcal{K}_{\mathcal{I}_l} = \prod_{j \in \mathcal{I}_l} (1 - \Delta_j)^{1/2}$$

which is equivalent to $\mathcal{L}_{\mathcal{I}_l}$ in the L^2 functional space. However, it is not so evident for the X functional space, not only because of the $L^p - L^q$ type functional space, but also the change of variable in the integration. Luckily, after generalization of Calderón-Zygmund inequality and observation of the special property of our functional space, we found out some useful inequalities in Section 2.3. Then, we have the following Theorem:

Theorem 1.8. *If u_0 has the fixed spin states σ , $\mathcal{K}_{\mathcal{I}_l}u_0 \in L^2((\mathbb{R}^3)^N)$, $l = 1, \dots, s$, and $0 < \alpha < 1/2$, $\frac{6}{3-2\alpha} < p, q \leq 6$, the solution of Equation (1.1) has a unique solution u with the same spin states σ , and $\mathcal{K}_{\mathcal{I}_l}u \in X(a)$ for $s \in I_a$.*

And there is a constant C_2 ($C_2 > C_1$) only dependent on α , \tilde{p} , p , \tilde{q} and q with $\frac{6}{1+2\alpha} < \tilde{p}, \tilde{q} \leq 6$ and $1/\theta > 0$, if T is small enough such that $C_2(\sum_{\mu} Z_{\mu} + N)NT^{1/\theta} < 1/2$, we have

$$\|\mathcal{K}_{\mathcal{I}_l}u\|_{L_t^{\infty}(L^2)} \leq \|\mathcal{K}_{\mathcal{I}_l}u\|_X \lesssim_{p,q} \|\mathcal{K}_{\mathcal{I}_l}u_0\|_{L^2}.$$

Remark 1.9. Indeed, the constant C_2 is such that the Inequality (4.5) holds.

1.3 The Numerical Analysis

Similar to [60], it is interesting to consider the numerical approximation of Equation (1.1).

We construct the projection firstly.

Define by $\Omega(R)$ the following hyperbolic cross space

$$\Omega(R) = \left\{ (\omega_1, \dots, \omega_N) \in (\mathbb{R}^3)^N \mid \sum_{1 \leq l \leq s} \prod_{i \in \mathcal{I}_l} (1 + |\omega_i|^2)^{1/2} \leq R \right\}.$$

And let $\chi : (\mathbb{R}^3)^N \rightarrow [0, 1]$ now be a symmetric function with the values $\chi_R(\omega) = 1$ for $\omega \in \Omega(R)$. Then, we have the following operator:

$$(P_{R,\chi}u)(x) = \left(\frac{1}{\sqrt{2\pi}} \right)^{3N} \int_{\omega \in (\mathbb{R}^3)^N} \chi_R(\omega) \hat{u}(\omega) \exp(i\omega \cdot x) d\omega.$$

For example, let $\chi_R(\omega) = \mathbb{1}_{\Omega(R)}(\omega)$, then the operator $P_{R,\chi}$ is a projector in Fourier space.

As the choice of χ_R has few influences to our result, we shorten $P_{R,\chi}$ by P_R without confusion. And then we have the following approximation of Equation (1.1):

$$\begin{cases} i\partial_t u_R = H_R(u_R), & t \in [-a, a] = I_a, x = (x_1, \dots, x_N) \in (\mathbb{R}^3)^N \\ u_R(0, x) = P_R(u_0)(x) \end{cases} \quad (1.10)$$

with

$$H_R(u) = \sum_{j=1}^N -\Delta_j u - \sum_{j=1}^N \sum_{\mu=1}^M P_R(V(x_j, t)u) + \sum_{k < j}^N P_R(W(x_j, x_k)u).$$

As a consequence of our main Theorem 1.5 and Theorem 1.8, we have:

Theorem 1.10. *If u_0 has the fixed spin states σ , $\mathcal{K}_{\mathcal{I}_l}u_0 \in L^2((\mathbb{R}^3)^N)$, $l = 1, \dots, s$, and $0 < \alpha < 1/2$, $\frac{6}{3-2\alpha} < p, q < 6$, then the solution of Equation (1.10) has unique solution u_R .*

And there is a constant C_3 ($C_3 > C_2$) only dependent on α , \tilde{p} , p , \tilde{q} and q with $\frac{6}{1+2\alpha} < \tilde{p}, \tilde{q} < 6$ and $1/\theta > 0$, if T small enough such that $C_3(\sum_{\mu} Z_{\mu} + N)NT^{1/\theta} < 1/2$, we have

$$\|u - u_R\|_{L_t^\infty(L^2)} \leq \|u - u_R\|_X \lesssim_{p,q} 1/R \sum_{l=1}^s \|\mathcal{K}_{\mathcal{I}_l}u_0\|_{L^2}, \quad (1.11)$$

where u is the solution of Equation (1.1).

Remark 1.11. Indeed, the constant C_3 is such that the Inequality (5.1) holds.

Indeed, it provides us several numerical methods, [22, 60]. For the numerical analysis, normally, we split $\Omega(R)$ into finitely many subdomains by means of a C^∞ -partition of unity $\sum_{l=1}^L \psi_l = 1$ on $\Omega(R)$ with $l \in (\mathbb{N}^3)^N$, i.e. each $\psi_l(\omega) \in C^\infty$ has compact support. It forms the basis of many possible approximation procedures that differ mainly

by the way that the partition of unity is actually chosen and that the parts are finally approximated by functions in finite dimensional spaces. Let

$$u_l(x) = \left(\frac{1}{\sqrt{2\pi}} \right)^{3N} \int \psi_l \widehat{u}(\omega) \exp(i\omega \cdot x) d\omega,$$

and

$$\psi_l(\omega) = (\widehat{\phi}_l)^2.$$

[60] tells us that the part u_l of u can be approximated arbitrarily well by the functions in the space

$$\mathcal{V}_l = \text{span}\{\phi_l(\cdot - D_l^{-1}k) | k \in \mathbb{Z}^{3N}\}$$

with

$$D_l \omega = \frac{4}{\pi} (2^{l_1} \omega_1, \dots, 2^{l_N} \omega_N).$$

Hence, taking the symmetric $\sum_{l=1}^L \psi_l$ and let $\chi_R = \sum_{l=1}^L \psi_l$. As a consequence, we get the P_R and then u_R which satisfies the Inequality (1.11).

Outline of the paper. Before giving the proofs of the main results, we pause to outline the structure of this paper.

- In Section 2 we introduce the tools that we need: the Hardy-type inequalities, the generalization of Strichartz estimates, and the Sobolev inequalities in $L^p - L^2$ functional spaces.
- In Section 3 we prove the existence of the general many-body Schrödinger equation, namely the Theorem 1.2.
- In Section 4, we return back to Coulombic potentials, and study its regularity. Under the assumption of the initial datum that u_0 has the fixed spin states σ , we get our main results: Theorem 1.5 and 1.8. The Sobolev inequalities play one central role in the proof of the Theorem 1.8.
- In Section 5, we design one new hyperbolic cross space approximation and derive the numerical analysis by using the Theorem 2.8.

2 Preliminary

2.1 Hardy Type Inequality

For the mixed regularity, we need to study the Hardy type inequalities. By a similar methods to [59, lemma 1], we generalize the Hardy inequality:

Lemma 2.1. *If $u \in C_0^\infty(\mathbb{R}^3 \setminus \{0\})$, then*

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

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

Proof. Let $d(x) = |x|$. We have the relationship:

$$(k-1) \frac{1}{d^k} = -\nabla \frac{1}{d^{k-1}} \cdot \nabla d,$$

and because of $\int_{\mathbb{R}^3} \frac{|u(x)|^2}{|x|^k} dx < \infty$, hence by the integration by part we obtain

$$(k-1) \int_{\mathbb{R}^3} \frac{1}{d^k} u^2 = \int_{\mathbb{R}^3} \frac{1}{d^{k-1}} \nabla \cdot (u^2 \nabla d) dx.$$

Using $\Delta d = \frac{2}{d}$ on the right hand, then

$$(k-1) \int_{\mathbb{R}^3} \frac{1}{d^k} u^2 dx = 2 \int_{\mathbb{R}^3} \frac{1}{d^{k-1}} u \nabla u \cdot \nabla d dx + 2 \int_{\mathbb{R}^3} \frac{1}{d^k} u^2 dx,$$

by the Cauchy-Schwarz inequality, we yield

$$\left| \frac{k-3}{2} \right| \int_{\mathbb{R}^3} \frac{1}{d^k} u^2 \leq \left(\int_{\mathbb{R}^3} \frac{1}{d^k} u^2 dx \right)^{1/2} \left(\int_{\mathbb{R}^3} \frac{1}{d^{k-2}} |\nabla d \cdot \nabla u|^2 dx \right)^{1/2}$$

and as $|\nabla d| = 1$, finally get the estimate. \square

Using Lemma 2.1 twice and the Fubini's Theorem, we have the following corollary.

Corollary 2.2. *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:*

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

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

When $k = 3$, from Lemma 2.1, we can only know

$$\int_{\mathbb{R}^3} \frac{|\nabla u(x)|^2}{|x|} dx \geq 0,$$

which means that $\int_{\mathbb{R}^3} \frac{|\nabla u(x)|^2}{|x|} dx$ has no relation with $\int_{\mathbb{R}^3} \frac{|u(x)|^2}{|x|^3} dx$.

Let $x = (x_1, x_2, x_3) \in \mathbb{R}^3$. Now, we consider the cylindrical coordinates in \mathbb{R}^3 , let

$$x_1 = r \cos \theta, \quad x_2 = r \sin \theta$$

then we have the following unit vectors

$$\vec{r} = (\cos \theta, \sin \theta, 0), \quad \vec{\theta} = (-\sin \theta, \cos \theta, 0).$$

Let $A = \vec{\theta}/r$. Indeed it is the Aharonov-Bohm magnetic vector potential. So we have the following covariant derivatives:

$$D_\alpha = -i\nabla + \alpha A.$$

Then, we have the magnetic Hardy-type inequality:

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

$$\int_{\mathbb{R}^3} \frac{|D_\alpha u(x)|^2}{|x|} dx \geq \min_{k \in \mathbb{Z}} (k - \alpha)^2 \int_{\mathbb{R}^3} \frac{|u(x)|^2}{|x|^3} dx.$$

Proof. Indeed, using the cylindrical coordinates (r, θ, x_3) we have $u(x_1, x_2, x_3) = (1/\sqrt{2\pi}) \sum_k u_k(r, x_3) e^{ik\theta}$. Therefore,

$$\begin{aligned} \int_{\mathbb{R}^3} \frac{|D_\alpha u(x)|^2}{|x|} dx &= \int_{\mathbb{R}_z} \int_0^\infty \int_0^{2\pi} \left(|u'_r|^2 + |u'_{x_3}|^2 + \left| \frac{i u'_\theta + \alpha u}{r} \right|^2 \right) d\theta dr dx_3 \\ &\geq \frac{1}{2\pi} \int_{\mathbb{R}_z} \int_0^\infty \int_0^{2\pi} \left| \sum_k \frac{\alpha - k}{r} u_k e^{ik\theta} \right|^2 d\theta dr dx_3 \\ &= \int_{\mathbb{R}_z} \int_0^\infty \sum_k \left| \frac{\alpha - k}{r} u_k \right|^2 dr dx_3 \\ &\geq \min_{k \in \mathbb{Z}} (k - \alpha)^2 \int_{\mathbb{R}^3} \frac{|u|^2}{|x|^3} dx. \end{aligned}$$

□

Remark 2.4. This kind of magnetic Hardy inequalities has been well developed for the 2d case, which can be used to study the many-body Hardy inequalities, see [45, 26].

2.2 Strichartz Estimate

At the beginning, we recall the free propagator $U_0 = \exp(it \sum_{j=1}^N \Delta)$.

Denoting the integral operator

$$(Su)(t) = \int_0^t U_0(t - \tau) u(\tau) d\tau.$$

and

$$Qu(t) = \sum_{j=1}^N (SV(x_j, \cdot)u)(t) - \sum_{j < k} (SW(x_j, x_k)u(\cdot))(t),$$

we consider the integral equation:

$$u(t) = U_0(t)u_0 + iQu(t). \quad (2.1)$$

Before the discussion about U_0 , we need the following properties.

Lemma 2.5.

$$\mathcal{R}_{i,j} \nabla_i = (\nabla_{d_{i,j}} + \nabla_{D_{i,j}}) \mathcal{R}_{i,j}, \quad \mathcal{R}_{i,j} \nabla_j = (\nabla_{D_{i,j}} - \nabla_{d_{i,j}}) \mathcal{R}_{i,j}$$

and

$$-\mathcal{R}_{i,j} \Delta_i = |\nabla_{d_{i,j}} + \nabla_{D_{i,j}}|^2 \mathcal{R}_{i,j}, \quad -\mathcal{R}_{i,j} \Delta_j = |\nabla_{d_{i,j}} - \nabla_{D_{i,j}}|^2 \mathcal{R}_{i,j}$$

Proof. We know $x_i = (d_{i,j} + D_{i,j})/2$ and $x_j = (D_{i,j} - d_{i,j})/2$, then

$$\nabla_{d_{i,j}} \mathcal{R}_{i,j} u = 1/2 \mathcal{R}_{i,j} (\nabla_i - \nabla_j) u,$$

and

$$\nabla_{D_{i,j}} \mathcal{R}_{i,j} u = 1/2 \mathcal{R}_{i,j} (\nabla_i + \nabla_j) u.$$

Then the first equation holds.

For the second, we just use the fact

$$-\Delta_i = \nabla_i^* \cdot \nabla_i = |\nabla_i|^2.$$

Together with the first equation, we yield the results. \square

Then the next integrability property of the free propagator $U_0(t)$ is fundamental in the following discussions.

Lemma 2.6 (Kato). *Let $2 \leq p \leq \infty$, then*

$$\|U_0(t)u\|_{L_D^{p,2}} \lesssim_p |t|^{-3(1/2-1/p)} \|u\|_{L_D^{p',2}}, \quad D \subset \{1, \dots, N\}, \quad 1 \leq |D| \leq 2.$$

Proof. For the case $|D| = 1$, it is just the normal Kato inequality. For the another case, let $D = \{i, j\}$. Notice that by Lemma 2.5

$$-\mathcal{R}_{i,j} \Delta_x - \mathcal{R}_{i,j} \Delta_y = -2\Delta_{d_{i,j}} \mathcal{R}_{i,j} - 2\Delta_{D_{i,j}} \mathcal{R}_{i,j}.$$

Then, we know

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

with $\tilde{U}_0(t) = \exp(-i(\sum_{k \neq i,j} \Delta_k + 2\Delta_{d_{i,j}} + 2\Delta_{D_{i,j}}))$.

Therefore,

$$\begin{aligned} \|U_0(t)u\|_{L_{i,j}^{p,2}} &= \|\mathcal{R}_{i,j} U_0(t)u\|_{L_{d_{i,j}}^{p,2}} \\ &= \|\tilde{U}_0(t) \mathcal{R}_{i,j} u\|_{L_{d_{i,j}}^{p,2}} \\ &\lesssim_p |t|^{-3(1/2-1/p)} \|\mathcal{R}_{i,j} u\|_{L_{d_{i,j}}^{p,2}} \\ &\lesssim_p |t|^{-3(1/2-1/p)} \|u\|_{L_{i,j}^{p,2}}. \end{aligned}$$

Get conclusion. \square

Then, we have the following Strichartz estimates:

Lemma 2.7 (Strichartz estimate). [58, 33] *For $D, D' \subset \{1, \dots, N\}, 1 \leq |D|, |D'| \leq 2$ and $2 \leq p, q \leq 6$, we have*

$$\|U_0(t)f\|_{L_t^{\theta_p}(L_D^{p,2})} \lesssim_p \|f\|_{L^2}, \quad (2.2a)$$

$$\left\| \int U(s)^* u(s) ds \right\|_{L^2} \lesssim_p \|u\|_{L_t^{\theta_p'}(L_D^{p',2})}, \quad (2.2b)$$

$$\|Su\|_{L_t^{\theta_p}(L_D^{p,2})} \lesssim_{p,q} \|u\|_{L_t^{\theta_q'}(L_{D'}^{q',2})}, \quad (2.2c)$$

Normally, the operator bounded in L^2 functional space is not bounded in the $L_D^{p,2}$ functional space. But the following theorem tells us that after applying the operator S , the bounded operator in L^2 is also bounded in $L_D^{p,2}$.

Theorem 2.8. *If $2 \leq p, q < 6$, for one operator P acting on $L^2(\mathbb{R}^{3N})$, if $[P, U_0] = 0$ and $\|Pf_0\|_{L^2} \leq \|f\|_{L^2}$, then*

$$\|PSf(\cdot, x)\|_{L_t^{\theta_p}(L_D^{p,2})} \lesssim_{p,q} \|f\|_{L_t^{\theta'_q}(L_{D'}^{q',2})}.$$

And this inequality has the same optimal constant with Inequality (2.2c).

Proof. It is to prove

$$\left\| P \int_0^t U_0(t-s)f(s, x)ds \right\|_{L_t^{\theta_p}(L_D^{p,2})} \lesssim_{p,q} \|f\|_{L_t^{\theta'_q}(L_{D'}^{q',2})}.$$

Then instead of proving this inequality, we prove the following one,

$$\left\| P \int_0^T U_0(t-s)f(s, x)ds \right\|_{L_t^{\theta_p}(L_D^{p,2})} \lesssim_{p,q} \|f\|_{L_t^{\theta'_q}(L_{D'}^{q',2})}$$

then by Christ-Kiselev lemma, get conclusion.

Since P and U_0 commute, we have

$$\left\| P \int_0^T U_0(t-s)f(s, x)ds \right\|_{L_t^{\theta_p}(L_D^{p,2})} = \left\| U_0(t)P \int_0^T U(s)^* f(s, x)ds \right\|_{L_t^{\theta_p}(L_D^{p,2})}.$$

By Inequality (2.2a), we have

$$\left\| P \int_0^T U_0(t-s)f(s, x)ds \right\|_{L_t^{\theta_p}(L_D^{p,2})} \lesssim_p \left\| P \int_0^T U(s)^* f(s, x)ds \right\|_{L^2}.$$

Then, by $\|Pf_0\|_{L^2} \leq \|f\|_{L^2}$, we have

$$\left\| P \int_0^T U_0(t-s)f(s, x)ds \right\|_{L_t^{\theta_p}(L_D^{p,2})} \lesssim_p \left\| \int_0^T U(s)^* f(s, x)ds \right\|_{L^2}.$$

By Inequality (2.2b), we have

$$\left\| P \int_0^T U_0(t-s)f(s, x)ds \right\|_{L_t^{\theta_p}(L_D^{p,2})} \lesssim_{p,q} \|f\|_{L_t^{\theta'_q}(L_{D'}^{q',2})}.$$

□

Corollary 2.9. *For $D, D' \subset \{1, \dots, N\}$, $1 \leq |D|, |D'| \leq 2$ and $2 \leq p, q < 6$, we have*

$$\|SP_R u\|_{L_t^{\theta_p}(L_D^{p,2})} \lesssim_{p,q} \|u\|_{L_t^{\theta'_q}(L_{D'}^{q',2})}, \quad (2.3a)$$

$$\|S(1 - P_R)u\|_{L_t^{\theta_p}(L_D^{p,2})} \lesssim_{p,q} 1/R \left\| \sum_{1 \leq l \leq s} \mathcal{K}_{\mathcal{I}_l} u \right\|_{L_t^{\theta'_q}(L_{D'}^{q',2})}. \quad (2.3b)$$

And these inequalities have the same optimal constant with Inequality (2.2c).

Proof. Obviously, by the definition of P_R , we have

$$[P_R, U_0] = 0$$

and

$$\|P_R u\|_{L^2} \leq \|u\|_{L^2}.$$

Let $P = P_R$, then we get the Inequality (2.3a). Besides,

$$\|(1 - P_R)u\|_{L^2} \leq \|\mathbb{1}_{\Omega(R)^c} \hat{u}\|_{L^2}$$

For all wave vector ω outside the domain $\Omega(R)$, we have

$$1 \leq 1/R \sum_{1 \leq l \leq s} \prod_{i \in \mathcal{I}_l} (1 + |\omega_i|^2)^{1/2}.$$

By the definition of norm, we know

$$\|(1 - P_R)u\|_{L^2} \leq 1/R \left\| \sum_{1 \leq l \leq s} \prod_{i \in \mathcal{I}_l} (1 + |\omega_i|^2)^{1/2} \hat{u} \right\|_{L^2} = 1/R \left\| \sum_{1 \leq l \leq s} \mathcal{K}_{\mathcal{I}_l} u \right\|_{L^2}.$$

Given $[\mathcal{K}_{\mathcal{I}_l}, U_0] = 0$, then take $P = R(1 - P_R) \left(\sum_{1 \leq l \leq s} \mathcal{K}_{\mathcal{I}_l} \right)^{-1}$, we get conclusion. \square

2.3 Sobolev Inequalities

Because of the unusuality of our functional space, we need to reconstruct some Sobolev inequalities which will be useful for the regularity. We generalized the Calderón-Zygmund inequality to satisfy the new functional space $L_i^{p,2}$ in Appendix. The following inequalities are the application of the new Calderón-Zygmund inequality and then we make it compatible for the functional space $L_{i,j}^{p,2}$.

Theorem 2.10. *For $1 < p < \infty$, the following inequalities hold:*

$$\|\nabla_i u\|_{L_i^{p,2}} \lesssim_p \|(1 - \Delta_i)^{1/2} u\|_{L_i^{p,2}}, \quad i = 1, \dots, N \quad (2.4a)$$

$$\|u\|_{L_i^{p,2}} \lesssim_p \|(1 - \Delta_i)^{1/2} u\|_{L_i^{p,2}}, \quad i = 1, \dots, N \quad (2.4b)$$

$$\|(1 - \nabla_i)u\|_{L_i^{p,2}} \lesssim_p \|(1 - \Delta_i)^{1/2} u\|_{L_i^{p,2}}, \quad i = 1, \dots, N \quad (2.4c)$$

$$\|\nabla_i u\|_{L_{i,j}^{p,2}} \lesssim_p \|(1 - \Delta_i)^{1/2} u\|_{L_{i,j}^{p,2}}, \quad i, j = 1, \dots, N \quad (2.4d)$$

$$\|u\|_{L_{i,j}^{p,2}} \lesssim_p \|(1 - \Delta_i)^{1/2} u\|_{L_{i,j}^{p,2}}, \quad i, j = 1, \dots, N \quad (2.4e)$$

$$\|(1 - \nabla_i)u\|_{L_{i,j}^{p,2}} \lesssim_p \|(1 - \Delta_i)^{1/2} u\|_{L_{i,j}^{p,2}}, \quad i = 1, \dots, N. \quad (2.4f)$$

Proof. For the first inequality, we only need to study equivalently the following inequality

$$\|\nabla_i (1 - \Delta_i)^{-1/2} u\|_{L_i^{p,2}} \lesssim_p \|u\|_{L_i^{p,2}}.$$

Obviously,

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

Using Theorem A.3, get conclusion. And since $\xi \in \mathbb{R}^3$, we know the optimal constant of this inequality is independent on N .

The second and third inequalities are similar.

For the fourth inequality, by Lemma 2.3, we know

$$\|\nabla_i u\|_{L_{i,j}^{p,2}} = \|\mathcal{R}_{i,j} \nabla_i u\|_{L_{d_{i,j}}^{p,2}} = \|(\nabla_{d_{i,j}} + \nabla_{D_{i,j}}) \mathcal{R}_{i,j} u\|_{L_{d_{i,j}}^{p,2}}.$$

Define the Fourier transform just for the variable $D_{i,j}$ by \mathcal{F}_D , and by Parseval's Theorem, then

$$\begin{aligned} \|\nabla_i u\|_{L_{i,j}^{p,2}} &= \|(\nabla_{d_{i,j}} - i\xi_{D_{i,j}}) \mathcal{F}_D \mathcal{R}_{i,j} u\|_{L_{d_{i,j}}^{p,2}} \\ &= \|\nabla_{d_{i,j}} \exp(-id_{i,j} \cdot \xi_{D_{i,j}}) \mathcal{F}_D \mathcal{R}_{i,j} u\|_{L_{d_{i,j}}^{p,2}} \\ &\lesssim_p \|(1 - \Delta_{d_{i,j}})^{1/2} \exp(-id_{i,j} \cdot \xi_{D_{i,j}}) \mathcal{F}_D \mathcal{R}_{i,j} u\|_{L_{d_{i,j}}^{p,2}}. \end{aligned}$$

So in order to get the result, we only need to prove for every u ,

$$(1 - \Delta_{d_{i,j}})^{1/2} \exp(-id_{i,j} \cdot \xi_{D_{i,j}}) u = \exp(-id_{i,j} \cdot \xi_{D_{i,j}}) (1 + |\nabla_{d_{i,j}} - i\xi_{D_{i,j}}|)^{1/2} u.$$

It is correct by the fact

$$(1 - \Delta)^{1/2} = 2/\pi \int_0^\infty \frac{1 - \Delta}{1 - \Delta + t^2} dt$$

and

$$(1 - \Delta + t^2)^{-1} = \int_0^\infty \exp(-(1 - \Delta + t^2)s) ds.$$

Finally, repeating the strategy of the fourth inequality, we get the fifth and sixth inequalities. \square

Remark 2.11. The inequalities we get in Theorem 2.10 work not only on i , but also on j .

3 Existence of Solution

Proof of Theorem 1.2. In fact, we just need to analyze the term $SW(x_i, x_j)u$. Since

$$W \in L_t^{\alpha p}(L^{p/(p-2)}) + L_t^{\beta p}(L^\infty),$$

we have

$$W = W_1 + W_2, \quad W_1 \in L_t^{\alpha p}(L^{p/(p-2)}), \quad W_2 \in L_t^{\beta p}(L^\infty)$$

then,

$$\begin{aligned} \| |W|^{1/2} u \|_{L^2}^2(t) &= \int |W|(t) |u|^2(t) dx \\ &\leq \int |W_1|(t) |u|^2(t) dx + \int |W_2|(t) |u|^2(t) dx \\ &\leq \|W_1\|_{L^{p/(p-2)}}(t) \|u\|_{L_{i,j}^{p,2}}^2(t) + \|W_2\|_{L^\infty}(t) \|u\|_{L^2}^2(t). \end{aligned}$$

Therefore, for every $v \in L_t^{\theta'_q}(L_D^{q',2})$ with $1 \leq |D| \leq 2$ and $2 \leq q < 6$.

$$\begin{aligned}
& \int_0^T \langle SW(x_i, x_j)u(t), v \rangle dt \\
&= \int_0^T \langle W(x_i, x_j)^{1/2}u, W(x_i, x_j)^{1/2}S^*v(s) \rangle ds \\
&\leq \int_0^T \left\| |W(x_i, x_j)|^{1/2}u \right\|_{L^2} \left\| |W(x_i, x_j)|^{1/2}S^*v \right\|_{L^2} ds \\
&\leq \int_0^T \left(\|W_2\|_{L^\infty}^{1/2} \|u\|_{L^2} + \|W_1\|_{L^{p/(p-2)}}^{1/2} \|u\|_{L_{i,j}^{p,2}} \right) \\
&\quad \left(\|W_2\|_{L^\infty}^{1/2} \|S^*v\|_{L^2} + \|W_1\|_{L^{p/(p-2)}}^{1/2} \|S^*v\|_{L_{i,j}^{p,2}} \right) ds \\
&\leq \int_0^T \left(\|W_2\|_{L^\infty} \|u\|_{L^2} + \|W_1\|_{L^{p/(p-2)}}^{1/2} \|W_2\|_{L^\infty}^{1/2} \|u\|_{L_{i,j}^{p,2}} \right) \|S^*v\|_{L^2} ds \\
&\quad + \int_0^T \left(\|W_1\|_{L^{p/(p-2)}}^{1/2} \|W_2\|_{L^\infty}^{1/2} \|u\|_{L^2} + \|W_1\|_{L^{p/(p-2)}} \|u\|_{L_{i,j}^{p,2}} \right) \|S^*v\|_{L_{i,j}^{p,2}} ds \\
&\lesssim_{p,q,W} T^{1/\theta_{\alpha,\beta}} \left(\|u\|_{L_t^\infty(L^2)} + \|u\|_{L_t^{\theta_p}(L_{i,j}^{p,2})} \right) \|v\|_{L_t^{\theta'_q}(L_D^{q',2})} \\
&\lesssim_{p,q,W} T^{1/\theta_{\alpha,\beta}} \|u\|_X \|v\|_{L_t^{\theta'_q}(L_D^{q',2})}.
\end{aligned}$$

Choosing one sequence $v_n \in L_t^{\theta'_q}(L_D^{q',2})$ with $\|v_n\|_{L_t^{\theta'_q}(L_D^{q',2})} = 1$, such that

$$\|SWu\|_{L_t^{\theta_q}(L_D^{q,2})} = \lim_{n \rightarrow \infty} \left| \langle SWu, v_n \rangle_{L_t^{\theta_q}(L_D^{q,2}), L_t^{\theta'_q}(L_D^{q',2})} \right| \lesssim_{p,q,W} T^{1/\theta_{\alpha,\beta}} \|u\|_X.$$

Let $L_t^{\theta_q}(L_D^{q,2}) = L_t^\infty(L^2)$ or $L_t^{\theta_p}(L_{i,j}^{p,2})$ or $L_t^{\theta_q}(L_k^{q,2})$. Then obviously,

$$\|SWu\|_X \lesssim_{p,q,W} T^{1/\theta_{\alpha,\beta}} \|u\|_X.$$

Similarly, we have

$$\|SVu\|_X \lesssim_{p,q,V} T^{1/\theta_{\alpha,\beta}} \|u\|_X$$

Hence, there is a constant C only dependent on p, q, V, W , such that

$$\|Qu\|_X \leq CT^{1/\theta_{\alpha,\beta}} N(N+1) \|u\|_X. \tag{3.1}$$

Let T small enough, such that $CT^{1/\theta_{\alpha,\beta}} N(N+1) < 1/2$, the operator Q is a contraction on X . Since, by Lemma 2.7, $u_0(t) = U_0(t)u_0 \in X$, for any $u_0 \in L^2$, it follows that the integral equation

$$u(t) = u_0(t) + iQu(t)$$

has a unique solution $u(t) = (\mathbb{1} - iQ)^{-1}u_0(t) \in X$. And

$$\|u\|_X \leq 2\|U_0(t)u_0\|_X \lesssim_{p,q} \|u_0\|_{L^2}.$$

Besides the standard continuation procedure for the solution of linear integral equations yields a global unique solution $u \in X(a)$. \square

4 Regularity of the Equation

Before analyzing this section, we study the following equation firstly:

$$\begin{cases} i\partial_t u_\epsilon = H_\epsilon u_\epsilon, & t \in [-a, a] = I_a, x = (x_1, \dots, x_N) \in (\mathbb{R}^3)^N \\ u_\epsilon(0, x) = v_0(x) \end{cases}$$

with

$$H_\epsilon = \sum_{j=1}^N -\Delta_j - \sum_{j=1}^N \sum_{\mu=1}^M V_\epsilon(x_j) + \sum_{k < j}^N W_\epsilon(x_j, x_k),$$

where

$$V_\epsilon(x_j) = \sum_{\mu=1}^M \frac{Z_\mu}{|x_j - a_\mu(t)| + \epsilon}$$

and

$$W_\epsilon(x_j, x_k) = \frac{1}{|x_k - x_j| + \epsilon}.$$

Let

$$Q_\epsilon u_\epsilon(t) = \sum_{j=1}^N (S V_\epsilon(x_j, \cdot) u_\epsilon)(t) - i \sum_{j < k} (S W_\epsilon(x_j, x_k) u_\epsilon(\cdot))(t), \quad (4.1)$$

Lemma 4.1. *For $\epsilon > 0$, if $v_0 \in C_0^\infty((\mathbb{R}^3)^N)$ has the fixed spin states σ , then the above equation has a unique solution with the same spin states and the solution $u_\epsilon \in C_0^\infty((\mathbb{R}^3)^N)$.*

Proof. Taking the all kinds of derivatives, the potential V_ϵ and W_ϵ are still smooth, hence in $L_t^\infty(L^{q/(q-2)} + L_t^\infty(L^\infty))$ and $L_t^\infty(L^{p/(p-2)} + L_t^\infty(L^\infty))$ respectively. From Theorem 1.2, we know the equation has a unique solution.

And by the smoothness of V_ϵ and W_ϵ , we know the solution $u_\epsilon \in C_0^\infty((\mathbb{R}^3)^N)$.

Let $P_{\mathcal{I}_l}$ is the permutation operator, denote \mathcal{A} by

$$\mathcal{A}u(x) = \frac{1}{|\mathcal{I}_l|!} \sum_{P_{\mathcal{I}_l}} \text{sign}(P_{\mathcal{I}_l}) u(P_{\mathcal{I}_l} x).$$

If u_ϵ is a solution, then $\mathcal{A}u_\epsilon(x)$ is another solution too. By the uniqueness of solution, we know u_ϵ has the same spin states. \square

Therefore, we can use Corollary 2.2 for u_ϵ .

Proof of Theorem 1.5. Taking the operator \mathcal{L} to the integral equation, we have

$$\mathcal{L}_{\mathcal{I}_l} u_\epsilon(t) = U_0(t) \mathcal{L}_{\mathcal{I}_l} v_0 + i \sum_{j=1}^N (S \mathcal{L}_{\mathcal{I}_l} V_\epsilon(x_j, \cdot) u_\epsilon)(t) - i \sum_{j < k} (S \mathcal{L}_{\mathcal{I}_l} W_\epsilon(x_j, x_k) u_\epsilon(\cdot))(t). \quad (4.2)$$

The key point is to study the term $S \mathcal{L}_{\mathcal{I}_l} W_\epsilon(x_j, x_k) u_\epsilon(\cdot)$ and $S \mathcal{L}_{\mathcal{I}_l} V_\epsilon(x_j, \cdot) u_\epsilon(\cdot)$, herein we use the Strichartz estimate. And in fact, we just need to deal with $S \mathcal{L}_{\mathcal{I}_l} W_\epsilon(x_j, x_k) u_\epsilon(\cdot)$, for the term $S \mathcal{L}_{\mathcal{I}_l} V_\epsilon(x, \cdot) u_\epsilon(\cdot)$ the method is same.

Similar to operator \mathcal{L} , we define the following operators:

$$\mathcal{L}_{\mathcal{I}_l, j} = \bigotimes_{i \in \mathcal{I}_l, i \neq j} \nabla_i, \quad \mathcal{L}_{\mathcal{I}_l, j, k} = \bigotimes_{i \in \mathcal{I}_l, i \neq j, k} \nabla_i.$$

For every $v \in L_t^{\theta'_q}(L_D^{q', 2})$ with $1 \leq |D| \leq 2$, we consider the following inner product:

$$\int_0^T \langle [S \mathcal{L}_{\mathcal{I}_l} W_\epsilon(x_j, x_k) u_\epsilon](t), v(t) \rangle dt.$$

If $j, k \notin \mathcal{I}_l$, we have

$$\mathcal{L}_{\mathcal{I}_l} W_\epsilon(x_j, x_k) u_\epsilon = W_\epsilon(x_j, x_k) \mathcal{L}_{\mathcal{I}_l} u_\epsilon.$$

And if $j \in \mathcal{I}_l$, and $k \notin \mathcal{I}_l$,

$$\mathcal{L}_{\mathcal{I}_l} W_\epsilon(x_j, x_k) u_\epsilon = W_\epsilon(x_j, x_k) \mathcal{L}_{\mathcal{I}_l} u_\epsilon + (\nabla_j W_\epsilon(x_j, x_k)) \mathcal{L}_{\mathcal{I}_l, j} u_\epsilon.$$

Analogously for $k \in \mathcal{I}_l$, and $j \notin \mathcal{I}_l$. Finally if $j, k \in \mathcal{I}_l$,

$$\begin{aligned} & \mathcal{L}_{\mathcal{I}_l} W_\epsilon(x_j, x_k) u_\epsilon \\ &= W_\epsilon(x_j, x_k) \mathcal{L}_{\mathcal{I}_l} u_\epsilon + (\nabla_j W_\epsilon(x_j, x_k)) \mathcal{L}_{\mathcal{I}_l, j} u_\epsilon \\ & \quad + (\nabla_k W_\epsilon(x_j, x_k)) \mathcal{L}_{\mathcal{I}_l, k} u_\epsilon + (\nabla_j \nabla_k W_\epsilon(x_j, x_k)) \mathcal{L}_{\mathcal{I}_l, j, k} u_\epsilon. \end{aligned}$$

Then, we have

$$\begin{aligned} & \int_0^T \langle [S \mathcal{L}_{\mathcal{I}_l} W_\epsilon(x_j, x_k) u_\epsilon](t), v(t) \rangle dt \\ & \lesssim \left| \int_0^T \langle [S W_\epsilon \mathcal{L}_{\mathcal{I}_l} u_\epsilon](t), v(t) \rangle dt \right| + \left| \int_0^T \langle [S (\nabla_j W_\epsilon) \mathcal{L}_{\mathcal{I}_l, j} u_\epsilon](t), v(t) \rangle dt \right| \\ & \quad + \left| \int_0^T \langle [S (\nabla_k W_\epsilon) \mathcal{L}_{\mathcal{I}_l, k} u_\epsilon](t), v(t) \rangle dt \right| + \left| \int_0^T \langle [S (\nabla_j \nabla_k W_\epsilon) \mathcal{L}_{\mathcal{I}_l, j, k} u_\epsilon](t), v(t) \rangle dt \right| \end{aligned}$$

For $\alpha \in (0, 1/2)$, by

$$\begin{aligned} |W_\epsilon(x_j, x_k)| & \leq \frac{1}{|x_j - x_k|}, \\ |\nabla_j W_\epsilon(x_j, x_k)| & \lesssim \frac{1}{|x_j - x_k|^2}, \\ |\nabla_j \nabla_k W_\epsilon(x_j, x_k)| & \lesssim \frac{1}{|x_j - x_k|^3}, \end{aligned}$$

we yield

$$\begin{aligned} & \int_0^T \langle [S W_\epsilon \mathcal{L}_{\mathcal{I}_l} u_\epsilon](t), v(t) \rangle dt \\ &= \int_0^T \left\langle \frac{1}{|x_j - x_k|^\alpha} \mathcal{L}_{\mathcal{I}_l} u_\epsilon(s), \frac{1}{|x_j - x_k|^{1-\alpha}} [S^* v](s) \right\rangle ds \\ & \lesssim \int_0^T \left\| \frac{1}{|x_j - x_k|^\alpha} \mathcal{L}_{\mathcal{I}_l} u_\epsilon \right\|_{L^2} \left\| \frac{1}{|x_j - x_k|^{1-\alpha}} [S^* v] \right\|_{L^2} ds; \end{aligned}$$

for the second and third term,

$$\begin{aligned}
& \int_0^T \langle [S(\nabla_j W_\epsilon) \mathcal{L}_{\mathcal{I}_l, j} u_\epsilon](t), v(t) \rangle dt \\
& \lesssim \int_0^T \left\| \frac{1}{|x_j - x_k|^{1+\alpha}} \mathcal{L}_{\mathcal{I}_l, j} u_\epsilon \right\|_{L^2} \left\| \frac{1}{|x_j - x_k|^{1-\alpha}} [S^* v] \right\|_{L^2} ds \\
& \lesssim 1/(1-2\alpha) \int_0^T \left\| \frac{1}{|x_j - x_k|^\alpha} \mathcal{L}_{\mathcal{I}_l} u_\epsilon \right\|_{L^2} \left\| \frac{1}{|x - y|^{1-\alpha}} [S^* v] \right\|_{L^2} ds;
\end{aligned}$$

and the fourth term

$$\begin{aligned}
& \int_0^T \langle [S(\nabla_j \nabla_k W_\epsilon) \mathcal{L}_{\mathcal{I}_l, j, k} u_\epsilon](t), v(t) \rangle dt \\
& \lesssim \int_0^T \left\| \frac{1}{|x_j - x_k|^{2+\alpha}} \mathcal{L}_{\mathcal{I}_l, j, k} u_\epsilon \right\|_{L^2} \left\| \frac{1}{|x_j - x_k|^{1-\alpha}} [S^* v] \right\|_{L^2} ds \\
& \lesssim 1/(1-2\alpha)^2 \int_0^T \left\| \frac{1}{|x_j - x_k|^\alpha} \mathcal{L}_{\mathcal{I}_l} u_\epsilon \right\|_{L^2} \left\| \frac{1}{|x_j - x_k|^{1-\alpha}} [S^* v] \right\|_{L^2} ds.
\end{aligned}$$

By the Hölder inequality, we have

$$\left\| \frac{v}{|x_j - x_k|^{1-\alpha}} \right\|_2 \leq \left\| \frac{1}{|x|^{1-\alpha}} \right\|_{L^{\tilde{r}}(\mathbb{B}(0,1))} \|v\|_{L_{j,k}^{\tilde{p},2}} + \|v\|_{L^2} \lesssim_{\alpha, \tilde{p}} \|v\|_{L_{j,k}^{\tilde{p},2}} + \|v\|_{L^2}, \quad (4.3a)$$

$$\left\| \frac{u_\epsilon}{|x_j - x_k|^\alpha} \right\|_2 \leq \left\| \frac{1}{|x|^\alpha} \right\|_{L^r(\mathbb{B}(0,1))} \|u_\epsilon\|_{L_{j,k}^{p,2}} + \|u_\epsilon\|_{L^2} \lesssim_{\alpha, p} \|u_\epsilon\|_{L_{j,k}^{p,2}} + \|u_\epsilon\|_{L^2}, \quad (4.3b)$$

for $1/2 = 1/p + 1/r$, $1/2 = 1/\tilde{p} + 1/\tilde{r}$, $\tilde{p}, p \leq 6$, $\alpha r < 3$, $(1-\alpha)\tilde{r} < 3$, namely

$$\frac{6}{1+2\alpha} < \tilde{p} \leq 6, \quad \frac{6}{3-2\alpha} < p \leq 6.$$

Then

$$\begin{aligned}
& \int_0^T \langle [S \mathcal{L}_{\mathcal{I}_l} W_\epsilon u_\epsilon](t), v(t) \rangle dt \\
& \lesssim_{\alpha, p, \tilde{p}} \int_0^T \left(\|\mathcal{L}_{\mathcal{I}_l} u_\epsilon\|_{L_{j,k}^{p,2}} + \|\mathcal{L}_{\mathcal{I}_l} u_\epsilon\|_{L^2} \right) \left(\|[S^* v]\|_{L_{j,k}^{\tilde{p},2}} + \|[S^* v]\|_{L^2} \right) ds \\
& \lesssim_{\alpha, p, \tilde{p}} \left(\|\mathcal{L}_{\mathcal{I}_l} u_\epsilon\|_{L_t^{\theta'_p}(L_{j,k}^{p,2})} + \|\mathcal{L}_{\mathcal{I}_l} u_\epsilon\|_{L_t^{\theta'_p}(L^2)} \right) \|[S^* v]\|_{L_t^{\theta_{\tilde{p}}}(L_{j,k}^{\tilde{p},2})} \\
& \quad + \left(\|\mathcal{L}_{\mathcal{I}_l} u_\epsilon\|_{L_t^1(L_{j,k}^{p,2})} + \|\mathcal{L}_{\mathcal{I}_l} u_\epsilon\|_{L_t^1(L^2)} \right) \|[S^* v]\|_{L_t^\infty(L^2)} \\
& \lesssim_{\alpha, p, \tilde{p}} T^{1/\theta'_p - 1/\theta_p} \left(\|\mathcal{L}_{\mathcal{I}_l} u_\epsilon\|_{L_t^{\theta_p}(L_{j,k}^{p,2})} + \|\mathcal{L}_{\mathcal{I}_l} u_\epsilon\|_{L_t^{\theta_p}(L^2)} \right) \|[S^* v]\|_{L_t^{\theta_{\tilde{p}}}(L_{j,k}^{\tilde{p},2})} \\
& \quad + T^{1-1/\theta_p} \left(\|\mathcal{L}_{\mathcal{I}_l} u_\epsilon\|_{L_t^1(L_{j,k}^{p,2})} + \|\mathcal{L}_{\mathcal{I}_l} u_\epsilon\|_{L_t^1(L^2)} \right) \|[S^* v]\|_{L_t^\infty(L^2)} \\
& \lesssim_{\alpha, p, \tilde{p}} T^{1/\theta} \|\mathcal{L}_{\mathcal{I}_l} u_\epsilon\|_X \|v\|_{L_t^{\theta'_q}(L_D^{q',2})}.
\end{aligned}$$

Choosing a sequence $\|v_n\|_{L_t^{\theta'_q}(L_D^{q',2})} = 1$, for $q = 2$ or $\frac{6}{3-2\alpha} < q \leq 6$ such that

$$\|S \mathcal{L}_{\mathcal{I}_l} W(x_j, x_k) u_\epsilon\|_{L_t^{\theta_q}(L_D^{q,2})} = \lim_{n \rightarrow \infty} \left| \langle S \mathcal{L}_{\mathcal{I}_l} W(x_j, x_k) u_\epsilon, v_n \rangle_{L_t^{\theta_q}(L_D^{q,2}), L_t^{\theta'_q}(L_D^{q',2})} \right|.$$

Let $L_t^{\theta_q}(L_D^{q,2}) = L_t^\infty(L^2)$ or $L_t^{\theta_p}(L_{i,j}^{p,2})$ or $L_t^{\theta_q}(L_k^{q,2})$. Then,

$$\|S\mathcal{L}_{\mathcal{I}_l}W(x_j, x_k)u_\epsilon\|_X \lesssim_{\alpha, p, \tilde{p}, q} T^{1/\theta} \|\mathcal{L}_{\mathcal{I}_l}u_\epsilon\|_X.$$

Similarly, there is a $\frac{6}{1+2\alpha} < \tilde{q} \leq 6$, such that

$$\begin{aligned} & \int_0^T \langle [S\mathcal{L}_{\mathcal{I}_l}V(x_j, \cdot)u_\epsilon](t), v(t) \rangle dt \\ & \lesssim_{\alpha, p, \tilde{q}, q} \sum_\mu Z_\mu T^{1/\theta} \|\mathcal{L}_{\mathcal{I}_l}u_\epsilon\|_X \|v\|_{L_t^{\theta'_p}(L_D^{p',2})}, \end{aligned}$$

and

$$\|S\mathcal{L}_{\mathcal{I}_l}V(x_j, \cdot)u_\epsilon\|_X \lesssim_{\alpha, \tilde{p}, p, \tilde{q}, q} \sum_\mu Z_\mu T^{1/\theta} \|\mathcal{L}_{\mathcal{I}_l}u_\epsilon\|_X.$$

Hence, there is a constant C_1 only dependent on α , \tilde{p} , p , \tilde{q} and q , such that

$$\|\mathcal{L}_{\mathcal{I}_l}Q_\epsilon u_\epsilon\|_X \leq C_1 \left(\sum_\mu Z_\mu + N \right) NT^{1/\theta} \|\mathcal{L}_{\mathcal{I}_l}u_\epsilon\|_X. \quad (4.4)$$

Let $C_1(\sum_\mu Z_\mu + N)NT^{1/\theta} < 1/2$, by Equation (4.2) we have

$$\|\mathcal{L}_{\mathcal{I}_l}u_\epsilon\|_X \leq \|U_0\mathcal{L}_{\mathcal{I}_l}v_0\|_X + 1/2\|\mathcal{L}_{\mathcal{I}_l}u_\epsilon\|_X,$$

thus,

$$\|\mathcal{L}_{\mathcal{I}_l}u_\epsilon\|_X \leq 2\|U_0\mathcal{L}_{\mathcal{I}_l}v_0\|_X \lesssim_{p,q} \|\mathcal{L}_{\mathcal{I}_l}v_0\|_{L^2}.$$

Let $\epsilon \rightarrow 0$ and $\mathcal{L}_{\mathcal{I}_l}v_0 \rightarrow \mathcal{L}_{\mathcal{I}_l}u_0$ in L^2 , we know

$$\|\mathcal{L}_{\mathcal{I}_l}u\|_X \lesssim_{p,q} \|\mathcal{L}_{\mathcal{I}_l}u_0\|_{L^2},$$

which implies

$$u_\epsilon \xrightarrow{*} u \text{ in } X.$$

We also have these other convergences:

$$V_\epsilon \rightarrow V \text{ in } L_t^\infty(L_x^\infty) + L_t^\infty(L_x^r),$$

and

$$W_\epsilon \rightarrow W \text{ in } L_t^\infty(L_x^\infty) + L_t^\infty(L_x^r).$$

with $0 < r < 3$.

Thus u is the solution in the sense of distributions and satisfies $\mathcal{L}_{\mathcal{I}_l}u \in X$. And the uniqueness is because of the uniqueness of the solution in L^2 . \square

Combining the Theorem 2.10, we can prove the Theorem 1.8.

Proof of Theorem 1.8. Denote

$$\mathcal{K}_{\mathcal{I}_l, j} = \prod_{i \neq j} (1 - \Delta_i)^{1/2}$$

and

$$\mathcal{K}_{\mathcal{I}_l, j, k} = \prod_{i \neq j, k} (1 - \Delta_i)^{1/2}.$$

Analogously, we study the term $SKW_\epsilon(x_j, x_k)u_\epsilon(\cdot)$ firstly. If $j, k \in \mathcal{I}_l$,

$$\mathcal{K}_{\mathcal{I}_l} \cdot \mathcal{K}_{\mathcal{I}_l} = \mathcal{K}_{\mathcal{I}_l, j, k} \cdot \mathcal{K}_{\mathcal{I}_l, j, k} (1 - \nabla_j \cdot \nabla_j - \nabla_k \cdot \nabla_k + (-\nabla_j \cdot \nabla_j)(-\nabla_k \cdot \nabla_k)),$$

then

$$\begin{aligned} & \int_0^T \langle SK_{\mathcal{I}_l} W_\epsilon(x_j, x_k) u_\epsilon, \mathcal{K}_{\mathcal{I}_l} v \rangle \\ &= \langle SW_\epsilon(x_j, x_k) \mathcal{K}_{\mathcal{I}_l, j, k} u_\epsilon, \mathcal{K}_{\mathcal{I}_l, j, k} v \rangle \\ &+ \langle S \nabla_j W_\epsilon(x_j, x_k) \mathcal{K}_{\mathcal{I}_l, j, k} u_\epsilon, \nabla_j \mathcal{K}_{\mathcal{I}_l, j, k} v \rangle \\ &+ \langle S \nabla_k W_\epsilon(x_j, x_k) \mathcal{K}_{\mathcal{I}_l, j, k} u_\epsilon, \nabla_k \mathcal{K}_{\mathcal{I}_l, j, k} v \rangle \\ &+ \langle S \nabla_j \nabla_k W_\epsilon(x_j, x_k) \mathcal{K}_{\mathcal{I}_l, j, k} u_\epsilon, \nabla_j \nabla_k \mathcal{K}_{\mathcal{I}_l, j, k} v \rangle. \end{aligned}$$

After calculation, we have

$$\begin{aligned} & \int_0^T \langle SK_{\mathcal{I}_l} W_\epsilon(x_j, x_k) u_\epsilon, \mathcal{K}_{\mathcal{I}_l} v \rangle \\ & \lesssim_{\alpha, p, \tilde{p}} \int_0^T \left(\|\mathcal{K}_{\mathcal{I}_l, j, k} u_\epsilon\|_{L_{\mathcal{I}_l, j, k}^{p, 2}} + \|\mathcal{K}_{\mathcal{I}_l, j, k} u_\epsilon\|_{L^2} \right) \\ & \quad \times \left(\| [S^* \mathcal{K}_{\mathcal{I}_l, j, k} v] \|_{L_{j, k}^{\tilde{p}, 2}} + \| [S^* \mathcal{K}_{\mathcal{I}_l, j, k} v] \|_{L^2} \right) ds \\ & + \int_0^T \left(\|\nabla_j \mathcal{K}_{\mathcal{I}_l, j, k} u_\epsilon\|_{L_{\mathcal{I}_l, j, k}^{p, 2}} + \|\nabla_j \mathcal{K}_{\mathcal{I}_l, j, k} u_\epsilon\|_{L^2} \right) \\ & \quad \times \left(\| [S^* \nabla_j \mathcal{K}_{\mathcal{I}_l, j, k} v] \|_{L_{j, k}^{\tilde{p}, 2}} + \| [S^* \nabla_j \mathcal{K}_{\mathcal{I}_l, j, k} v] \|_{L^2} \right) ds \\ & + \int_0^T \left(\|\nabla_k \mathcal{K}_{\mathcal{I}_l, j, k} u_\epsilon\|_{L_{j, k}^{p, 2}} + \|\nabla_k \mathcal{K}_{\mathcal{I}_l, j, k} u_\epsilon\|_{L^2} \right) \\ & \quad \times \left(\| [S^* \nabla_k \mathcal{K}_{\mathcal{I}_l, j, k} v] \|_{L_{j, k}^{\tilde{p}, 2}} + \| [S^* \nabla_k \mathcal{K}_{\mathcal{I}_l, j, k} v] \|_{L^2} \right) ds \\ & + \int_0^T \left(\|\nabla_j \nabla_k \mathcal{K}_{\mathcal{I}_l, j, k} u_\epsilon\|_{L_{j, k}^{p, 2}} + \|\nabla_j \nabla_k \mathcal{K}_{\mathcal{I}_l, j, k} u_\epsilon\|_{L^2} \right) \\ & \quad \times \left(\| [S^* \nabla_j \nabla_k \mathcal{K}_{\mathcal{I}_l, j, k} v] \|_{L_{\mathcal{I}_l, j, k}^{\tilde{p}, 2}} + \| [S^* \nabla_j \nabla_k \mathcal{K}_{\mathcal{I}_l, j, k} v] \|_{L^2} \right) ds \end{aligned}$$

By the Theorem 2.10, we have for $p, \tilde{p} = 2$ or $\frac{6}{3-2\alpha} < p, \tilde{p} \leq 6$

$$\|\nabla_j^{l_1} \nabla_k^{l_2} \mathcal{K}_{\mathcal{I}_l, j, k} v\|_{L_{\mathcal{I}_l, j, k}^{\tilde{p}, 2}} \lesssim_{\tilde{p}} \|\mathcal{K}_{\mathcal{I}_l} v\|_{L_{j, k}^{\tilde{p}, 2}}, \quad l_1, l_2 = 0, 1.$$

and same for u_ϵ . Then, we yield

$$\begin{aligned} & \int_0^T \langle SK_{\mathcal{I}_l} W_\epsilon(x_j, x_k) u_\epsilon, \mathcal{K}_{\mathcal{I}_l} v \rangle \\ & \lesssim_{\alpha, p, \tilde{p}} \int_0^T \left(\|\mathcal{K}_{\mathcal{I}_l} u_\epsilon\|_{L_{j, k}^{p, 2}} + \|\mathcal{K}_{\mathcal{I}_l} u_\epsilon\|_{L^2} \right) \\ & \quad \times \left(\| [S^* \mathcal{K}_{\mathcal{I}_l} v] \|_{L_{j, k}^{p, 2}} + \| [S^* \mathcal{K}_{\mathcal{I}_l} v] \|_{L^2} \right) ds. \end{aligned}$$

If $j \in \mathcal{I}_l$ and $k \notin \mathcal{I}_l$,

$$\mathcal{K}_{\mathcal{I}_l} \cdot \mathcal{K}_{\mathcal{I}_l} = \mathcal{K}_{\mathcal{I}_l, j} \cdot \mathcal{K}_{\mathcal{I}_l, j} (1 - \nabla_j \cdot \nabla_j)$$

then

$$\begin{aligned} & \int_0^T \langle S \mathcal{K}_{\mathcal{I}_l} W_\epsilon(x_j, x_k) u_\epsilon, \mathcal{K}_{\mathcal{I}_l} v \rangle \\ &= \langle S W_\epsilon(x_j, x_k) \mathcal{K}_{\mathcal{I}_l, j} u_\epsilon, \mathcal{K}_{\mathcal{I}_l, j} v \rangle \\ & \quad + \langle S \nabla_j W_\epsilon(x_j, x_k) \mathcal{K}_{\mathcal{I}_l, j} u_\epsilon, \nabla_j \mathcal{K}_{\mathcal{I}_l, j} v \rangle. \end{aligned}$$

Repeating the above calculation and by Theorem 2.10, we have

$$\begin{aligned} & \int_0^T \langle S \mathcal{K}_{\mathcal{I}_l} W_\epsilon(x_j, x_k) u_\epsilon, \mathcal{K}_{\mathcal{I}_l} v \rangle \\ & \lesssim_{\alpha, p, \tilde{p}} \int_0^T \left(\|\mathcal{K}_{\mathcal{I}_l} u_\epsilon\|_{L_{j,k}^{p,2}} + \|\mathcal{K}_{\mathcal{I}_l} u_\epsilon\|_{L^2} \right) \\ & \quad \times \left(\|[S^* \mathcal{K}_{\mathcal{I}_l} v]\|_{L_{j,k}^{\tilde{p},2}} + \|[S^* \mathcal{K}_{\mathcal{I}_l} v]\|_{L^2} \right) ds. \end{aligned}$$

Analogously for $j \notin \mathcal{I}_l$ and $k \in \mathcal{I}_l$. Finally if $i, k \notin \mathcal{I}_l$, obviously

$$\int_0^T \langle S \mathcal{K}_{\mathcal{I}_l} W_\epsilon(x_j, x_k) u_\epsilon, \mathcal{K}_{\mathcal{I}_l} v \rangle = \langle S W_\epsilon(x_j, x_k) \mathcal{K}_{\mathcal{I}_l} u_\epsilon, \mathcal{K}_{\mathcal{I}_l} v \rangle.$$

after calculation, we have

$$\begin{aligned} & \int_0^T \langle S \mathcal{K}_{\mathcal{I}_l} W_\epsilon(x_j, x_k) u_\epsilon, \mathcal{K}_{\mathcal{I}_l} v \rangle \\ & \lesssim_{p, \tilde{p}} \int_0^T \left(\|\mathcal{K}_{\mathcal{I}_l} u_\epsilon\|_{L_{j,k}^{p,2}} + \|\mathcal{K}_{\mathcal{I}_l} u_\epsilon\|_{L^2} \right) \\ & \quad \times \left(\|[S^* \mathcal{K}_{\mathcal{I}_l} v]\|_{L_{j,k}^{\tilde{p},2}} + \|[S^* \mathcal{K}_{\mathcal{I}_l} v]\|_{L^2} \right) ds. \end{aligned}$$

Thus, for any $1 \leq j < k \leq N$, we have

$$\begin{aligned} & \int_0^T \langle S \mathcal{K}_{\mathcal{I}_l} W_\epsilon(x_j, x_k) u_\epsilon, \mathcal{K}_{\mathcal{I}_l} v \rangle \\ & \lesssim_{\alpha, \tilde{p}, p, \tilde{q}, q} \int_0^T \left(\|\mathcal{K}_{\mathcal{I}_l} u_\epsilon\|_{L_{j,k}^{p,2}} + \|\mathcal{K}_{\mathcal{I}_l} u_\epsilon\|_{L^2} \right) \\ & \quad \times \left(\|[S^* \mathcal{K}_{\mathcal{I}_l} v]\|_{L_{j,k}^{\tilde{p},2}} + \|[S^* \mathcal{K}_{\mathcal{I}_l} v]\|_{L^2} \right) ds. \end{aligned}$$

And similarly for the term $S \mathcal{K}_{\mathcal{I}_l} V_\epsilon u_\epsilon$.

Repeating the same procedure of Theorem 1.5, there is a constant C_2 only dependent on $\alpha, \tilde{p}, p, \tilde{q}$ and q such that

$$\|\mathcal{K}_{\mathcal{I}_l} Q_\epsilon u_\epsilon\|_X \leq C_2 \left(\sum_\mu Z_\mu + N \right) N T^{1/\theta} \|\mathcal{K}_{\mathcal{I}_l} u_\epsilon\|_X. \quad (4.5)$$

And if $C_2 (\sum_\mu Z_\mu + N) N T^{1/\theta} < 1/2$, we can get

$$\|\mathcal{K}_{\mathcal{I}_l} u_\epsilon\|_X \lesssim_{p,q} \|\mathcal{K}_{\mathcal{I}_l} v_0\|_{L^2}.$$

Taking $\epsilon \rightarrow 0$ and $\mathcal{L}_{\mathcal{I}_l} v_0 \rightarrow \mathcal{L}_{\mathcal{I}_l} u_0$ in L^2 , we have

$$\|\mathcal{K}_{\mathcal{I}_l} u\|_X \lesssim_{p,q} \|\mathcal{K}_{\mathcal{I}_l} u_0\|_{L^2}.$$

Consequently, u is the solution in the sense of distribution and satisfies $\mathcal{K}_{\mathcal{I}_l} u \in X$. \square

5 Numerical Analysis

Lemma 5.1. *Under the assumption of Theorem 1.10, we have*

$$\|u - P_R u\|_X \lesssim_{p,q} 1/R \sum_{1 \leq l \leq s} \|\mathcal{K}_{\mathcal{I}_l} u_0\|_{L^2}$$

Proof. By the Equation (2.1), we know

$$(P_R u)(t) = (P_R U_0(t) u_0) + i(P_R Q u(t)).$$

Thus,

$$\|u - P_R u\|_X \leq \|(1 - P_R) U_0 u_0\|_X + \|(1 - P_R) Q u\|_X.$$

By the definition of P_R and Lemma 2.7, we know

$$\|(1 - P_R) U_0 u\|_X \lesssim_{p,q} \|(1 - P_R) u_0\|_{L^2} \lesssim_{p,q} 1/R \sum_{1 \leq l \leq s} \|\mathcal{K}_{\mathcal{I}_l} u_0\|_{L^2}.$$

Instead of studying $(1 - P_R) Q u$ directly, we study $(1 - P_R) Q_\epsilon u_\epsilon$ with the initial datum $v_0 \in C_0^\infty((\mathbb{R}^3)^N)$, and then take them to the limit. So we just need to consider the term $(1 - P_R) S(V_\epsilon(j, \cdot) u_\epsilon)$ and $(1 - P_R) S(W_\epsilon(x_j, x_k) u_\epsilon)$. They are similar, so we just deal with the latter.

We consider the following inner product

$$\begin{aligned} & \int_0^T \left\langle (1 - P_R) S(W_\epsilon(x_j, x_k) u_\epsilon), \sum_{1 \leq l \leq s} \mathcal{K}_{\mathcal{I}_l} v \right\rangle dt \\ &= \sum_{1 \leq l \leq s} \int_0^T \langle \mathcal{K}_{\mathcal{I}_l} S(W_\epsilon(x_j, x_k) u_\epsilon), (1 - P_R) v \rangle dt. \end{aligned}$$

Let

$$\tilde{\mathcal{K}}_{\mathcal{I}_l, j} = (1 + \nabla_j) \prod_{l \neq j} (1 - \Delta_l)^{1/2},$$

$$\tilde{\mathcal{K}}_{\mathcal{I}_l, j, k} = (1 + \nabla_j) \otimes (1 + \nabla_k) \prod_{l \neq j, k} (1 - \Delta_l)^{1/2},$$

and

$$\tilde{\mathcal{K}}^j = \frac{(1 - \nabla_j)}{(1 - \Delta_j)^{1/2}}.$$

$$\tilde{\mathcal{K}}^{j, k} = \frac{(1 - \nabla_j) \otimes (1 - \nabla_k)}{(1 - \Delta_j)^{1/2} (1 - \Delta_k)^{1/2}}.$$

Then,

$$\mathcal{K}_{\mathcal{I}_l} = \tilde{\mathcal{K}}^j \cdot \tilde{\mathcal{K}}_{\mathcal{I}_l, j} = \tilde{\mathcal{K}}^{j, k} \cdot \tilde{\mathcal{K}}_{\mathcal{I}_l, j, k}.$$

If $j, k \in \mathcal{I}_l$, we consider the following inner product

$$\begin{aligned} & \int_0^T \langle \mathcal{K}_{\mathcal{I}_l} S(W_\epsilon(x_j, x_k)u_\epsilon), (1 - P_R)v \rangle dt \\ &= \int_0^T \langle \tilde{\mathcal{K}}_{\mathcal{I}_l, j, k}^* (W_\epsilon(x_j, x_k)u_\epsilon), S^*(1 - P_R)\tilde{\mathcal{K}}^{j, k}v \rangle ds \\ &= \int_0^T \langle (1 - \nabla_j)(1 - \nabla_k)(W_\epsilon(x_j, x_k)\mathcal{K}_{\mathcal{I}_l, j, k}u_\epsilon), S^*(1 - P_R)\tilde{\mathcal{K}}^{j, k}v \rangle ds. \end{aligned}$$

Or if $j \in \mathcal{I}_l$ and $k \notin \mathcal{I}_l$, we consider the following inner product

$$\begin{aligned} & \int_0^T \langle \mathcal{K}_{\mathcal{I}_l} S(W_\epsilon(x_j, x_k)u_\epsilon), (1 - P_R)v \rangle dt \\ &= \int_0^T \langle \tilde{\mathcal{K}}_{\mathcal{I}_l, j}^* (W_\epsilon(x_j, x_k)u_\epsilon), S^*(1 - P_R)\tilde{\mathcal{K}}^jv \rangle ds \\ &= \int_0^T \langle (1 - \nabla_j)(W_\epsilon(x_j, x_k)\mathcal{K}_{\mathcal{I}_l, j, k}u_\epsilon), S^*(1 - P_R)\tilde{\mathcal{K}}^jv \rangle ds. \end{aligned}$$

Analogously for $j \notin \mathcal{I}_l$ and $k \in \mathcal{I}_l$. And finally, if $j, k \notin \mathcal{I}_l$,

$$\int_0^T \langle \mathcal{K}_{\mathcal{I}_l} S(W_\epsilon(x_j, x_k)u_\epsilon), (1 - P_R)v \rangle dt = \int_0^T \langle (W_\epsilon(x_j, x_k)\mathcal{K}_{\mathcal{I}_l}u_\epsilon), S^*(1 - P_R)v \rangle dt.$$

Before repeating the proof of Theorem 1.8, we only need to deal with

$$\|S^*(1 - P_R)\tilde{\mathcal{K}}^jv\|_{L_t^{\theta_{\tilde{p}}}(L_{j, k}^{\tilde{p}, 2})}$$

and

$$\|S^*(1 - P_R)\tilde{\mathcal{K}}^{j, k}v\|_{L_t^{\theta_{\tilde{p}}}(L_{j, k}^{\tilde{p}, 2})}.$$

By Theorem 2.10 and Corollary 2.9, we know

$$\begin{aligned} \|S^*(1 - P_R)\tilde{\mathcal{K}}^jv\|_{L_t^{\theta_{\tilde{p}}}(L_{j, k}^{\tilde{p}, 2})} &\lesssim_{\tilde{p}, p, q} \|S^*(1 - P_R)v\|_{L_t^{\theta_{\tilde{p}}}(L_{j, k}^{\tilde{p}, 2})} \\ &\lesssim_{\tilde{p}, p, q} 1/R \left\| \sum_l \mathcal{K}_{\mathcal{I}_l}v \right\|_{L_t^{\theta'_q}(L_D^{q', 2})} \end{aligned}$$

and

$$\begin{aligned} \|S^*(1 - P_R)\tilde{\mathcal{K}}^{j, k}v\|_{L_t^{\theta_{\tilde{p}}}(L_{j, k}^{\tilde{p}, 2})} &\lesssim_{\tilde{p}, p, q} \|S^*(1 - P_R)v\|_{L_t^{\theta_{\tilde{p}}}(L_{j, k}^{\tilde{p}, 2})} \\ &\lesssim_{\tilde{p}, p, q} 1/R \left\| \sum_l \mathcal{K}_{\mathcal{I}_l}v \right\|_{L_t^{\theta'_q}(L_D^{q', 2})}. \end{aligned}$$

Now, we know

$$\begin{aligned} & \int_0^T \langle \mathcal{K}_{\mathcal{I}_l} S(W_\epsilon(x_j, x_k)u_\epsilon), (1 - P_R)v \rangle dt \\ &\lesssim_{\alpha, \tilde{p}, p, \tilde{q}, q} T^{1/\theta} / R \| \mathcal{K}_{\mathcal{I}_l}u_\epsilon \|_X \left\| \sum_l \mathcal{K}_{\mathcal{I}_l}v \right\|_{L_t^{\theta'_q}(L_D^{q', 2})}. \end{aligned}$$

Thus,

$$\begin{aligned} & \int_0^T \left\langle (1 - P_R)S(W_\epsilon(x_j, x_k)u_\epsilon), \sum_{1 \leq l \leq s} \mathcal{K}_{\mathcal{I}_l} v \right\rangle dt \\ & \lesssim_{\alpha, \tilde{p}, p, \tilde{q}, q} T^{1/\theta} / R \left(\sum_{1 \leq l \leq s} \|\mathcal{K}_{\mathcal{I}_l} u_\epsilon\|_X \right) \left\| \sum_l \mathcal{K}_{\mathcal{I}_l} v \right\|_{L_t^{\theta'_q} (L_D^{q', 2})}. \end{aligned}$$

Therefore,

$$\|(1 - P_R)S(W_\epsilon(x_j, x_k)u_\epsilon)\|_X \lesssim_{\alpha, \tilde{p}, p, \tilde{q}, q} T^{1/\theta} / R \sum_{1 \leq l \leq s} \|\mathcal{K}_{\mathcal{I}_l} u_\epsilon\|_X.$$

Similarly for the term $(1 - P_R)S(V_\epsilon(x_j, \cdot)u_\epsilon)$

Hence, there is a constant $C_3 > C_2$ only dependent on $\alpha, \tilde{p}, p, \tilde{q}$ and q , such that

$$\|(1 - P_R)Q_\epsilon u_\epsilon\|_X \leq C_3 \left(\sum_\mu Z_\mu + N \right) NT^{1/\theta} / R \sum_{1 \leq l \leq s} \|\mathcal{K}_{\mathcal{I}_l} u_\epsilon\|_X. \quad (5.1)$$

If $C_3(\sum_\mu Z_\mu + N)NT^{1/\theta} < 1/2$, then $C_2(\sum_\mu Z_\mu + N)NT^{1/\theta} < 1/2$. By Theorem 1.8 we have

$$\|\mathcal{K}_{\mathcal{I}_l} u_\epsilon\|_X \lesssim_{p, q} \|\mathcal{K}_{\mathcal{I}_l} u_0\|_{L^2}.$$

Thus

$$\|(1 - P_R)Q_\epsilon u_\epsilon\|_X \leq 1/R \sum_{1 \leq l \leq s} \|\mathcal{K}_{\mathcal{I}_l} u_\epsilon\|_X \lesssim_{p, q} 1/R \sum_{1 \leq l \leq s} \|\mathcal{K}_{\mathcal{I}_l} u_0\|_{L^2}.$$

Therefore,

$$\|u_\epsilon - P_R u_\epsilon\|_X \lesssim_{p, q} 1/R \sum_{1 \leq l \leq s} \|\mathcal{K}_{\mathcal{I}_l} u_0\|_{L^2}.$$

Finally, taking $\epsilon \rightarrow 0$, we have

$$\|u - P_R u\|_X \lesssim_{p, q} 1/R \sum_{1 \leq l \leq s} \|\mathcal{K}_{\mathcal{I}_l} u_0\|_{L^2}.$$

□

Proof of Theorem 1.10. The proof of existence is similar to Theorem 1.2 except the following modification:

$$\int_0^T \langle P_R S W(x_i, x_j) u(t), v \rangle dt = \int_0^T \langle S W(x_i, x_j) u(t), P_R v \rangle ds$$

Given the symmetry of the projector P_R , we know if the Equation (1.10) has a solution, the solution u_R keeps the spin states. For the existence, we only need study the term

$$\|P_R S^* v\|_{L_t^{\theta'_p} (L_D^{\tilde{p}', 2})}.$$

By the Corollary 2.9, we have

$$\|P_R S^* v\|_{L_t^{\theta'_q} (L_D^{q, 2})} \lesssim_{\tilde{p}, p} \|v\|_{L_t^{\theta'_p} (L_D^{\tilde{p}', 2})}.$$

Thus by Theorem 1.2 and under the assumption of Theorem 1.10, for the Equation (1.10), there exists a unique solution u_R , such that

$$\|u\|_X \lesssim_{p, q} \|u_0\|_{L^2}.$$

Instead of studying $\|u - u_R\|_X$ directly, we consider $\|P_R - u_R\|_X$ at the beginning. By the Formula 2.1, we know

$$u_R - P_R u = iP_R Q(u - u_R)$$

Repeating the above process, and under the assumption of Theorem 1.8, we know

$$\|u_R - P_R u\|_X \leq 1/2 \|u - u_R\|_X \leq 1/2 \|u_R - P_R u\|_X + 1/2 \|u - P_R u\|_X$$

Then,

$$\|u_R - P_R u\|_X \leq \|u - P_R u\|_X \lesssim_{p,q} 1/R \sum_{1 \leq l \leq s} \|\mathcal{K}_{\mathcal{I}_l} u_0\|_{L^2}.$$

Finally, we know

$$\|u - u_R\|_X \leq \|u - P_R u\|_X + \|u_R - P_R u\|_X \lesssim_{p,q} 1/R \sum_{1 \leq l \leq s} \|\mathcal{K}_{\mathcal{I}_l} u_0\|_{L^2}.$$

□

A The Calderón-Zygmund Inequality

Unlike the usual Calderón-Zygmund inequality, we need to prove a new one which is compatible for our special functional space. But the proof is similar, so we just give the sketch of proof, for the details, see [52, p.27-38].

Definition A.1. Let $n \in \mathbb{N}$ and let $\Delta_n := \{(x, y) \in \mathbb{R}^n \times \mathbb{R}^n | x = y\}$ be the diagonal in $\mathbb{R}^n \times \mathbb{R}^n$. Fix two constants $C > 0$ and $0 < \sigma \leq 1$. A Calderón-Zygmund pair on \mathbb{R}^n with constants C and σ is a pair (T_x, K) , consisting of a bounded linear operator $T_x : L^2(\mathbb{R}^n, \mathbb{C}) \rightarrow L^2(\mathbb{R}^n, \mathbb{C})$ working on variable $x \in \mathbb{R}^n$ and a continuous function $K : (\mathbb{R}^n \times \mathbb{R}^n) \setminus \Delta_n \rightarrow \mathbb{C}$, satisfying the following axioms.

- $\|T_x f\|_{L^2} \leq C \|f\|_{L^2}$ for all $f \in L^2(\mathbb{R}^n \times \mathbb{R}^m, \mathbb{C})$.
- For $(x, z) \in \mathbb{R}^n \times \mathbb{R}^m$, if $f(x, z) : \mathbb{R}^n \times \mathbb{R}^m \rightarrow \mathbb{C}$ is a continuous function with compact support then

$$(T_x f)(x, z) = \int_{\mathbb{R}^n} K(x, y) f(y, z) dy.$$

- Let $x, y \in \mathbb{R}^n$ such that $x \neq y$. Then

$$|K(x, y)| \leq \frac{C}{|x - y|^n}.$$

- Let $x, x', y, y' \in \mathbb{R}^n$ such that $x \neq y$, $x' \neq y'$, and $x' \neq y$. Then

$$|y - y'| < \frac{1}{2} |x - y| \implies |K(x, y) - K(x, y')| \leq \frac{C |y - y'|^\sigma}{|x - y|^{n+\sigma}},$$

$$|x - x'| < \frac{1}{2} |x - y| \implies |K(x, y) - K(x', y)| \leq \frac{C |x - x'|^\sigma}{|x - y|^{n+\sigma}}.$$

Theorem A.2. Fix an integer $m, n \in \mathbb{N}$, a real number $1 < p < \infty$, and two constants $C > 0$ and $0 < \sigma \leq 1$. Then there exists a constant $c = c(n, p, \sigma, C)$ such that every Calderón-Zygmund pair (T_x, K) working only on the variable $x \in \mathbb{R}^n$ with constant C and σ satisfies the inequality

$$\|T_x f(x, y)\|_{L^p(\mathbb{R}^n, L^2(\mathbb{R}^m))} \leq c \|f(x, y)\|_{L^p(\mathbb{R}^n, L^2(\mathbb{R}^m))}$$

for all $f \in L^2(\mathbb{R}^{n+m}, \mathbb{C}) \cap L^p(\mathbb{R}^n, L^2(\mathbb{R}^m))$.

Sketch of proof. Let $b_f(x) = \left(\int_{\mathbb{R}^m} |f(x, y)|^2 dy\right)^{1/2}$, and μ the Lebesgue measure on \mathbb{R}^n . Then define the function $\kappa_f : (0, \infty) \rightarrow [0, \infty]$ by

$$\kappa_f(t) := \mu(\{t \geq 0 \mid |b_f(x)| > t\}) \quad \text{for } t > 0.$$

We shorten the operator T_x by T without confusion.

Step 1. (Calderón Zygmund Decomposition).

Decompose $b_f(x)$ in place of $f(x, y)$ directly. Then for $t > 0$, there exists a countable collection of closed cubes $Q_i \subset \mathbb{R}^n$ with pairwise disjoint interiors such that

$$\mu(Q_i) < \frac{1}{t} \int_{Q_i} |b_f(x)| dx \leq 2^n \mu(Q_i) \quad \text{for all } i \in \mathbb{N}$$

and

$$|b_f(x)| \leq t \quad \text{for almost all } x \in \mathbb{R}^n \setminus B$$

where $B := \cup_{i=1}^{\infty} Q_i$.

Step 2. (Construction of function).

Define $g, h : \mathbb{R}^n \times \mathbb{R}^m \rightarrow \mathbb{R}$ by

$$g(x, y) := f(x, y) \mathbb{1}_{\mathbb{R}^n \setminus B} + \sum_i \frac{\int_{Q_i} f(x, y) dx}{\mu(Q_i)} \mathbb{1}_{Q_i}, \quad h := f - g.$$

Then,

$$b_g(x) = b_f(x) \leq t \quad \text{for almost all } x \in \mathbb{R}^n \setminus B, \tag{A.1}$$

and by Minkowski's inequality,

$$\begin{aligned} b_g(x) &= \frac{1}{\mu(Q_i)} \left(\int_{\mathbb{R}^m} \left| \int_{Q_i} f dx \right|^2 dy \right)^{1/2} \\ &\leq \frac{1}{\mu(Q_i)} \int_{Q_i} |b_f(x)| dx \quad \text{for } x \in B. \\ &\leq 2^n t \end{aligned} \tag{A.2}$$

Combining Equation (A.1) and Equation (A.2) together, we know

$$\|g\|_{L^1(L^2)} = \|b_g\|_{L^1} \leq \|b_f\|_{L^1} = \|f\|_{L^1(L^2)}, \quad \|h\|_{L^1(L^2)} \leq 2\|f\|_{L^1(L^2)}. \tag{A.3}$$

Hence, we have

$$\kappa_{Tg} \leq \frac{1}{t^2} \int_{\mathbb{R}^n} |b_g(x)|^2 dx \leq \frac{2^n}{t} \int_{\mathbb{R}^n} |b_g(x)| dx \leq \frac{2^n}{t} \int_{\mathbb{R}^n} |b_f(x)| dx \leq \frac{2^n}{t} \|f\|_{L^1(L^2)}.$$

Step 3. (Estimate for κ_{Th}). Define $h_i(x)$ by

$$h_i(x, y) = h(x, y) \mathbb{1}_{Q_i}.$$

Denote by $q_i \in Q_i$ the center of the cube Q_i and by $2r_i > 0$ its length. Then $|x - q_i| \leq \sqrt{n}r_i$ for all Q_i . Then we have

$$(Th_i)(x, y) = \int_{Q_i} K(x, z) h_i(z, y) dz = \int_{Q_i} (K(x, z) - K(x, q_i)) h_i(z, y) dz.$$

Hence, by Minkowski's inequality

$$b_{Th_i}(x) \leq \int_{Q_i} |K(x, z) - K(x, q_i)| |b_{h_i}(z)| dz.$$

Then, by the standard proof of Calderón-Zygmund inequality, we know, there is a constant c dependent on n such that

$$\kappa_{Th}(t) \leq c \left(\mu(B) + \frac{1}{t} \|b_h\|_{L^1} \right) \quad \text{for all } t > 0.$$

Besides,

$$\mu(B) = \sum_i \mu(Q_i) \leq \frac{1}{t} \sum_i \int_{Q_i} |b_f(x)| dx \leq \frac{1}{t} \|f\|_{L^1(L^2)}.$$

Together with Equation (A.3),

$$\kappa_{Th}(t) \leq \frac{3c}{t} \|f\|_{L^1(L^2)}.$$

By the triangle inequality, we know

$$b_{Tf}(x) \leq b_{Tg} + b_{Th},$$

therefore,

$$\kappa_{Tf}(2t) \leq \kappa_{Tg}(t) + \kappa_{Th}(t) \leq \frac{2^{n+1} + 6c}{2t} \|f\|_{L^1(L^2)}.$$

Finally, using the standard method, we get conclusion. \square

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

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

given by

$$T_a u := \widetilde{a\check{u}}$$

for $u \in L^2(\mathbb{R}^n \times \mathbb{R}^m, \mathbb{C})$, and \check{u} is the inverse Fourier Transform.

Theorem A.3. *For every integer $m, n \in \mathbb{N}$, every constant $C > 0$, and every real number $1 < p < \infty$, there exists a constant $c = c(n, p, C)$ with the following significance. Let $a : \mathbb{R}^n \setminus \{0\} \rightarrow \mathbb{C}$ be a C^{n+2} function that satisfies the inequality*

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

for every $\xi \in \mathbb{R}^n \setminus \{0\}$ and every multi-index $\alpha = (\alpha_1, \dots, \alpha_n) \in \mathbb{N}_0^n$ with $|\alpha| \leq n + 2$. Then

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

for all $f \in L^2(\mathbb{R}^n \times \mathbb{R}^m), \mathbb{C} \cap L^p(\mathbb{R}^n, L^2(\mathbb{R}^m))$.

The proof is same with the normal Mihlin Multiplier Theorem except using the Theorem A.2 instead of the normal one.

Part II

The Dirac-Fock models for crystals

Chapter 3

Existence of minimizers for Dirac-Fock models in crystals

In this paper, we introduce a relativistic crystal model inspired both from the atomic and molecular Dirac-Fock models and the non-relativistic Hartree-Fock type models for crystals. And we give a new definition for the ground state of this model by considering the Lieb's relaxed functional and the Fermi level. By Séré's retraction, the existence of minimizers for this model are proved, and every minimizer is the solution of a self-consistent equation.

1 Introduction

Whereas different models exist in the mathematical and physics literature for non-relativistic crystals, we are not aware of any for relativistic crystals. The aim of this paper is to propose a Dirac-Fock type model for ground states energies of relativistic crystals.

A natural way of building quantum models for the crystalline phase is to consider the so-called thermodynamic limit of quantum molecular models. Roughly speaking it consists in considering a finite but large piece of the (infinite and neutral) crystal. The thermodynamic law predicts that the ground state energy of the obtained large neutral molecule is proportional to the volume of this finite piece (which turns out to be also proportional to the total number of particles composing the molecule). The energy for the whole crystal is then identified with the limit – if it exists - of the energy per unit volume (or equivalently per particle) of the large molecule when the size of the considered piece goes to infinity.

This method has been successfully applied by different authors for different well-known models from quantum chemistry [43, 9, 7, 8]-see also [6] for a review- but always for non-relativistic crystals.

Concerning relativistic models, the atomic and molecular Dirac-Fock (DF) is the most attracting one since it has been formally justified by Mittleman [48], and gives

numerical results in excellent agreement with experimental data [34, 21, 10]. The mathematical study of this model has been done in [14, 49], but the situation, compared to the non-relativistic models, is different: The existence result for bound states only holds if the total positive charge Z is not too large (with physical units, $Z \leq 124$). On the other hand, relativistic effects have to be taken into account essentially for molecules with heavy atoms. This causes an important problem if we try to find a thermodynamic limit for the Dirac-Fock model, since we do not even know if there are bound states for large systems. Moreover, the energy functional of the atomic DF is strongly indefinite and the notion of ground state has to be handled very carefully (cf. [14])-anyway, no minimization procedure is available in this case. The similar procedure for crystals is harder than the atomic one.

On the other hand, Esteban and Séré [13] showed that certain solutions of the Dirac-Fock equations converge towards the energy-minimizing solutions of the non-relativistic Hartree-Fock equations when the speed of light tends to infinity. This allows mathematicians to define the notion of ground state solutions and ground state energy of the Dirac-Fock equations. By a simple fixed point theory and this new definition of the ground state of Dirac-Fock model, a similar result of Dirac-Fock model has been done by Huber and Siedentop [29]. Finally, Séré provided directly a retraction technique in [53] to construct the ground state of Dirac-Fock. Recently, based on Séré's retraction, the scott correction for Dirac-Fock models has been studied in [15]. Based on the work [53], we propose a ground state of Dirac-Fock model for crystals, and prove its existence.

Outline of the paper

Before giving the main statement, we pause to outline the structure of this paper:

- We first propose in Section 2 a Dirac-Fock-type periodic functional. This functional is simply derived from the periodic Hartree-Fock functional introduced in [7] in the same manner that the Dirac-Fock model for molecules is derived from the Hartree-Fock one; that is, again roughly speaking (see Section 2 for precise formulation), by replacing the Laplace operator by the Dirac operator and the functional space accordingly. Since the Dirac operator is not bounded below, we have to redefine the ground state: instead of defining it in the whole functional space by the critical point theory, we define it in the positive spectra of the periodic Dirac-Fock operator $D_{\gamma,\xi}$, namely $\Gamma_q^+ := \{\gamma; \text{Tr}_{L^2} \gamma = q, \mathbb{1}_{[0,\infty)}(D_{\gamma,\xi})\gamma = \gamma\}$. At the end, our main result is Theorem 2.13, and the solution also solves a self-consistent equation.
- In Section 3, we give some fundamental estimates which are useful for the next sections.
- In section 4, analogously to [53], we construct the bounded positive level of the energy $\Gamma_{\leq q}^+$ by using Séré's retraction: taking $T(\gamma) = \mathbb{1}_{[0,\infty)}(D_\gamma)\gamma\mathbb{1}_{[0,\infty)}(D_\gamma)$, and

we will see under some conditions, $T^n(\gamma) \rightarrow \theta(\gamma) \in \Gamma_{\leq q}^+$ with $\Gamma_{\leq q}^+ := \{\gamma; \text{Tr}_{L^2} \gamma \leq q, \mathbb{1}_{[0, \infty)}(D_{\gamma, \xi})\gamma = \gamma\}$ as n goes to infinity.

- Finally, in Section 5, we prove the existence of minimizers. Because of the complexity of the exchange terms in this model, we consider first the existence of minimizers in $\Gamma_{\leq q}^+ \cap B_R$ with B_R a ball of radius R . We will see that there is a $R_0 > 0$ such that for any $R \geq R_0$ the minimizers in $\Gamma_{\leq q}^+ \cap B_R$ will be indeed in the ball B_{R_0} . Thus the existence of minimizers in $\Gamma_{\leq q}^+$ is equivalent to the existence of minimizers in $\Gamma_{\leq q}^+ \cap B_{R_0}$. And this minimizer is indeed in Γ_q^+ . Now we only need to prove the existence in $\Gamma_{\leq q}^+ \cap B_R$:

For every $\gamma \in \Gamma_{\leq q}^+$, by Bloch decomposition, the corresponding operators D_γ can be decomposed into a direct integral of operators $D_{\gamma, \xi}$ acting on $L_\xi^2(Q_l; \mathbb{C}^4)$ for $\xi \in Q_l^*$. The k -th eigenvalue (counted with multiplicity) of $D_{\gamma, \xi}$ is bounded and both the upper and lower bounds are independent of $\xi \in Q_l^*$ and the choice of γ . Besides, the minimizing sequence γ_n can be decomposed into higher parts and lower parts in terms of the spectrum of the operator D_{γ_n} . The higher parts will disappear when n goes to infinity while the lower parts have a weak-star convergent subsequence. Based on this convergent sequence, we construct some other kinds of convergent subsequences for the potentials which make the sequence pass the limit in the energy and keep the minimizer $\gamma_* \in \Gamma_{\leq q}^+ \cap B_R$. Consequently, we proved the existence of minimizers in $\Gamma_{\leq q}^+ \cap B_R$, and every minimizer solves a self-adjoint equation.

2 General setting of the models and main results

2.1 Preliminaries-Functional framework

We first introduce some notation. We consider only the case of a **cubic** crystal with only one point-like nucleus per unit cell for simplicity, but the reader should keep in mind that the general case could be handled as well. Let $l > 0$ denote the length of the elementary cell $Q_l =]-\frac{l}{2}, \frac{l}{2}]^3$. The nuclei with positive charge z , which are treated as classical particles with infinite mass, are located at each point of $l\mathbb{Z}^3$. The electrons are treated quantum mechanically and we ask the electronic density to be a Q_l -periodic function with L^1 norm equals to q over the elementary cell. Especially if $q = z$, the electrons are "periodically distributed among the nuclei" such that electrical neutrality is ensured.

Throughout the paper, we choose units for which $m = c = \hbar = 1$, where m is the mass of the electron, c the speed of light, and \hbar the Planck constant. The Dirac operator can be written as $D_0 = -i \sum_{k=1}^3 \alpha_k \partial_k + \beta$, with 4×4 complex matrices $\alpha_1, \alpha_2, \alpha_3$ and

β , whose standard forms are:

$$\beta = \begin{pmatrix} \mathbb{1}_2 & 0 \\ 0 & -\mathbb{1}_2 \end{pmatrix}, \alpha = \begin{pmatrix} 0 & \sigma_k \\ \sigma_k & 0 \end{pmatrix},$$

where the σ_k are the well-known 2×2 Pauli matrices

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

The operator D_0 acts on 4-spinors – that is on functions from \mathbb{R}^3 to \mathbb{C}^4 – and it is self-adjoint in $L^2(\mathbb{R}^3; \mathbb{C}^4)$, with domain $H^1(\mathbb{R}^3, \mathbb{C}^4)$ and form domain $H^{1/2}(\mathbb{R}^3; \mathbb{C}^4)$. Its spectrum is $\sigma(D_0) = (-\infty, -1] \cup [+1, \infty)$. Following the notation in [14, 49], we denote by Λ^+ and $\Lambda^- = \mathbb{1}_{L^2} - \Lambda^+$ respectively the two orthogonal projectors on $L^2(\mathbb{R}^3; \mathbb{C}^4)$ corresponding to the positive and negative eigenspace of D_0 , and such that

$$\begin{cases} D_0 \Lambda^+ = \Lambda^+ D_0 = \Lambda^+ \sqrt{1 - \Delta} = \sqrt{1 - \Delta} \Lambda^+; \\ D_0 \Lambda^- = \Lambda^- D_0 = -\Lambda^- \sqrt{1 - \Delta} = -\sqrt{1 - \Delta} \Lambda^-. \end{cases}$$

According to the Floquet theory [50], the underlying Hilbert space $L^2(\mathbb{R}^3; \mathbb{C}^4)$ is unitarily equivalent to $L^2(Q_l^*) \otimes L^2(Q_l; \mathbb{C}^4)$, where $Q_l^* = [-\frac{\pi}{l}, \frac{\pi}{l}]^3$ is the so-called dual cell of the lattice. The unitary Floquet transform \mathcal{U} is given by

$$(\mathcal{U} \cdot \phi)_\xi = \sum_{k \in \mathbb{Z}^3} e^{-ilk \cdot \xi} \phi(\cdot + kl)$$

for every $\xi \in Q_l^*$ and ϕ in $L^2(\mathbb{R}^3; \mathbb{C}^4)$, and $(\mathcal{U} \cdot \phi)_\xi$ belongs to $L_\xi^2(Q_l, \mathbb{C}^4)$, $\xi \in Q^*$, where

$$L_\xi^2(Q_l; \mathbb{C}^4) = \{\psi \in L_{loc}^2(\mathbb{R}^3; \mathbb{C}^4); e^{-i\xi \cdot x} \psi \text{ is } Q_l\text{-periodic}\}.$$

Functions ψ of this form are called Bloch waves or Q_l -quasi-periodic functions with quasi-momentum $\xi \in Q_l^*$. Operators L on $L^2(\mathbb{R}^3; \mathbb{C}^4)$ which commute with the translations of $l\mathbb{Z}^3$ may be decomposed into a direct integral of operators L_ξ acting on $L_\xi^2(Q_l; \mathbb{C}^4)$ according to

$$L_\xi(\mathcal{U} \cdot \phi)_\xi = (\mathcal{U} \cdot L\phi)_\xi \quad (2.1)$$

for every ϕ in $L^2(\mathbb{R}^3; \mathbb{C}^4)$ (see [50] for more details). The operator L is then denoted by $\frac{l^3}{(2\pi)^3} \int_{Q_l^*}^\oplus L_\xi d\xi$. In particular, the Dirac operator is unitary equivalent to the direct integral of self-adjoint operator D_ξ on $L_\xi^2(Q_l; \mathbb{C}^4)$, with domain

$$H_\xi^1(Q_l, \mathbb{C}^4) = L_\xi^2(Q_l; \mathbb{C}^4) \cap H_{loc}^1(\mathbb{R}^3; \mathbb{C}^4)$$

and form-domain

$$H_\xi^{1/2}(Q_l; \mathbb{C}^4) = L_\xi^2(Q_\xi; \mathbb{C}^4) \cap H_{loc}^{1/2}(\mathbb{R}^3; \mathbb{C}^4).$$

(To simplify the notation, we shall simply write L_ξ^2 , H_ξ^1 and $H_\xi^{1/2}$ when there is no ambiguity.) Note that $D_\xi^2 = 1 - \Delta_\xi$, where $-\Delta = \frac{l^3}{(2\pi)^3} \int_{Q_l^*}^\oplus -\Delta_\xi d\xi$. The spectrum $\sigma(D_\xi)$

of D_ξ is composed of two sequences of eigenvalues $(d_n^-(\xi))_{n \geq 1}$ and $(d_n^+(\xi))_{n \geq 1}$ such that $(d_n^-(\xi))_{n \geq 1} \leq -1$, $(d_n^+(\xi))_{n \geq 1} \geq 1$, $\lim_{n \rightarrow \infty} (d_n^-(\xi))_{n \geq 1} = -\infty$, $\lim_{n \rightarrow \infty} (d_n^+(\xi))_{n \geq 1} = +\infty$ and

$$\cup_{\xi \in Q_l^*} \sigma(D_\xi) = \sigma(D_0) = (-\infty, -1] \cup [+1, +\infty).$$

By analogy with the Hartree-Fock model for crystals introduced in [7] our energy functional will be defined on a set \mathcal{T} of admissible one-particle density matrices γ .

Définition 2.1 (Definition of \mathcal{T}). A family of self-adjoint operators γ_ξ , ($\xi \in Q_l^*$) on $L_\xi^2(Q_l)$ enjoys the following properties, for almost every $\xi \in Q_l^*$:

$$(H2') \quad 0 \leq \gamma_\xi \leq \mathbb{1}_{L_\xi^2(Q_l)};$$

$$(H3) \quad \text{the operators } \gamma_\xi \text{ have finite traces and satisfy } \frac{l^3}{(2\pi)^3} \int_{Q_l^*} \text{Tr}_{L_\xi^2(Q_l)} \gamma_\xi d\xi < \infty;$$

$$(H4) \quad \text{Tr}_{L_\xi^2(Q_l)} (|D_\xi| \gamma_\xi) < +\infty \text{ and } \frac{l^3}{(2\pi)^3} \int_{Q_l^*} \text{Tr}_{L_\xi^2(Q_l)} (|D_\xi| \gamma_\xi) d\xi < +\infty$$

To every such family of operators is associated, in a unique way, a self-adjoint operator γ in $L^2(\mathbb{R}^3)$, denoted by $\gamma = \frac{l^3}{(2\pi)^3} \int_{Q_l^*}^\oplus \gamma_\xi d\xi$, such that

$$(H1) \quad \gamma \text{ commutes with the translations of } l\mathbb{Z}^3;$$

$$(H2) \quad 0 \leq \gamma \leq \mathbb{1}_{L^2}.$$

We denote by \mathcal{T} the set of operators $\gamma = \frac{l^3}{(2\pi)^3} \int_{Q_l^*}^\oplus \gamma_\xi d\xi$ which satisfy the conditions (H2'), (H3) and (H4), and we shall call γ a Q_l -periodic density matrix.

Remark 2.2. For almost every ξ in Q^* , there exists a complete set of eigenfunctions $(u_n(\xi, \cdot))_{n \geq 1}$ of γ_ξ in $L_\xi^2(Q)$ corresponding to the non-decreasing sequence of eigenvalues $0 \leq \lambda_n(\xi) \leq 1$ (counted with their multiplicity) such that $u_n(\xi, \cdot) \in H_\xi^{1/2}(Q)$, and such that

$$\gamma_\xi(x, y) = \sum_{n \geq 1} \lambda_n(\xi) u_n(\xi, x) u_n^*(\xi, y), \quad (2.2)$$

for almost every ξ in Q^* .

Remark 2.3. It has been proved in [7] that, for every γ in \mathcal{T} , the kernel of γ is given by

$$\gamma(x, y) = \frac{l^3}{(2\pi)^3} \int_{Q_l^*} \gamma_\xi(x, y) d\xi.$$

Moreover, for every k in \mathbb{Z}^3 ,

$$\gamma(\cdot + kl, \cdot + kl) = \gamma(\cdot, \cdot)$$

This is simply the formulation in terms of kernels of the fact that the operator γ commutes with the translations of $l\mathbb{Z}^3$.

Définition 2.4. Let γ belong to \mathcal{T} . Then we may define in a unique way a Q_l -periodic density ρ_γ associated to γ by

$$\rho_\gamma(x) = \frac{l^3}{(2\pi)^3} \int_{Q_l^*} \text{Tr}_4 \gamma_\xi(x, x) d\xi. \quad (2.3)$$

By the way, if $\gamma_\xi = \sum_{i=1}^{\infty} \lambda_i(\xi) u_i(\xi, x) \otimes u_i^*(\xi, y)$ for almost every $\xi \in Q_l^*$, we have

$$\rho_\gamma(x) = \frac{l^3}{(2\pi)^3} \int_{Q_l^*} \sum_{i=1}^{\infty} \lambda_i(\xi) |u_i(\xi, x)|^2 d\xi,$$

where $|\cdot|$ denotes the usual norm in \mathbb{C}^4 , and $\lambda_i \geq 0$ for all $i \in \mathbb{N}$.

Now, the following functional spaces associated with the γ and γ_ξ are introduced:

•

$$\sigma_s(\xi) = \left\{ \gamma_\xi \in \mathcal{B}(L_\xi^2(Q_l)); \text{Tr}_{L_\xi^2}(|\gamma_\xi|^s) < \infty \right\}$$

endowed with the norm

$$\|\gamma_\xi\|_{\sigma_s(\xi)} = \left(\text{Tr}_{L_\xi^2}(|\gamma_\xi|^s) \right)^{1/s}.$$

•

$$\sigma_{s,t} = \left\{ \gamma; \gamma = \frac{l^3}{(2\pi)^3} \int_{Q_l^*}^{\oplus} \gamma_\xi d\xi, \gamma_\xi \in \mathcal{B}(L_\xi^2(Q_l)), \gamma_\xi \in \sigma_s(\xi), \int_{Q_l^*} \|\gamma_\xi\|_{\sigma_s(\xi)}^t d\xi < \infty \right\}$$

endowed with

$$\|\gamma\|_{\sigma_{s,t}} = \left(\frac{l^3}{(2\pi)^3} \int_{Q_l^*} \|\gamma_\xi\|_{\sigma_s(\xi)}^t d\xi \right)^{1/t}.$$

Particularly, $\sigma_{\infty,\infty} = L^\infty(Q_l^*; \mathcal{B}(L_\xi^2))$.

•

$$X^\alpha(\xi) = \left\{ \gamma_\xi \in \mathcal{B}(L_\xi^2(Q_l)); |D_\xi|^{\alpha/2} \gamma_\xi |D_\xi|^{\alpha/2} \in \sigma_1(\xi) \right\}$$

endowed with the norm

$$\|\gamma_\xi\|_{X^\alpha(\xi)} = \| |D_\xi|^{\alpha/2} \gamma_\xi |D_\xi|^{\alpha/2} \|_{\sigma_1(\xi)};$$

•

$$X_s^\alpha = \left\{ \gamma; \gamma = \frac{l^3}{(2\pi)^3} \int_{Q_l^*}^{\oplus} \gamma_\xi d\xi, (\gamma_\xi)_{\xi \in Q_l^*} \in \mathcal{T}, \int_{Q_l^*} \| |D_\xi|^{\alpha/2} \gamma_\xi |D_\xi|^{\alpha/2} \|_{\sigma_1(\xi)}^s d\xi < \infty \right\}$$

endowed with the norm

$$\|\gamma\|_{X_s^\alpha} = \left(\frac{l^3}{(2\pi)^3} \int_{Q_l^*} \| |D_\xi|^{\alpha/2} \gamma_\xi |D_\xi|^{\alpha/2} \|_{\sigma_1(\xi)}^s d\xi \right)^{1/s};$$

For convenience, we use $X(\xi)$, X and Y to represent $X^1(\xi)$, $X_1^1, \sigma_{\infty, \infty}$ respectively. Therefore, we obtain the intersected functional space $\sigma_{1,1} \cap \sigma_{1,4}$ and $X \cap Y$, endowed with the norm

$$\|\gamma\|_{\sigma_{1,1} \cap \sigma_{1,4}} = \max(\|\gamma\|_{\sigma_{1,1}}, \|\gamma\|_{\sigma_{1,4}}),$$

and

$$\|\gamma\|_{X \cap Y} = \max(\|\gamma\|_X, \|\gamma\|_Y).$$

And in addition to the functional space for operators, we also introduce the functional space for functions

$$\begin{aligned} & W^{\alpha,1}(Q_l^*; H^s(Q_l^2)) \\ & = \left\{ f(\xi, x, y); \int_{Q_l^*} \|f(\xi, \cdot, \cdot)\|_{H_\xi^s(Q_l^2)} d\xi + \int_{Q_l^*} \|\nabla_\xi^\alpha f(\xi, \cdot, \cdot)\|_{H_\xi^s(Q_l^2)} d\xi < \infty \right\} \end{aligned}$$

with the norm

$$\|f\|_{W^{\alpha,1}(H^s)} = \frac{l^3}{(2\pi)^3} \int_{Q_l^*} \|f(\xi, \cdot, \cdot)\|_{H_\xi^s(Q_l^2)} d\xi + \frac{l^3}{(2\pi)^3} \int_{Q_l^*} \|\nabla_\xi^\alpha f(\xi, \cdot, \cdot)\|_{H_\xi^s(Q_l^2)} d\xi.$$

Remark 2.5. For every $\gamma \in \mathcal{T}$, in fact, $\|\gamma\|_{\sigma_{1,1}} = \|\gamma\|_{\sigma_1}$, and $\| |D_0|^{1/2} \gamma |D_0|^{1/2} \|_{\sigma_1} = \|\gamma\|_X$.

By Floquet decomposition, we have that for any orthonormal basis $(u_n(x))_{n \geq 1}$, we have that

$$(Uu)_\xi(x) = \sum_{k \in \mathbb{Z}^3} e^{-ik \cdot \xi} u(x+k),$$

and

$$\gamma_\xi(Uu)_\xi = (U\gamma u)_\xi.$$

By virtue of

$$(u, v)_{L^2(\mathbb{R}^3)} = \frac{l^3}{(2\pi)^2} \int_{Q_l^*} \langle (Uu)_\xi, (Uv)_\xi \rangle_{L^2(Q_l)} d\xi$$

we know that $(Uu_n)_{n,\xi}$ is still an orthonormal basis, and

$$\begin{aligned} \|\gamma\|_{\sigma_1} &= \sum_{n \geq 1} \langle u_n, \gamma u_n \rangle_{L^2(\mathbb{R}^3)} \\ &= \frac{l^3}{(2\pi)^2} \int_{Q_l^*} \langle (Uu_n)_\xi, (U\gamma u_n)_\xi \rangle_{L^2(Q_l)} d\xi, \\ &= \frac{l^3}{(2\pi)^2} \int_{Q_l^*} \langle (Uu_n)_\xi, \gamma_\xi (Uu_n)_\xi \rangle_{L^2(Q_l)} d\xi, \\ &= \|\gamma\|_{\sigma_{1,1}}. \end{aligned}$$

For another equation, the proof is similar.

Let

$$\Gamma_{\leq q} := \{\gamma \in \mathcal{T}; \gamma \in X \cap Y, \|\gamma\|_{\sigma_{1,1}} \leq q\},$$

and

$$\Gamma_q := \{\gamma \in \mathcal{T}; \gamma \in X \cap Y, \|\gamma\|_{\sigma_{1,1}} = q\}.$$

The condition $\gamma \in X \cap Y$ can be removed since if $\gamma \in \mathcal{T}$, obviously $\gamma \in X \cap Y$.

Now, we introduce the periodic Dirac-Fock model.

2.2 The periodic Dirac-Fock models

For every $\gamma \in \Gamma_{\leq q}$, we now define the periodic Dirac operator with potential by:

$$D_{\gamma, \xi} := D_\xi - \alpha z G_l + \alpha V_{\gamma, \xi}$$

where D_ξ is defined by (2.1) and

$$V_{\gamma, \xi} = \rho_\gamma * G_l(x) - W_{\gamma, \xi}$$

with

$$\rho_\gamma * G_l(x) = \int_{Q_l} G_l(y-x) \rho_\gamma(y) dy = \text{Tr}_{L^2(Q_l)}(G_l(\cdot-x)\gamma)$$

and

$$W_{\gamma, \xi} \psi_\xi(x) = \frac{l^3}{(2\pi)^3} \int_{Q_l^*} d\xi' \int_{Q_l} W_l^\infty(\xi' - \xi, x-y) \gamma_{\xi'}(x, y) \psi_\xi(y) dy.$$

The so-called fine structure constant α is a dimensionless positive constant (the physical value is approximately 1/137).

The operator D_ξ have a simple expression in Fourier series: Given any $\phi_\xi \in H_\xi^{1/2}$, we have

$$\phi_\xi(x) = \sum_{k \in \mathbb{Z}^3} \hat{\phi}_{k+\xi} e^{(2i\pi k/l + i\xi) \cdot x},$$

with

$$\hat{\phi}_{k+\xi} = \frac{1}{l^3} \int_{Q_l} \phi_\xi(y) e^{-(2i\pi k/l + i\xi) \cdot y} dy$$

and

$$D_\xi \phi_\xi(x) = \sum_{k \in \mathbb{Z}^3} \left[\left(\frac{2\pi}{l} k + \xi \right) \cdot \alpha + \beta \right] \hat{\phi}_{k+\xi} e^{(2i\pi k/l + i\xi) \cdot x},$$

where $(k + \xi) \cdot \alpha = \sum_{j=1}^3 (k_j + \xi_j) \alpha_j \in \mathcal{M}_4(\mathbb{C})$.

Thus, the functional framework in this discrete setting should be set:

Définition 2.6. The space of $H^{1/2}(\mathbb{T}, \mathbb{C}^4)$ will be simply denoted by $H_\#^{1/2}(Q_l)$. Recall that

$$H_\#^{1/2}(Q_l) = \left\{ \psi \in L^2(\mathbb{T}, \mathbb{C}^4); \sum_{k \in \mathbb{Z}^3} \sqrt{1 + \frac{4\pi^2 k^2}{l^2}} |\hat{\psi}_k|^2 < \infty \right\},$$

endowed with the norm

$$\|\psi\|_{H_\#^{1/2}(Q_l)}^2 = \sum_{k \in \mathbb{Z}^3} \sqrt{1 + \frac{4\pi^2 k^2}{l^2}} |\hat{\psi}_k|^2.$$

In this periodic setting, the Coulomb-like interaction between periodic distributions of particles is described through the Q_l -periodic potential G_l that is uniquely defined by

$$-\Delta G_l = 4\pi \left[-\frac{1}{l^3} + \sum_{k \in \mathbb{Z}^3} \delta_{lk} \right] \quad (2.4)$$

and

$$\int_{Q_l} G_l = 0. \quad (2.5)$$

G_l is actually the Green function of the periodic Laplace operator on Q_l . The Fourier series of G_l reads, for $x \in \mathbb{R}^3$,

$$G_l(x) = \frac{1}{\pi l} \sum_{\substack{p \in \mathbb{Z}^3 \\ p \neq 0}} \frac{e^{\frac{2i\pi}{l} p \cdot x}}{|p|^2}. \quad (2.6)$$

The following scaling property, for any $\lambda > 0$,

$$G_{\lambda l}(x) = \frac{1}{\lambda} G_l\left(\frac{x}{\lambda}\right) \quad (2.7)$$

is easily checked.

And the potential W_l^∞ which enters the definition of the exchange term is defined by

$$W_l^\infty(\eta, x) = \frac{4\pi}{l^3} \sum_{k \in \mathbb{Z}^3} \frac{1}{\left|\frac{2\pi k}{l} - \eta\right|^2} e^{i\left(\frac{2\pi k}{l} - \eta\right) \cdot x} = \lambda W_{\lambda l}^\infty\left(\frac{\eta}{\lambda}, \lambda x\right), \quad \eta \in \mathbb{R}^3, x \in \mathbb{R}^3 \quad (2.8)$$

(see [7] for a formal derivation of this exchange term from its analogue for molecules). It is Q_l^* periodic with respect to η and quasi-periodic with quasi-momentum η with respect to x .

Remark 2.7. $\gamma(\cdot, \cdot)$ belongs to $L^2(Q_l \times \mathbb{R}^3)$ and the exchange term is also

$$\begin{aligned} & \frac{l^6}{(2\pi)^6} \iint_{(Q_l^*)^2} d\xi d\xi' \iint_{Q_l^2} \text{Tr}_4[\gamma_\xi(x, y) \gamma_{\xi'}(y, x)] W_l^\infty(\xi - \xi', x - y) dx dy \\ &= \int_{Q_l} \int_{\mathbb{R}^3} \frac{\text{Tr}_4(\gamma(x, y) \gamma(y, x))}{|x - y|} dy. \end{aligned}$$

where the trace Tr_4 which appears in the last term (the exchange term) denotes the trace of a 4×4 matrix.

Finally, let

$$P_{\gamma, \xi}^\pm := \mathbb{1}_{\mathbb{R}^\pm}(D_{\gamma, \xi}), \quad P_\gamma^\pm = \frac{l^3}{(2\pi)^3} \int_{Q_l^*}^\oplus P_{\gamma, \xi}^\pm d\xi,$$

and

$$P_\gamma^\pm \gamma' := \int_{Q_l^*}^\oplus P_{\gamma, \xi}^\pm \gamma_\xi d\xi.$$

Note that by definition $P_{0, \xi}^\pm = \mathbb{1}_{\mathbb{R}^\pm}(D_\xi - \alpha z G)$.

Now, define

$$\Gamma_{\leq q}^+ := \{\gamma \in \Gamma_{\leq q}; P_\gamma^- \gamma = 0\},$$

and

$$\Gamma_q^+ := \{\gamma \in \Gamma_q; P_\gamma^- \gamma = 0\}.$$

Our goal is to give a new definition of the ground state of the periodic Dirac-Fock functional

$$\begin{aligned}
& \mathcal{E}^{DF}(\gamma) \\
&= \frac{l^3}{(2\pi)^3} \int_{Q_l^*} \text{Tr}_{L_\xi^2}(D_\xi \gamma_\xi) d\xi - \alpha z \int_{Q_l} G_l(x) \rho_\gamma(x) dx + \frac{\alpha}{2} \iint_{Q_l^2} \rho_\gamma(x) G_l(x-y) \rho_\gamma(y) dx dy \\
&\quad - \frac{\alpha}{2} \frac{l^6}{(2\pi)^6} \iint_{(Q_l^*)^2} d\xi d\xi' \iint_{Q_l^2} \text{Tr}_4[\gamma_\xi(x, y) \gamma_{\xi'}(y, x)] W_l^\infty(\xi - \xi', x - y) dx dy,
\end{aligned} \tag{2.9}$$

Even though we restrict our study of ground state to q electrons, this functional is indeed defined on the closed convex set $\Gamma_{\leq q}$. When q is integers, $\Gamma_{\leq q}$ is the set of all Dirac-Fock states of a system of q -electrons. The relation between \mathcal{E}^{DF} and $D_{\gamma, \xi}$ is the following: if γ and $\gamma + h$ are in $\Gamma_{\leq q}$ with, then the right derivative of $f(t) = \mathcal{E}^{DF}(\gamma + th)$ at $t = 0$ is $\int_{Q_l^*} d\xi \text{Tr}_{L_\xi^2}(D_{\gamma, \xi} h_\xi)$.

Mimicking [53], we impose that the ground state lies in $\Gamma_{\leq q}^+$. However, the direct computation implies that zero minimizes the problem rather than the real ground states. To overcome this problem, we add a penalization term $\epsilon_F \text{Tr}_{L^2}(\gamma)$, and study the penalized functional

$$\mathcal{E}^{DF}(\gamma) - \epsilon_F \text{Tr}_{L^2}(\gamma)$$

in $\Gamma_{\leq q}^+$.

A fundamental tool in our definition of a ground state will be a map that we denote θ . It is a retraction of a certain closed subset F of $\Gamma_{\leq q}$ onto $F \cap \Gamma_{\leq q}^+$. The set F will be large enough, so that it will contain the "ground state" of the Dirac-Fock functional. Moreover θ will have an extension on an open neighborhood of F in $X \cap Y$ and this extension will be of class C^1 . Note that the map θ will be easy to implement numerically. More precisely, for $\gamma \in F$, let $\gamma_0 = \gamma$ and $\gamma_{p+1} = P_{\gamma_p}^+ \gamma_p P_{\gamma_p}^+$. Then we define $\theta(\gamma)$ as the limit, if it exists, of the sequence (γ_p) for the topology of $X \cap Y$.

2.3 Main results

At the beginning, we recall the main properties of the periodic potential G_l and W_l^∞ . In fact, we prove the Hardy-type estimates in section 3 that will be used all along the proof, and we prove the main technical results concerning the operators.

First of all, and it is a major difference with $\frac{1}{|x|}$, the periodic Coulomb potential G_l is no more positive, but is bounded below:

Proposition 2.8. *There exists a positive constant C_0 such that, for any $l > 0$, $x \in Q_l$, we have*

$$G_l(x) \geq -\frac{C_0}{l}. \tag{2.10}$$

Moreover, we have the following Hardy-type estimates concerning the periodic potential G , and the proof is given in subsection 3.1:

Lemma 2.9. *There exists $C_H > 0$ and $C'_H > 0$, such that, for any $\xi \in Q_l^*$ and any $\psi_\xi \in H_\xi^{1/2}(Q_l; \mathbb{C}^4)$, we have:*

$$(\psi_\xi, G_l \psi_\xi)_{L^2(Q_l)} \leq C_H (\psi_\xi, |D_\xi| \psi_\xi)_{Q_l}, \quad (2.11a)$$

$$(\psi_\xi, |G_l| \psi_\xi)_{L^2(Q_l)} \leq C'_H (\psi_\xi, |D_\xi| \psi_\xi)_{Q_l}, \quad (2.11b)$$

Moreover, there exists $C_G \geq C'_H > 0$, such that, for any $\xi \in Q_l^*$ and any $\phi_\xi \in H_\xi^1(Q_l; \mathbb{C}^4)$, we have:

$$\|G_l \phi_\xi\|_{L^2(Q_l)} \leq C_G \| |D_\xi| \phi_\xi \|_{L_\xi^2(Q_l)}. \quad (2.12)$$

Remark 2.10. Note that, as a difference with the atomic case, we do not know the best constants C_H , C'_H and C_G .

We will need, for the proof of Lemma 2.11 the following result, quoted in [7]: we can separate the singularities of W_l^∞ w.r.t. η and x :

$$W_l^\infty(\eta, x) = e^{-i\eta \cdot x} G_l(x) + 4\pi \frac{e^{-i\eta \cdot x}}{|\eta|^2} + f_l(\eta, x), \quad (2.13)$$

where

$$f_l(\eta, x) = \frac{2\pi}{l} e^{-i\eta \cdot x} \sum_{m \in \mathbb{Z}^3 \setminus \{0\}} e^{2i\pi m/l \cdot x} \frac{4\pi l \eta \cdot m - l^2 |\eta|^2}{|l\eta - 2\pi m|^2 |2\pi m|^2}$$

is a bounded function on $Q_l^* \times (2Q_l)$. We have that

$$f_l(\eta, x) = \lambda f_{\lambda l} \left(\frac{\eta}{\lambda}, \lambda x \right),$$

and as $f(\eta, x)$ is harmonic in $(1 + \epsilon)Q_l$ for any ϵ small enough, then for any $x \in Q_l$

$$|f_l(\eta, x)| \leq \frac{1}{l} |f_1(\eta, x)| \leq \frac{c}{l} \|f_1(\eta, \cdot)\|_{L^2(Q_l)}^{1/2}.$$

Furthermore, $f_l \in W^{1,\infty}(Q_l^*; L_\eta^\infty(Q_l))$. We notice that $\nabla_\eta f(\eta, x)$ is equally harmonic in $(1 + \epsilon)Q_l$, since

$$-\Delta_x \nabla_\eta f_l(\eta, x) = 4\pi \sum_{k \in \mathbb{Z}^3 \setminus \{0\}} -ik e^{-ik \cdot \eta} \delta_k(x).$$

By virtue of the mean-value property, we finally obtain for every $x \in Q_l$,

$$\begin{aligned} |\nabla_\eta f_l(\eta, x)|^2 &\leq \left(\int_{x+\epsilon Q_l} |\nabla_\eta f_l(\eta, y)| dy \right)^2 \\ &\leq C \|\nabla_\eta f_l(\eta, \cdot)\|_{L_\eta^2(Q_l)}^2 \leq C \sum_{\mathbb{Z}^3 \setminus \{0\}} \frac{1 + |m|^2}{|l\eta - 2\pi m|^4 |2\pi m|^2}. \end{aligned} \quad (2.14)$$

And, for the exchange term,

$$\begin{aligned} W_l^\infty(\xi - \xi', (x - y)/l) &= e^{-i(\xi - \xi') \cdot (x - y)} G_l(x - y) \\ &\quad + 4\pi \sum_{m \in \mathbb{Z}^3, |m|_\infty \leq 1} \frac{e^{-i(\xi - \xi' - 2\pi m/l) \cdot (x - y)}}{|\xi - \xi' - 2\pi m/l|^2} + g_l(\xi - \xi', x - y), \end{aligned} \quad (2.15)$$

And analogously to f_l , g_l is a bounded function on $Q_l^* \times (2Q_l)$ as well as

$$g(\eta, x) \in W^{1,\infty}((Q_l^*)^2, L_\xi^\infty(Q_l)). \quad (2.16)$$

We have the following estimates for W , and the proof is given in subsection 3.2:

Lemma 2.11. *For any $\psi_\xi \in H_\xi^{1/2}$, there are constants C_W, C'_W, C''_W such that for any $\xi \in Q_l^*$:*

- if $\gamma \in X \cap Y$,

$$\|W_{\gamma,\xi}\psi_\xi\|_{L_\xi^2} \leq C_W \|\gamma\|_{X \cap Y} \|\psi_\xi\|_{L_\xi^2}. \quad (2.17)$$

- if $\gamma \in \sigma_{1,1} \cap Y$,

$$\|W_{\gamma,\xi}\psi_\xi\|_{L_\xi^2} \leq C'_W \|\gamma\|_{\sigma_{1,1} \cap Y} \|D_\xi|\psi_\xi\|_{L_\xi^2} \quad (2.18)$$

- if $\gamma \in \sigma_{1,1} \cap \sigma_{1,4}$,

$$\|W_\gamma\psi_\xi\|_{L_\xi^2} \leq C''_W \|\gamma\|_{\sigma_{1,1} \cap \sigma_{1,4}} \|\psi_\xi\|_{L_\xi^2}, \quad (2.19)$$

Before stating the theorem, we need the following assumption:

Assumption 2.12. Let $q^+ = \max\{q, 1\}$, $\kappa := \alpha((C'_H(z+q) + C'_W q^+))$, $C_{EE} := C'_H + C_W$, $A > \frac{1}{4}\alpha(1-\kappa)^{-2}(1+\kappa)C_{EE}$ and

$$c^*(k) := \sup_{\xi \in Q_l^*} \inf_{\substack{\dim V = k \\ V \subset \Lambda_\xi^+ H_\xi^{1/2}}} \sup_{u_\xi^+ \in V} \frac{\| |D_\xi|^{1/2} u_\xi^+ \|_{L_\xi^2}}{\|u_\xi^+\|_{L_\xi^2}}.$$

We assume that

1. $\kappa < 1 - 1/2\alpha C_{EE} q^+$,
2. $\kappa' := \alpha(C_G(z+q) + C'_W q^+) < 1$,
3. $A\sqrt{\max\{(1-\kappa - 1/2\alpha C_{EE} q^+)^{-1}(1-\kappa)^{-1}c^*(q+1)q, 1\}}q^+ < 1$.

We have

Theorem 2.13. *Under Assumption 2.12, there exists $\gamma_* \in \Gamma_q^+$ such that*

$$\mathcal{E}^{DF}(\gamma_*) = I := \min_{\gamma \in \Gamma_q^+} \mathcal{E}^{DF}(\gamma). \quad (2.20)$$

Besides, γ_* solves the following nonlinear self-consistent equation:

$$\begin{cases} \gamma = \mathbb{1}_{[0,\nu]}(D_\gamma) + \delta \\ D_\gamma = \frac{l^3}{(2\pi)} \int_{Q_l^*}^\oplus d\xi D_{\gamma,\xi}, \end{cases} \quad (2.21)$$

where $0 \leq \delta \leq \mathbb{1}_{\{\nu\}}(D_\gamma)$ and $0 \leq \nu \leq (1-\kappa)^{-1}c^*(q+1)$.

Remark 2.14. In solid state physics, the length of the unit cell is about a few Angstroms. And in our system of unit, $\hbar = m = c = 1$, thus $\alpha \approx \frac{1}{137}$ and $l \approx 1000$. Under the condition $q = z$ for electrical neutrality, we find that the Assumption 2.12 is satisfied for $q \leq 4$, and the details can be found in Appendix E. Moreover, our estimates are far from optimal and one can expect that the ideas of this paper apply to higher values of q .

Remark 2.15. Unlike the Hartree-Fock model for crystals [20], when q is integer, we can not yield $\delta = \epsilon \mathbb{1}_{\{\nu\}}(D_\gamma)$ where $\epsilon \in \{0, 1\}$, since our restriction $\gamma \in \Gamma_q^+$ is non-linear.

3 Fundamental estimates

3.1 Lemma 2.9 and its corollaries

proof of .

Estimates of C_H and C'_H

Let ξ be fixed in Q_l^* and let $\phi_\xi \in H_\xi^{1/2}(Q_l; \mathbb{C}^4)$. We write ϕ_ξ on the form $\phi_\xi = e^{i\xi \cdot x} u(x)$ with u Q -periodic. Then, denoting by $\hat{u}(k)$ the k -th Fourier coefficient of u in its Fourier series expansion, we have, on the other hand,

$$(\phi_\xi, |D_\xi| \phi_\xi)_{L_\xi^2} = l^3 \sum_{k \in \mathbb{Z}^3} \sqrt{1 + |\xi + \frac{2\pi}{l} k|^2} |\hat{u}(k)|^2.$$

On the other hand, using Equation (2.6), we obtain

$$(\phi_\xi, G_l \phi_\xi)_{L^2(Q_l)} = \frac{l^2}{\pi} \sum_{\substack{k, k' \in \mathbb{Z}^3 \\ k \neq k'}} \frac{\hat{u}(k) \hat{u}^*(k')}{|k - k'|^2}.$$

Let ϑ a positive number to be determined later. By Cauchy-Schwarz' inequality, we have

$$\begin{aligned} \sum_{\substack{k, k' \in \mathbb{Z}^3 \\ k \neq k'}} \frac{\hat{u}(k) \hat{u}^*(k')}{|k - k'|^2} &= \sum_{\substack{k \neq k' \\ k \neq 0, k' \neq 0}} \frac{\hat{u}(k) |k|^\vartheta}{|k - k'| |k'|^\vartheta} \frac{\hat{u}^*(k') |k'|^\vartheta}{|k - k'| |k|^\vartheta} + \sum_{k' \neq 0} \frac{\hat{u}(0) \hat{u}^*(k')}{|k'|^2} + \sum_{k \neq 0} \frac{\hat{u}^*(0) \hat{u}(k)}{|k|^2} \\ &\leq \sum_{\substack{k \neq k' \\ k \neq 0}} \frac{|\hat{u}|^2(k) |k|^{2\vartheta}}{|k'|^{2\vartheta} |k - k'|^2} + 2\Re \left(\hat{u}(0) \sum_{k \neq 0} \frac{\hat{u}^*(k)}{|k|^2} \right), \end{aligned} \tag{3.1}$$

with $\Re(z)$ denoting the real part of the complex number z for $z \in \mathbb{C}$. We first bound from above the second term in the right hand side of Equation (3.1), thanks again to the Cauchy-Schwarz inequality by:

$$\begin{aligned} 2\Re \left(\hat{u}(0) \sum_{k \neq 0} \frac{\hat{u}^*(k)}{|k|^2} \right) &\leq 2|\hat{u}(0)| \left(\sum_{k \in \mathbb{Z}^3} |\hat{u}|^2(k) |k| \right)^{1/2} \left(\sum_{k \neq 0} \frac{1}{|k|^5} \right)^{1/2} \\ &\leq \left(\sum_{k \neq 0} \frac{1}{|k|^5} \right)^{1/2} \left(|\hat{u}|^2(0) + \sum_{k \in \mathbb{Z}^3} |\hat{u}|^2(k) |k| \right). \end{aligned}$$

For the first term, we proceed as follows:

$$\sum_{k \in \mathbb{Z}^3} |\hat{u}|^2(k) |k|^{2\vartheta} \sum_{\substack{k' \neq k \\ k' \neq 0}} \frac{1}{|k'|^{2\vartheta} |k - k'|^2} = \sum_{k \in \mathbb{Z}^3} |\hat{u}|^2(k) |k| \left[\frac{1}{|k|^3} \sum_{\substack{k' \neq k \\ k' \neq 0}} \frac{1}{\left(\frac{|k'|}{|k|}\right)^{2\vartheta} \left|\frac{k}{|k|} - \frac{k'}{|k|}\right|^2} \right].$$

Herein we choose $\vartheta = 1$. By Appendix D.1, we know that

$$\sum_{k \in \mathbb{Z}^3} |\hat{u}|^2(k) |k|^{2\vartheta} \sum_{\substack{k' \neq k \\ k' \neq 0}} \frac{1}{|k'|^2 |k - k'|^2} \leq 59.235 \sum_{k \in \mathbb{Z}^3} |k| |\hat{u}|^2(k) \quad (3.2)$$

We now observe that, for every k in \mathbb{Z}^3 , and ξ in Q_l^* ,

$$|k| \leq \left(\sqrt{3} + \frac{l}{2\pi}\right) \sqrt{1 + \left|\xi + \frac{2\pi}{l}k\right|^2},$$

since

$$|k| \leq \left|k + \frac{l}{2\pi}\xi\right| + \frac{l}{2\pi}|\xi| \leq \left|k + \frac{l}{2\pi}\xi\right| + \sqrt{3}.$$

Now we can conclude that

$$\begin{aligned} (\phi_\xi, G_l \phi_\xi)_{L_\xi^2(Q_l)} &\leq C \frac{l^2}{\pi} \left(|\hat{u}|^2(0) + \sum_{\substack{q \in \mathbb{Z}^3 \\ q \neq 0}} |\hat{u}|^2(q) |q| \right) \\ &\leq \left(\sqrt{3} + \frac{l}{2\pi}\right) C \frac{l^2}{\pi} \sum_{k \in \mathbb{Z}^3} \sqrt{1 + \left|\frac{2\pi}{l}k + \xi\right|^2} |\hat{u}|^2(k) \\ &= \frac{C}{\pi l} \left(\sqrt{3} + \frac{l}{2\pi}\right) (\phi_\xi, |D_\xi| \phi_\xi)_{L_\xi^2(Q_l)}, \end{aligned}$$

with

$$C = \left(\sum_{k \neq 0} \frac{1}{|k|^5} \right)^{1/2} + 59.235.$$

Hence,

$$C_H = \frac{1}{\pi} \left(\frac{\sqrt{3}}{l} + \frac{1}{2\pi}\right) \left[\left(\sum_{k \neq 0} \frac{1}{|k|^5} \right)^{1/2} + 59.235 \right].$$

The second Hardy inequality (2.11b) is easily deduced from (2.11a) and (2.10) by taking

$$C'_H = C_H + 2 \frac{C_0}{l}.$$

Estimates of C_G

The proof of (2.12) follows the same patterns as the proof of (2.11a). As

$$(\phi_\xi, G_l^2 \phi_\xi)_{L^2(Q_l)} = \frac{l}{\pi^2} \sum_{\substack{p, k, k' \in \mathbb{Z}^3 \\ k, k' \neq p}} \frac{\hat{u}(k) \hat{u}^*(k')}{|k - p|^2 |k' - p|^2}.$$

Then by Cauchy-Schwarz's inequality, we have

$$\begin{aligned}
& \sum_{\substack{p,k,k' \in \mathbb{Z}^3 \\ p \neq k, k'}} \frac{\hat{u}(k)\hat{u}^*(k')}{|k-p|^2|k'-p|^2} \\
& \leq \sum_{\substack{k,k' \neq 0 \\ p \neq k, k'}} \frac{\hat{u}(k)|k|^\vartheta}{|p-k|^2|k'|^\vartheta} \frac{\hat{u}^*(k')|k'|^\vartheta}{|p-k|^2|k|^\vartheta} + \sum_{p \neq 0} \frac{|\hat{u}|^2(0)}{|p|^4} \\
& \quad + \sum_{\substack{k,p \in \mathbb{Z}^3 \\ k,p \neq 0 \\ p \neq k}} \frac{\hat{u}(k)\hat{u}^*(0)}{|p-k|^2|p|^2} + \sum_{\substack{k',p \in \mathbb{Z}^3 \\ k',p \neq 0 \\ p \neq k'}} \frac{\hat{u}(0)\hat{u}^*(k')}{|p-k'|^2|p|^2} \\
& \leq \sum_{\substack{p,k,k' \in \mathbb{Z}^3 \\ p \neq k, k' \\ k, k' \neq 0}} \frac{|\hat{u}|^2(k)|k|^{2\vartheta}}{|p-k|^2|p-k'|^2|k'|^{2\vartheta}} + 2\Re \left(\hat{u}(0) \sum_{\substack{p,k \in \mathbb{Z}^3 \\ p \neq 0, p \neq k}} \frac{\hat{u}^*(k)}{|p-k|^2|p|^2} \right) + \sum_{p \neq 0} \frac{|\hat{u}|^2(0)}{|p|^4}.
\end{aligned}$$

By virtue of Cauchy-Schwarz's inequality again,

$$\begin{aligned}
2\Re \left(\hat{u}(0) \sum_{\substack{p,k \in \mathbb{Z}^3 \\ k,p \neq 0 \\ k \neq p}} \frac{\hat{u}^*(k)}{|p-k|^2|p|^2} \right) & \leq 2|\hat{u}(0)| \left(\sum_{k \in \mathbb{Z}^3 \setminus \{0\}} |\hat{u}|^2(k)|k|^2 \right)^{1/2} \left(\sum_{\substack{p \neq k \\ k,p \neq 0}} \frac{1}{|p-k|^4|p|^4|k|^2} \right)^{1/2} \\
& \leq \left(\sum_{\substack{p \neq k \\ k,p \neq 0}} \frac{1}{|p-k|^4|p|^4|k|^2} \right)^{1/2} \left(|\hat{u}|^2(0) + \sum_{k \in \mathbb{Z}^3 \setminus \{0\}} |\hat{u}|^2(k)|k|^2 \right).
\end{aligned}$$

And for the first term, we proceed as follows:

$$\sum_{\substack{p,k,k' \in \mathbb{Z}^3 \\ k,k' \neq p \\ k,k' \neq 0}} \frac{|\hat{u}|^2(k)|k|^{2\vartheta}}{|p-k|^2|p-k'|^2|k'|^{2\vartheta}} = \sum_{k \in \mathbb{Z}^3} |\hat{u}|^2(k)|k|^2 \sum_{\substack{p \neq k', k \\ k, k' \neq 0}} \frac{1}{|k|^6} \frac{1}{\left| \frac{p}{|k|} - \frac{k}{|k|} \right|^2 \left| \frac{p}{|k|} - \frac{k'}{|k|} \right|^2 \left| \frac{k'}{|k|} \right|^{2\vartheta}}.$$

Herein, we take $\vartheta = 1.25$. And by Appendix D.2, we get that

$$\iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{1}{|x-e|^2|y-x|^2|y|^{2.5}} dx dy \leq 122498.747 + \sum_{p \neq 0} \frac{1}{|p|^{4.5}}. \quad (3.3)$$

Now, we conclude that

$$\begin{aligned}
(\phi_\xi, G_l^2 \phi_\xi)_{L^2(Q_l)} & \leq C' \frac{l}{\pi^2} \left(|\hat{u}|^2(0) + \sum_{k \neq 0} |\hat{u}|^2(k)|k|^2 \right) \\
& \leq \left(3 + \frac{l^2}{4\pi^2} \right) C' \frac{l}{\pi^2} \sum_{k \in \mathbb{Z}^3} \left(1 + \left| \frac{2\pi}{l}k + \xi \right|^2 \right) |\hat{u}|^2(k) \\
& = \frac{C'}{\pi^2} \left(\frac{3}{l^2} + \frac{1}{4\pi^2} \right) \| |D_\xi| \phi_\xi \|_{L_\xi^2(Q_l)}^2,
\end{aligned}$$

with

$$C' = \sum_{p \neq 0} \frac{1}{|p|^4} + \left(\sum_{\substack{p \neq k \\ k, p \neq 0}} \frac{1}{|p-k|^4 |p|^4 |k|^2} \right)^{1/2} + 22498.747 + \sum_{p \neq 0} \frac{1}{|p|^{4.5}}.$$

Hence,

$$C_G = \frac{1}{\pi} \max\left(\frac{\sqrt{3}}{l}, \frac{1}{2\pi}\right) \left(\sum_{p \neq 0} \frac{1}{|p|^4} + \left(\sum_{\substack{p \neq k \\ k, p \neq 0}} \frac{1}{|p-k|^4 |p|^4 |k|^2} \right)^{1/2} + 22498.747 + \sum_{p \neq 0} \frac{1}{|p|^{4.5}} \right)^{1/2}.$$

□

As a result of Lemma 2.9, we can directly get

Corollary 3.1. *For any $\gamma, \gamma_1, \gamma_2 \in X$, we get:*

$$\|\rho_\gamma * G_l\|_{\mathcal{B}(L_\xi^2)} \leq C'_H \|\gamma\|_X \quad (3.4)$$

and

$$\|(\rho_{\gamma_1} - \rho_{\gamma_2}) * G_l\|_{\mathcal{B}(L_\xi^2)} \leq C'_H \|\gamma_1 - \gamma_2\|_X. \quad (3.5)$$

Proof. From Lemma 2.9, we know

$$|G_l| \leq C'_H |D_\xi|.$$

Thus,

$$\begin{aligned} & |\rho_\gamma * G_l|(x) \\ &= |\mathrm{Tr}_{L^2}(G_l(\cdot - x)\gamma)|(x) \\ &\leq \int_{Q_i^*} |\mathrm{Tr}_{L_\xi^2}(G_l(\cdot - x)\gamma_\xi)| d\xi \\ &= \int_{Q_i^*} |\mathrm{Tr}_{L_\xi^2}(|D_\xi|^{-1/2} G_l(\cdot - x) |D_\xi|^{-1/2} |D_\xi|^{1/2} \gamma_\xi |D_\xi|^{1/2})| d\xi \\ &\leq \int_{Q_i^*} \| |G_l|^{1/2}(\cdot - x) |D_\xi|^{-1/2} \|_{\mathcal{B}(L_\xi^2)}^2 \| |D_\xi|^{1/2} \gamma_\xi |D_\xi|^{1/2} \|_{\sigma_1(\xi)} d\xi \\ &\leq C'_H \|\gamma\|_X \end{aligned}$$

And similarly, we have

$$|(\rho_{\gamma_1} - \rho_{\gamma_2}) * G_l|(x) \leq C'_H \|\gamma_1 - \gamma_2\|_X.$$

Repeating the proof of the first inequality, we get the conclusion. □

3.2 Lemma 2.11 and its corollaries

proof of Lemma 2.11. As

$$\|W_{\gamma,\xi}\psi_\xi\|_{L_\xi^2} = \sup_{\substack{\phi_\xi \in L_\xi^2 \\ \|\phi_\xi\|_{L_\xi^2}=1}} |(W_{\gamma,\xi}\psi_\xi, \phi_\xi)|,$$

we only need to study the inner product $(W_{\gamma,\xi}\psi_\xi, \phi_\xi)$. Hence, we can separate $W_{\gamma,\xi}$ in three parts:

- one term with all singularity in z : by Cauchy-Schwarz' inequality

$$|\gamma|(x, y) \leq \rho^{1/2}(x)\rho^{1/2}(y)$$

and Corollary 3.1,

$$\begin{aligned} & \int_{Q_i^*} d\xi' \int_{Q_i^2} e^{-i(\xi'-\xi)(x-y)} G(x-y)\gamma_{\xi'}(x, y)\psi_\xi(y)\overline{\phi_\xi}(x)dx dy \\ & \leq \int_{Q_i^*} d\xi' \int_{Q_i^2} |G(x-y)||\gamma_{\xi'}|(x, y)|\psi_\xi(y)|\overline{\phi_\xi}(x)dx dy \\ & \leq \int_{Q_i^*} d\xi' \left(\int_{Q_i} |\psi_\xi|^2(y) \int_{Q_i} |G(x-y)||\rho_{\gamma_{\xi'}}|(x)dx dy \right)^{1/2} \\ & \quad \times \left(\int_{Q_i} |\overline{\phi_\xi}|^2(x) \int_{Q_i} |G(x-y)||\rho_{\gamma_{\xi'}}|(y)dx dy \right)^{1/2} \\ & \leq \int_{Q_i^*} \|\gamma_\xi\|_{X(\xi)} d\xi' \left(\int_{Q_i^2} |\psi_\xi|^2(y)dx dy \right)^{1/2} \left(\int_{Q_i^2} |\overline{\phi_\xi}|^2(x)dx dy \right)^{1/2} \\ & \leq C'_H \|\gamma\|_X \|\psi_\xi\|_{L_\xi^2} \end{aligned}$$

or

$$\begin{aligned} & \int_{Q_i^*} d\xi' \int_{Q_i} e^{-i(\xi'-\xi)(x-y)} G(x-y)\gamma_{\xi'}(x, y)\psi_\xi(y)\overline{\phi_\xi}(x)dx dy \\ & \leq \int_{Q_i^*} d\xi' \left(\int_{Q_i^2} |\rho_{\xi'}|(x)|\psi_\xi|^2(y)dx dy \right)^{1/2} \left(\int_{Q_i} |\rho_{\xi'}|(y) \int_{Q_i} |G(x-y)|^2|\overline{\phi_\xi}|^2(x)dx dy \right)^{1/2} \\ & \leq C_G \|\gamma\|_{\sigma_{1,1}} \|D_\xi\|\psi_\xi\|_{L_\xi^2} \end{aligned}$$

- the second term, carrying the singularity in η :

$$\begin{aligned}
& \int_{Q_l^*} d\xi' \int_{Q_l^2} 4\pi \sum_{m \in \mathbb{Z}^3, |m|_\infty \leq 1} \frac{e^{-i(\xi' - \xi - 2\pi m/l) \cdot (x-y)}}{|\xi' - \xi - 2\pi m/l|^2} \gamma_{\xi'}(x, y) \psi_\xi(y) \overline{\phi_\xi}(x) dx dy \\
& \leq 4\pi \sum_{m \in \mathbb{Z}^3, |m|_\infty \leq 1} \int_{Q_l^*} d\xi' \int_{Q_l^2} \frac{1}{|\xi' - \xi - 2\pi m/l|^2} \rho_{\gamma_{\xi'}}^{1/2}(x) \rho_{\gamma_{\xi'}}^{1/2}(y) |\psi_\xi|(y) |\overline{\phi_\xi}|(x) dx dy \\
& \leq 4\pi \left(\sum_{m \in \mathbb{Z}^3, |m|_\infty \leq 1} \int_{Q_l^*} \int_{Q_l^2} |\xi' - \xi - 2\pi m/l|^{-2} \rho_{\gamma_{\xi'}}(x) |\psi_\xi|(y)^2 d\xi' dx dy \right)^{1/2} \\
& \quad \times \left(\sum_{m \in \mathbb{Z}^3, |m|_\infty \leq 1} \int_{Q_l^*} \int_{Q_l^2} |\xi' - \xi - 2\pi m/l|^{-2} \rho_{\gamma_{\xi'}}(x) |\overline{\phi_\xi}|(y)^2 d\xi' dx dy \right)^{1/2} \\
& \leq 4\pi \left(3 \int_{4Q_l^*} |\eta|^{-8/3} d\eta \right)^{3/4} \|\gamma\|_{\sigma_{1,4}} \|\psi_\xi\|_{L_\xi^2} \\
& \leq C_l' \|\gamma\|_{\sigma_{1,4}} \|\psi_\xi\|_{L_\xi^2}.
\end{aligned}$$

or by $0 \leq \gamma_{\xi'} \leq \mathbb{1}_{L_{\xi'}^2}$ with $\gamma_{\xi'} f_{\xi'}(x) = \int_{Q_l} \gamma_{\xi'}(x, y) f_{\xi'}(y) dy$,

$$\begin{aligned}
& \int_{Q_l^*} d\xi' \int_{Q_l^2} 4\pi \sum_{m \in \mathbb{Z}^3, |m|_\infty \leq 1} \frac{e^{-i(\xi' - \xi - 2\pi m/l) \cdot (x-y)}}{|\xi' - \xi - 2\pi m/l|^2} \gamma_{\xi'}(x, y) \psi_\xi(y) \overline{\phi_\xi}(x) dx dy \\
& \leq 4\pi \sum_{m \in \mathbb{Z}^3, |m|_\infty \leq 1} \int_{Q_l^*} d\xi' \frac{1}{|\xi' - \xi - 2\pi m/l|^2} \\
& \quad \times \left| \left\langle \gamma_{\xi'} e^{-i(\xi' - \xi - 2\pi m/l) \cdot (\cdot)} \overline{\phi_\xi}(\cdot), e^{-i(\xi' - \xi - 2\pi m/l) \cdot (\cdot)} \overline{\psi_\xi}(\cdot) \right\rangle \right| \\
& \leq C_l \sup \operatorname{ess}_{\xi' \in Q_l^*} \|\gamma_{\xi'}\|_{\mathcal{B}(L_{\xi'}^2)} \|\psi_\xi\|_{L_\xi^2} \|\phi_\xi\|_{L_\xi^2} \\
& \leq C_l \|\gamma\|_Y \|\psi_\xi\|_{L_\xi^2},
\end{aligned}$$

with

$$C_l = \sup_{\xi \in Q_l^*} \sum_{m \in \mathbb{Z}^3, |m|_\infty \leq 1} \int_{Q_l^*} d\xi' \frac{4\pi}{|\xi' - \xi - 2\pi m/l|^2}.$$

- the last term, corresponding to g . Obviously, since $g \in L^\infty$,

$$\int_{Q_l^*} d\xi' \int_{Q_l} g(\xi' - \xi, x - y) \gamma_{\xi'}(x, y) \psi_\xi(y) \overline{\phi_\xi}(x) dx dy \leq \|g\|_{L^\infty} \|\gamma\|_{\sigma_{1,1}} \|\psi_\xi\|_{L_\xi^2}$$

As a result, there is a constant C_W and C_W' , such that

•

$$\|W_\gamma \psi_\xi\|_{L_\xi^2} \leq C_W \|\gamma\|_{X \cap Y} \|\psi_\xi\|_{L_\xi^2},$$

as $\|\gamma\|_{\sigma_{1,1}} \leq \|\gamma\|_X$;

•

$$\|W_\gamma \psi_\xi\|_{L_\xi^2} \leq C_W' \|\gamma\|_{\sigma_{1,1} \cap Y} \|D_\xi |\psi_\xi|\|_{L_\xi^2};$$

- and

$$\|W_\gamma \psi_\xi\|_{L_\xi^2} \leq C_W'' \|\gamma\|_{\sigma_{1,1} \cap \sigma_{1,4}} \| |D_\xi| \psi_\xi \|_{L_\xi^2},$$

where

$$C_W = C_H' + \|f\|_{L^\infty} + C_l, \quad C_W' = C_G + \|f\|_{L^\infty} + C_l, \quad C_W'' = C_H' + \|f\|_{L^\infty} + C_l'.$$

□

Similarly, we have

Corollary 3.2. *Let $\psi_\xi \in H_\xi^{1/2}$, then*

- if $\gamma_1, \gamma_2 \in X \cap Y$,

$$\|W_{\gamma_1 - \gamma_2, \xi} \psi_\xi\|_{L_\xi^2} \leq C_W \|\gamma_1 - \gamma_2\|_{X \cap Y} \|\psi_\xi\|_{L_\xi^2} \quad (3.6)$$

- if $\gamma_1, \gamma_2 \in \sigma_{1,1} \cap Y$,

$$\|W_{\gamma_1 - \gamma_2, \xi} \psi_\xi\|_{L_\xi^2} \leq C_W' \|\gamma_1 - \gamma_2\|_{\sigma_{1,1} \cap Y} \| |D_\xi| \psi_\xi \|_{L_\xi^2} \quad (3.7)$$

- if $\gamma_1, \gamma_2 \in \sigma_{1,1} \cap \sigma_{1,4}$,

$$\|W_{\gamma_1 - \gamma_2, \xi} \psi_\xi\|_{L_\xi^2} \leq C_W'' \|\gamma_1 - \gamma_2\|_{\sigma_{1,1} \cap \sigma_{1,4}} \|\psi_\xi\|_{L_\xi^2} \quad (3.8)$$

4 Retraction for the periodic Dirac-Fock model

In this section, we repeat the ideas of Séré [53], and construct the set $\Gamma_{\leq q}^+$.

Recall that $q^+ = \max\{q, 1\}$.

Lemma 4.1. *Let $\gamma \in \Gamma_{\leq q}$. For almost every $\xi \in Q_l^*$, then*

1. $\|V_{\gamma, \xi}\|_{\mathcal{B}(L_\xi^2)} \leq C_{EE} \|\gamma\|_{X \cap Y}$, with $C_{EE} = C_H' + C_W$;

2. for $u \in H_\xi^1$,

$$\|V_{\gamma, \xi} u_\xi\|_{L_\xi^2} \leq C_{EE}' \|\gamma\|_{\sigma_{1,1} \cap Y} \| |D_\xi| u \|_{L_\xi^2} \quad (4.1)$$

with $C_{EE}' = C_G + C_W'$;

3. if $q > 1$,

$$\| |D_{\gamma, \xi}|^{1/2} |D_\xi|^{-1/2} \|_{\mathcal{B}(L_\xi^2)} \leq (1 + \alpha(C_H'(z + q) + C_W' q^+))^{1/2};$$

4. if $\alpha(C_H'(z + q) + C_W' q^+) < 1$, then

$$\| |D_\xi|^{1/2} |D_{\gamma, \xi}|^{-1/2} \|_{\mathcal{B}(L_\xi^2)} \leq (1 - \alpha(C_H'(z + q) + C_W' q^+))^{-1/2};$$

5. if $\alpha(C_H'(z + q) - C_W' q^+) < 1$, then $D_{\gamma, \xi}$ is a self-adjoint operator.

Proof. For the first inequality, it is just the combination of Corollary 3.1 inequality (3.4) and Lemma 2.11 inequality (2.18). And

$$C_{EE} = C'_H + C_W.$$

For the second, we use the Lemma 2.9 and Lemma 2.11, with a small modification:

$$\|G_l * \rho_\gamma u_\xi\|_{L_\xi^2} \leq \|\rho\|_{L^1} \|G_l u_\xi\|_{L_\xi^2} \leq C_G \|\gamma\|_{\sigma_{1,1}} \|D_\xi |u_\xi|\|_{L_\xi^2}.$$

Now,

$$\|V_{\gamma,\xi} u_\xi\|_{L_\xi^2} \leq (C_G \|\gamma\|_{\sigma_{1,1}} + C'_W \|\gamma\|_{\sigma_{1,1} \cap Y}). \quad (4.2)$$

Thus,

$$\|V_{\gamma,\xi} u_\xi\|_{L_\xi^2} \leq C'_{EE} \|\gamma\|_{\sigma_{1,1} \cap Y} \|D_\xi |u_\xi|\|_{L_\xi^2}.$$

where

$$C'_{EE} = C_G + C'_W.$$

And the next two estimates are based on the following inequality:

$$|D_{\gamma,\xi} - D_\xi| \leq \alpha z |G_l| + \alpha |\rho_\gamma * G_l| + \alpha |W_{\gamma,\xi}|.$$

As $\|\gamma\|_Y \leq 1$ and $\|\gamma\|_{\sigma_{1,1}} \leq q$, thus $\|\gamma\|_{\sigma_{1,1} \cap Y} \leq q^+$. By Lemma 2.9 and inequality (4.2), we yield

$$|D_{\gamma,\xi} - D_\xi| \leq \alpha (C'_H(z+q) + C'_W q^+) |D_\xi|. \quad (4.3)$$

Thus, for the third inequality,

$$|D_{\gamma,\xi}| \leq |D_{\gamma,\xi} - D_\xi| + |D_\xi| \leq (1 + \alpha (C'_H(z+q) + C'_W q^+)) |D_\xi|;$$

and the fourth inequality,

$$|D_\xi| \leq |D_{\gamma,\xi} - D_\xi| + |D_{\gamma,\xi}| \leq \alpha (C'_H(z+q) - C'_W q^+) |D_\xi| + |D_{\gamma,\xi}|,$$

namely

$$|D_\xi| \leq (1 - \alpha (C'_H(z+q) - C'_W q^+))^{-1} |D_{\gamma,\xi}|.$$

Finally, the last statement is just application of the Kato-Rellich Theorem. \square

Recall that $P_{0,\xi}^+ = \mathbb{1}_{\mathbb{R}^+} (D_0 + \alpha z G_l)$

Lemma 4.2. *Assume that $\kappa = \alpha (C'_H(z+q) + C'_W q^+) < 1$. Let $a > \frac{\alpha}{2} C_{EE} (1 - \kappa)^{-1}$. Then for $r > 0$ small enough, the map*

$$Q : \gamma \rightarrow (P_\gamma^+ - P_0^+)$$

is defined by

$$Q_\xi(\gamma) := (P_{\gamma,\xi}^+ - P_{0,\xi}^+) \gamma_\xi$$

and

$$Q(\gamma) := (P_\gamma^+ - P_0^+) \gamma = \frac{l^3}{(2\pi)^3} \int_{Q_i^*}^\oplus Q_\xi(\gamma) d\xi.$$

This map is well-defined and of class $C^{1,1}$ on $\mathcal{D} := \Gamma_{\leq q} + B_{X \cap Y}(r)$, open subset of $X \cap Y$, with values in the Banach space Y . We have the estimates

- $\forall \gamma \in \mathcal{D}, h \in X \cap Y: \| |D_0|^{1/2} DQ(\gamma)h |D_0|^{1/2} \|_Y \leq a \|h\|_{X \cap Y};$
- $\forall \gamma, \gamma' \in \mathcal{D}, \| |D_0|^{1/2} [DQ(\gamma)h - DQ(\gamma')h] |D_0|^{1/2} \|_Y \leq K \|\gamma - \gamma'\|_{X \cap Y} \|h\|_{X \cap Y}.$

Proof. For every $\gamma \in \mathcal{D}$, we know that $\gamma = \gamma_1 + \gamma_2$ with $\gamma_1 \in \Gamma_{\leq q}$ and $\gamma_2 \in B_{X \cap Y}(r)$, thus

$$\|\gamma\|_{\sigma_{1,1}} \leq \|\gamma_1\|_{\sigma_{1,1}} + \|\gamma_2\|_{X \cap Y} \leq q + r.$$

Obviously, as $\kappa < 1$, there is a $R > 0$ small enough, such that $\tilde{\kappa}(r) := \alpha(C'_H(z + q + r) + C'_W(q^+ + r)) < 1$ for every $r \in [0, R)$.

By Lemma 4.1, $D_{\gamma,\xi}$ is a self-adjoint operator for all $\gamma \in \mathcal{D}$, then by Taylor's Formula [32, Chapter VI.5, Lemma 5.6] or [23] we have

$$P_{\gamma,\xi}^+ = \frac{1}{2} + \frac{1}{2\pi} \int_{-\infty}^{+\infty} (D_{\gamma,\xi} - iz)^{-1} dz. \quad (4.4)$$

and

$$Q_\xi(\gamma) = -\frac{\alpha}{2\pi} \int_{-\infty}^{+\infty} (D_{\gamma,\xi} - iz)^{-1} V_{\gamma,\xi} (D_{0,\xi} - iz)^{-1} dz.$$

Hence,

$$DQ_\xi(\gamma)h = -\frac{\alpha}{2\pi} \int_{-\infty}^{+\infty} (D_{\gamma,\xi} - iz)^{-1} V_{h,\xi} (D_{\gamma,\xi} - iz)^{-1} dz.$$

Now, by the Lemma 4.1,

$$\begin{aligned} & \| |D_\xi|^{1/2} Q_\xi(\gamma)h |D_\xi|^{1/2} \|_{\mathcal{B}(L_\xi^2)} \\ & \leq \frac{\alpha}{2\pi} \int_{-\infty}^{+\infty} \| |D_\xi|^{1/2} (D_{\gamma,\xi} - iz)^{-1} V_{h,\xi} (D_{\gamma,\xi} - iz)^{-1} |D_\xi|^{1/2} \|_{\mathcal{B}(L_\xi^2)} dz \\ & \leq \frac{\alpha}{2\pi} \|V_{h,\xi}\|_{\mathcal{B}(L_\xi^2)} \| |D_\xi|^{1/2} |D_{\gamma,\xi}|^{-1/2} \|_{\mathcal{B}(L_\xi^2)}^2 \int_{-\infty}^{+\infty} \| |D_{\gamma,\xi}|^{1/2} |D_{\gamma,\xi} - iz|^{-1} \|_{\mathcal{B}(L_\xi^2)}^2 dz \\ & \leq \frac{\alpha}{2\pi} C_{EE} (1 - \kappa)^{-1} \|h\|_{X \cap Y} \int_{-\infty}^{+\infty} \| |D_{\gamma,\xi}|^{1/2} |D_{\gamma,\xi} - iz|^{-1} \|_{\mathcal{B}(L_\xi^2)}^2 dz. \end{aligned} \quad (4.5)$$

For any $u_\xi \in L_\xi^2(Q_l)$, we have that

$$\int_{-\infty}^{+\infty} \left(u_\xi, (|D_{\gamma,\xi}|^2 + |z|^2)^{-1/2} |D_{\gamma,\xi}| (|D_{\gamma,\xi}|^2 + |z|^2)^{-1/2} u_\xi \right)_{(L_\xi^2, L_\xi^2)} dz = \frac{\pi}{2} \|u_\xi\|_{L_\xi^2}^2,$$

which means that

$$\int_{-\infty}^{+\infty} \| |D_{\gamma,\xi}|^{1/2} |D_{\gamma,\xi} - iz|^{-1} \|_{\mathcal{B}(L_\xi^2)}^2 dz = \pi.$$

Now, we yield

$$\| |D_0|^{1/2} Q(\gamma)h |D_0|^{1/2} \|_Y = \| |D_\xi|^{1/2} Q_\xi(\gamma)h |D_\xi|^{1/2} \|_{L^\infty(Q_l^*; \mathcal{B}(L_\xi^2))} \leq \frac{\alpha}{2} C_{EE} (1 - \tilde{\kappa}(r))^{-1} \|h\|_{X \cap Y}.$$

And for every $a > \frac{\alpha}{2} C_{EE} (1 - \kappa)^{-1}$, obviously there is a $0 < r_0 < R$, such that

$$a \geq \frac{\alpha}{2} C_{EE} (1 - \tilde{\kappa}(r_0))^{-1}.$$

Now, we have finished the first estimate.

For the second, we have that

$$\begin{aligned} & DQ_\xi(\gamma)h - DQ_\xi(\gamma') \\ &= -\frac{\alpha^2}{2\pi} \int_{-\infty}^{+\infty} (D_{\gamma,\xi} - iz)^{-1} V_{\gamma'-\gamma,\xi} (D_{\gamma',\xi} - iz)^{-1} V_{h,\xi} (D_{\gamma,\xi} - iz)^{-1} dz \\ &\quad - \frac{\alpha^2}{2\pi} \int_{-\infty}^{+\infty} (D_{\gamma',\xi} - iz)^{-1} V_{h,\xi} (D_{\gamma,\xi} - iz)^{-1} V_{\gamma'-\gamma,\xi} (D_{\gamma',\xi} - iz)^{-1} dz \end{aligned}$$

Now, we only need to calculate the first term in the right hand of the above equality. For the other term, the estimate is same.

Given

$$\begin{aligned} & \frac{\alpha^2}{2\pi} \left\| \int_{-\infty}^{+\infty} |D_\xi|^{1/2} (D_{\gamma,\xi} - iz)^{-1} V_{\gamma'-\gamma,\xi} (D_{\gamma',\xi} - iz)^{-1} V_{h,\xi} (D_{\gamma,\xi} - iz)^{-1} |D_\xi|^{1/2} dz \right\|_{\mathcal{B}(L_\xi^2)} \\ & \leq \frac{\alpha^2}{2\pi} \|V_{h,\xi}\|_{\mathcal{B}(L_\xi^2)} \|V_{\gamma'-\gamma,\xi}\|_{\mathcal{B}(L_\xi^2)} \| |D_\xi|^{1/2} |D_{\gamma',\xi}|^{-1/2} \|_{\mathcal{B}(L_\xi^2)}^2 \| |D_{\gamma',\xi}|^{-1} \|_{\mathcal{B}(L_\xi^2)} \\ & \quad \times \int_{-\infty}^{+\infty} dz \| |D_{\gamma,\xi}|^{1/2} (D_{\gamma,\xi} - iz)^{-1} \|_Y^2 \\ & \leq \frac{\alpha^2}{2} C_{EE}^2 (1 - \tilde{\kappa}(r))^{-2} \|h\|_{X \cap Y} \|\gamma - \gamma'\|_{X \cap Y}. \end{aligned}$$

Now we have

$$\| |D_0|^{1/2} [DQ(\gamma) - DQ(\gamma')] h |D_0|^{1/2} \|_Y \leq \alpha^2 C_{EE}^2 (1 - \tilde{\kappa}(r))^{-2} \|h\|_{X \cap Y} \|\gamma - \gamma'\|_{X \cap Y}.$$

Letting $K = \alpha^2 C_{EE}^2 (1 - \tilde{\kappa}(r))^{-2}$, we get the conclusion. \square

As a consequence of these estimates, we have the following inequality:

Proposition 4.3. *Assume that $\kappa = \alpha(C'_H(z+q) + C'_W q^+) < 1$ and $C_{EE} = C'_H + C_W$.*

Let

$$A > \frac{\alpha C_{EE} (1 + \kappa)^{1/2}}{(1 - \kappa)^{3/2}}.$$

Then for $r > 0$ small enough, the map $T : \gamma \rightarrow P_\gamma^+ \gamma P_\gamma^+$ is well-defined of class $C^{1,1}$ on $\mathcal{D} = \Gamma_{\leq q} + B_{X \cap Y}(r)$ with values in $X \cap Y$, and for any $\gamma \in T^{-1}(\mathcal{D})$:

$$\|T^2(\gamma) - T(\gamma)\|_{X \cap Y} \leq A \|T(\gamma)\|_{\sigma_{1,1} \cap Y}^{1/2} \|T(\gamma)\|_{X \cap Y}^{1/2} \|\gamma - T(\gamma)\|_{X \cap Y}. \quad (4.6)$$

Moreover, for any $R > 0$:

$$\|DT(\gamma)\|_{\mathcal{B}(X \cap Y)} \text{ and } \|T(\gamma) - \gamma\|_{X \cap Y} \text{ are bounded on } \mathcal{D} \cap B_{X \cap Y}(R+r). \quad (4.7)$$

$$\exists L_R > 0, \forall \gamma, \gamma' \in \mathcal{D} \cap B_{X \cap Y}(R+r), \quad \|DT(\gamma) - DT(\gamma')\|_{\mathcal{B}(X \cap Y)} \leq L_R \|\gamma' - \gamma\|_{X \cap Y}. \quad (4.8)$$

Remark 4.4. Notice that

$$T(\gamma) = P_\gamma^+ \gamma P_\gamma^+ = \frac{l^3}{(2\pi)^3} \int_{Q^*}^\oplus P_{\gamma,\xi}^+ \gamma_\xi P_{\gamma,\xi}^+ d\xi = \frac{l^3}{(2\pi)^3} \int_{Q^*}^\oplus T_\xi(\gamma_\xi) d\xi$$

Proof. Since $Q(\gamma)$ is $C^{1,1}$, then $T(\gamma)$ is $C^{1,1}$.

Now we prove (4.6).

$$T^2(\gamma) - T(\gamma) = (P_{T(\gamma)}^+ - P_\gamma^+)T(\gamma)P_{T(\gamma)}^+ + P_\gamma^+T(\gamma)(P_{T(\gamma)}^+ - P_\gamma^+)$$

Then

$$\|T^2(\gamma) - T(\gamma)\|_{X \cap Y} \leq \|(P_{T(\gamma)}^+ - P_\gamma^+)T(\gamma)P_{T(\gamma)}^+\|_{X \cap Y} + \|P_\gamma^+T(\gamma)(P_{T(\gamma)}^+ - P_\gamma^+)\|_{X \cap Y},$$

and

$$\|P_\gamma^+T(\gamma)(P_{T(\gamma)}^+ - P_\gamma^+)\|_X \leq \| |D_0|^{1/2}(P_{T(\gamma)}^+ - P_\gamma^+) |D_0|^{1/2} \|_Y \|T(\gamma)P_{T(\gamma)}^+ |D_0|^{1/2}\|_{\sigma_{1,1}},$$

$$\|P_\gamma^+T(\gamma)(P_{T(\gamma)}^+ - P_\gamma^+)\|_Y \leq \| |D_0|^{1/2}(P_{T(\gamma)}^+ - P_\gamma^+) |D_0|^{1/2} \|_Y \|T(\gamma)P_{T(\gamma)}^+\|_Y.$$

For the term $T(\gamma)P_{T(\gamma)}^+ |D_0|^{1/2}$, by Lemma 4.1, we have that

$$\begin{aligned} \|T_\xi(\gamma)P_{T(\gamma),\xi}^+ |D_\xi|^{1/2}\|_{\sigma_1(\xi)} &\leq \| |D_{T(\gamma),\xi}|^{-1/2} |D_\xi|^{1/2} \|_{\mathcal{B}(L_\xi^2)} \|T_\xi(\gamma)P_{T(\gamma),\xi}^+ |D_{T(\gamma),\xi}|^{1/2}\|_{\sigma_1(\xi)} \\ &\leq (1 - \kappa)^{-1/2} \|T_\xi(\gamma) |D_{T(\gamma),\xi}|^{1/2} P_{T(\gamma),\xi}^+\|_{\sigma_1(\xi)} \\ &\leq (1 - \kappa)^{-1/2} \|T_\xi(\gamma) |D_{T(\gamma),\xi}|^{1/2}\|_{\sigma_1(\xi)} \\ &\leq (1 - \kappa)^{-1/2} (1 + \kappa)^{1/2} \|T_\xi(\gamma) |D_\xi|^{1/2}\|_{\sigma_1(\xi)} \\ &\leq (1 - \kappa)^{-1/2} (1 + \kappa)^{1/2} \|T_\xi(\gamma)\|_{\sigma_1(\xi)}^{1/2} \|T_\xi(\gamma)\|_{X(\xi)}^{1/2}. \end{aligned} \tag{4.9}$$

Thus

$$\|T(\gamma)P_{T(\gamma)}^+ |D_0|^{1/2}\|_{\sigma_{1,1}} \leq (1 - \kappa)^{-1/2} (1 + \kappa)^{1/2} \|T_\xi(\gamma)\|_{\sigma_{1,1}}^{1/2} \|T_\xi(\gamma)\|_X^{1/2}.$$

And as $\gamma, T(\gamma) \in \mathcal{D}$, thus $\gamma + t(T(\gamma) - \gamma) \in \mathcal{D}$ for $0 \leq t \leq 1$,

$$|D_0|^{1/2}(P_{T(\gamma)}^+ - P_\gamma^+) |D_0|^{1/2} = \int_0^1 |D_0|^{1/2} DQ_\xi(\gamma + t(T(\gamma) - \gamma))(T(\gamma) - \gamma) |D_0|^{1/2} dt,$$

we deduce that

$$\| |D_0|^{1/2}(P_{T(\gamma)}^+ - P_\gamma^+) |D_0|^{1/2} \|_Y \leq \| |D_0|^{1/2} DQ(\gamma) |D_0|^{1/2} \|_Y \|\gamma - T(\gamma)\|_{X \cap Y}, \tag{4.10}$$

by Lemma 4.2 we yield

$$\|T^2(\gamma) - T(\gamma)\|_{X \cap Y} \leq 2a(1 - \kappa)^{-1/2} (1 + \kappa)^{1/2} \|T(\gamma)\|_{\sigma_{1,1} \cap Y}^{1/2} \|T(\gamma)\|_{X \cap Y}^{1/2} \|\gamma - T(\gamma)\|_{X \cap Y}.$$

For statement (4.7), by Lemma 4.2, for any $R > 0$, and for any $\gamma \in \mathcal{D} \cap B_{X \cap Y}(R+r)$, obviously

$$\|T(\gamma) - \gamma\|_{X \cap Y} \leq 2\|\gamma\|_{X \cap Y} \leq 2(R+r).$$

As

$$DT(\gamma)h = (DP_\gamma h)\gamma P_\gamma + P_\gamma \gamma (DP_\gamma h) + P_\gamma h P_\gamma,$$

then by Lemma 4.2 and inequality (4.9), we yield for r small enough,

$$\|DT(\gamma)h\|_{X \cap Y} \leq \left((1 - \tilde{\kappa}(r))^{-1} (1 + \tilde{\kappa}(r)) + A \|T_\xi(\gamma)\|_{\sigma_{1,1} \cap Y}^{1/2} \|T_\xi(\gamma)\|_{X \cap Y}^{1/2} \right) \|h\|_{X \cap Y}$$

Thus, $\|DT(\gamma)h\|_{\mathcal{B}(X \cap Y)}$ is bounded.

Finally, for the term $DT(\gamma') - DT(\gamma)$, we have

$$\begin{aligned} & DT_\xi(\gamma')h - DT_\xi(\gamma)h \\ &= (DP_{\gamma,\xi}h)\gamma_\xi P_{\gamma,\xi} + P_{\gamma,\xi}\gamma_\xi(DP_{\gamma,\xi}h) + P_{\gamma,\xi}h_\xi P_{\gamma,\xi} \\ & \quad - (DP_{\gamma',\xi}h)\gamma'_\xi P_{\gamma',\xi} - P_{\gamma',\xi}\gamma'_\xi(DP_{\gamma',\xi}h) - P_{\gamma',\xi}h_\xi P_{\gamma',\xi}. \end{aligned}$$

By Lemma 4.2, the inequality (4.9) and the inequality (4.10), we notice that there is a constant $C_{\tilde{\kappa},r,1}$, such that for r small enough

$$\begin{aligned} & \|(DP_{\gamma,\xi}h)\gamma_\xi P_{\gamma,\xi} - (DP_{\gamma',\xi}h)\gamma'_\xi P_{\gamma',\xi}\|_{X(\xi)} \\ & \leq \|[(DP_{\gamma,\xi}h) - (DP_{\gamma',\xi}h)]\gamma_\xi P_{\gamma,\xi}\|_{X(\xi)} + \|(DP_{\gamma',\xi}h)(\gamma_\xi - \gamma'_\xi)P_{\gamma,\xi}\|_{X(\xi)} \\ & \quad + \|(DP_{\gamma',\xi}h)\gamma'_\xi(P_{\gamma,\xi} - P_{\gamma',\xi})\|_{X(\xi)} \\ & \leq (1 - \tilde{\kappa}(r))^{-1/2}(1 + \tilde{\kappa}(r))^{1/2}\|\gamma_\xi\|_{\sigma_1(\xi)}^{1/2}\|\gamma_\xi\|_{X(\xi)}^{1/2}\|D_\xi|^{1/2}[(DP_{\gamma,\xi}h) - (DP_{\gamma',\xi}h)]\|_{\mathcal{B}(L_\xi^2)} \\ & \quad + (1 - \tilde{\kappa}(r))^{-1/2}(1 + \kappa(r))^{1/2}\|D_\xi|^{1/2}(DP_{\gamma',\xi}h)\|_{\mathcal{B}(L_\xi^2)}\|D_\xi|^{1/2}(\gamma_\xi - \gamma'_\xi)\|_{\sigma_1(\xi)} \\ & \quad + \|D_\xi|^{1/2}(DP_{\gamma',\xi}h)\|_{\mathcal{B}(L_\xi^2)}\|\gamma'_\xi\|_{\sigma_1(\xi)}\|D_\xi|^{1/2}(P_{\gamma,\xi} - P_{\gamma',\xi})\|_{\mathcal{B}(L_\xi^2)} \\ & \leq C_{\tilde{\kappa},r,1} \left(1 + \|\gamma_\xi\|_{\sigma_1(\xi)}^{1/2}\|\gamma_\xi\|_{X(\xi)}^{1/2} + \|\gamma'_\xi\|_{\sigma_1(\xi)}\right) \|\gamma - \gamma'\|_{X \cap Y} \|h\|_{X \cap Y}, \end{aligned}$$

and

$$\begin{aligned} & \|(DP_{\gamma,\xi}h)\gamma_\xi P_{\gamma,\xi} - (DP_{\gamma',\xi}h)\gamma'_\xi P_{\gamma',\xi}\|_{\mathcal{B}(L_\xi^2)} \\ & \leq \|[(DP_{\gamma,\xi}h) - (DP_{\gamma',\xi}h)]\gamma_\xi P_{\gamma,\xi}\|_{\mathcal{B}(L_\xi^2)} + \|(DP_{\gamma',\xi}h)(\gamma_\xi - \gamma'_\xi)P_{\gamma,\xi}\|_{\mathcal{B}(L_\xi^2)} \\ & \quad + \|(DP_{\gamma',\xi}h)\gamma'_\xi(P_{\gamma,\xi} - P_{\gamma',\xi})\|_{\mathcal{B}(L_\xi^2)} \\ & \leq \|\gamma_\xi\|_{\mathcal{B}(L_\xi^2)}\|D_\xi|^{1/2}(DP_{\gamma,\xi}h) - (DP_{\gamma',\xi}h)\|_{\mathcal{B}(L_\xi^2)} \\ & \quad + \|D_\xi|^{1/2}DP_{\gamma',\xi}h\|_{\mathcal{B}(L_\xi^2)}\|\gamma_\xi - \gamma'_\xi\|_{\mathcal{B}(L_\xi^2)} \\ & \quad + \|D_\xi|^{1/2}DP_{\gamma',\xi}h\|_{\mathcal{B}(L_\xi^2)}\|\gamma'_\xi\|_{\mathcal{B}(L_\xi^2)}\|D_\xi|^{1/2}(P_{\gamma,\xi} - P_{\gamma',\xi})\|_{\mathcal{B}(L_\xi^2)} \\ & \leq C_{\tilde{\kappa},r,1}\|\gamma - \gamma'\|_{X \cap Y} \|h\|_{X \cap Y}. \end{aligned}$$

Then,

$$\begin{aligned} & \|(DP_\gamma h)\gamma P_\gamma - (DP_{\gamma'} h)\gamma' P_{\gamma'}\|_{X \cap Y} \\ & \leq 2C_{\tilde{\kappa},r,1} (1 + \|\gamma\|_{X \cap Y}) \|\gamma - \gamma'\|_{X \cap Y} \|h\|_{X \cap Y}. \end{aligned}$$

Analogously, we have

$$\begin{aligned} & \|P_\gamma \gamma (DP_\gamma h) - P_{\gamma'} \gamma' (DP_{\gamma'} h)\|_{X \cap Y} \\ & \leq 2C_{\tilde{\kappa},r,1} (1 + \|\gamma_\xi\|_{X \cap Y}) \|\gamma - \gamma'\|_{X \cap Y} \|h\|_{X \cap Y}. \end{aligned}$$

And by inequality (4.10), there is a constant $C_{\tilde{\kappa},r,2}$

$$\|P_\gamma h P_\gamma - P_{\gamma'} h P_{\gamma'}\|_{X \cap Y} \leq C_{\tilde{\kappa},r,2} \|h\|_{X \cap Y} \|\gamma - \gamma'\|_{X \cap Y}.$$

Therefore,

$$\|DT(\gamma')h - DT(\gamma)h\|_{X \cap Y} \leq C_{\tilde{\kappa}, r} (1 + 2\|\gamma\|_{X \cap Y}) \|\gamma - \gamma'\|_{X \cap Y} \|h\|_{X \cap Y}$$

with $C_{\tilde{\kappa}, r} = 2C_{\tilde{\kappa}, r, 1} + C_{\tilde{\kappa}, r, 2}$.

For $\gamma \in \mathcal{D} \cap B_{X \cap Y}(R + r)$, we know

$$\|DT(\gamma') - DT(\gamma)\|_{\mathcal{B}(X \cap Y)} \leq C_{\tilde{\kappa}, r} (1 + 2R + 2r) \|\gamma - \gamma'\|_{X \cap Y}.$$

Herein, $L_R = C_{\tilde{\kappa}, r} (1 + 2R + 2r)$. □

We now define a closed set invariant for T and an open neighborhood \mathcal{U} of F .

Proposition 4.5. *Let κ and A as in Proposition 4.3, and assume $\kappa < 1$. Let $1 < R < \frac{1}{A^2 q^+}$ and*

$$F := \left\{ \gamma \in \Gamma_{\leq q}; \|\gamma\|_{X \cap Y} + \frac{\|T(\gamma) - \gamma\|_{X \cap Y}}{1 - A\sqrt{q^+}R} \leq R \right\}.$$

Let $\mathcal{U} := F + B_{X \cap Y}(r)$, r small enough.

Then \mathcal{U} and F satisfy the assumption of Séré's retraction [53] with $k := A\sqrt{q^+}R$.

Remark 4.6. Here we impose the condition $R > 1$. By Formula (5.3), the solution of our problem γ_* satisfies $\|\gamma_*\|_Y = 1$ if $1 \leq q$. Thus if $R = 1$, then $\|T(\gamma) - \gamma\|_{X \cap Y} \leq 0$ which means $F \subset \Gamma_{\leq q}^+$; and if $R < 1$, $F = \emptyset$. However F should be sufficiently large, hence we choose $R > 1$.

Proof. We only need to prove

$$k := A\|T(\gamma)\|_{\sigma_{1,1} \cap Y}^{1/2} \|T(\gamma)\|_{X \cap Y}^{1/2} < 1.$$

We have

$$\|T(\gamma)\|_{X \cap Y} \leq \|\gamma\|_{X \cap Y} \leq R.$$

Thus, under the assumption,

$$k \leq A\sqrt{q^+}R < 1.$$

□

Theorem 4.7. *Let κ and A as in Proposition 4.3, and assume $1 < R < \frac{1}{A^2 q^+}$, and $\kappa < 1$. Then there exists an open neighborhood \mathcal{V} of F in $X \cap Y$ with $T(\mathcal{V}) \subset \mathcal{V}$ and such that the sequence of iterated maps $(T^p)_{p \geq 0}$ converges for the topology of $C^{1,1}(\mathcal{V}, \mathcal{V})$, with the estimate*

$$\forall \gamma \in \mathcal{V}, \|\theta(\gamma) - T^p(\gamma)\|_{X \cap Y} \leq \frac{k^p}{1 - k} \|T(\gamma) - \gamma\|_{X \cap Y}.$$

In this way, we obtain a retraction θ of \mathcal{V} onto $\text{Fix}(T) \cup \mathcal{V}$ whose restriction to F is a retraction of F onto $\text{Fix}(T) \cap F$. This map and its differential are bounded and uniformly continuous on \mathcal{V} .

Moreover, for any $\gamma \in \theta(F)$, by Floquet-Bloch decomposition, we have

$$\gamma = \frac{l^3}{(2\pi)^3} \int_{Q_l^*}^{\oplus} \gamma_{\xi} d\xi$$

with $\gamma_{\xi} \in \theta_{\xi}(F)$ and $\theta_{\xi}(\gamma) = \gamma_{\xi}$. Then, for any $h \in X \cap Y$ with the operator $S_{\xi} = D\theta_{\xi}(\gamma)h$ satisfies

$$P_{\gamma,\xi}^+ S_{\xi} P_{\gamma,\xi}^+ = P_{\gamma,\xi}^+ h_{\xi} P_{\gamma,\xi}^+ \quad \text{and} \quad P_{\gamma,\xi}^- S_{\xi} P_{\gamma,\xi}^- = 0$$

In other words, the splitting $L_{\xi}^2 = P_{\gamma,\xi}^+ L_{\xi}^2 \oplus P_{\gamma,\xi}^- L_{\xi}^2$ gives a block decomposition of $D\theta_{\xi}(\gamma)h$ of the form

$$D\theta_{\xi}(\gamma)h = \begin{pmatrix} P_{\gamma,\xi}^+ h_{\xi} P_{\gamma,\xi}^+ & b_{\gamma,\xi}(h)^* \\ b_{\gamma,\xi}(h) & 0 \end{pmatrix} \quad (4.11)$$

Proof. It is just application of Séré's retraction A.1. And we only need to prove the equation (4.11).

As $P_{\gamma,\xi}^+ = (P_{\gamma,\xi}^+)^2$, we have

$$DP_{\gamma,\xi}^+ h = P_{\gamma,\xi}^+ (DP_{\gamma,\xi}^+ h) + (DP_{\gamma,\xi}^+ h) P_{\gamma,\xi}^+.$$

Thus,

$$P_{\gamma,\xi}^- (DP_{\gamma,\xi}^+ h) P_{\gamma,\xi}^- = 0,$$

and

$$P_{\gamma,\xi}^+ (DP_{\gamma,\xi}^+ h) P_{\gamma,\xi}^+ = 2P_{\gamma,\xi}^+ (DP_{\gamma,\xi}^+ h) P_{\gamma,\xi}^+,$$

which means that

$$P_{\gamma,\xi}^+ (DP_{\gamma,\xi}^+ h) P_{\gamma,\xi}^+ = 0.$$

Now, for $DT_{\xi}(\gamma)h$, we have

$$DT_{\xi}(\gamma)h = (DP_{\gamma,\xi}^+ h) \gamma_{\xi} P_{\gamma,\xi}^+ + P_{\gamma,\xi}^+ h_{\xi} P_{\gamma,\xi}^+ + P_{\gamma,\xi}^+ \gamma_{\xi} (DP_{\gamma,\xi}^+ h).$$

As $\gamma \in \theta(F)$, it is clear that

$$\gamma = T(\gamma) = \theta(\gamma), \quad \gamma_{\xi} = T_{\xi}(\gamma) = \theta_{\xi}(\gamma).$$

Hence,

$$\begin{aligned} D\theta_{\xi}(\gamma)h &= DT_{\xi}(\gamma)h \\ &= (DP_{\gamma,\xi}^+ h) \gamma_{\xi} P_{\gamma,\xi}^+ + P_{\gamma,\xi}^+ h_{\xi} P_{\gamma,\xi}^+ + P_{\gamma,\xi}^+ \gamma_{\xi} (DP_{\gamma,\xi}^+ h) \\ &= (DP_{\gamma,\xi}^+ h) P_{\gamma,\xi}^+ \gamma_{\xi} P_{\gamma,\xi}^+ + P_{\gamma,\xi}^+ h_{\xi} P_{\gamma,\xi}^+ + P_{\gamma,\xi}^+ \gamma_{\xi} P_{\gamma,\xi}^+ (DP_{\gamma,\xi}^+ h) \end{aligned}$$

Now,

$$\begin{aligned} P_{\gamma,\xi}^+ D\theta_{\xi}(\gamma)h P_{\gamma,\xi}^+ &= P_{\gamma,\xi}^+ h_{\xi} P_{\gamma,\xi}^+ \\ P_{\gamma,\xi}^- D\theta_{\xi}(\gamma)h P_{\gamma,\xi}^+ &= P_{\gamma,\xi}^- (DP_{\gamma,\xi}^+ h) P_{\gamma,\xi}^+ \gamma_{\xi} P_{\gamma,\xi}^+ \\ P_{\gamma,\xi}^+ D\theta_{\xi}(\gamma)h P_{\gamma,\xi}^- &= P_{\gamma,\xi}^+ \gamma_{\xi} P_{\gamma,\xi}^+ (DP_{\gamma,\xi}^+ h) P_{\gamma,\xi}^- \\ P_{\gamma,\xi}^- D\theta_{\xi}(\gamma)h P_{\gamma,\xi}^- &= 0. \end{aligned}$$

□

The question we address now is whether a minimizing sequence for $\mathcal{E}^{DF}(\gamma) - \epsilon_F \text{Tr}_{L^2}(\gamma)$ in $\Gamma_{\leq q}^+$ lies in the set F . For this purpose we need the following result.

Lemma 4.8. *Assume that $\kappa = \alpha(C'_H(z+q) + C'_W q) < 1$. There is a minimizing sequence $\gamma_n \in \Gamma_{\leq q}^+$ of $\min_{\gamma \in \Gamma_{\leq q}^+} (\mathcal{E}^{DF}(\gamma) - \epsilon_F \text{Tr}_{L^2}(\gamma))$, such that*

$$\mathcal{E}^{DF}(\gamma_n) - \epsilon_F \text{Tr}_{L^2}(\gamma_n) \leq 0.$$

And moreover, if $\kappa < 1 - 1/2\alpha C_{EE}q^+$, then we have

$$\|\gamma_n\|_{X \cap Y} \leq \max\{(1 - \kappa - 1/2\alpha C_{EE}q^+)^{-1}\epsilon_F q, 1\}. \quad (4.12)$$

Proof. Note that the operator 0 belongs to $\Gamma_{\leq q}^+$ and satisfies that $\mathcal{E}^{DF}(0) - \epsilon_F \text{Tr}_{L^2}(0) = 0$. It is also belongs to the interior of F in $\Gamma_{\leq q}$.

Thus, $\min_{\gamma \in \Gamma_{\leq q}^+} (\mathcal{E}^{DF}(\gamma) - \epsilon_F \text{Tr}_{L^2}(\gamma)) \leq 0$. And there is a minimizing sequence, such that

$$\mathcal{E}^{DF}(\gamma_n) - \epsilon_F \text{Tr}_{L^2}(\gamma_n) \leq 0.$$

Especially, if $\min_{\gamma \in \Gamma_{\leq q}^+} (\mathcal{E}^{DF}(\gamma) - \epsilon_F \text{Tr}_{L^2}(\gamma)) = 0$, then $\gamma_n = 0$ could be the sequence.

As

$$\frac{l^3}{(2\pi)^2} \int_{Q_l^*} \text{Tr}_{L^2_\xi}((D_{\gamma_n, \xi} - \epsilon_F - 1/2\alpha V_{\gamma_n, \xi})\gamma_n, \xi) d\xi = \mathcal{E}^{DF}(\gamma_n) - \epsilon_F \text{Tr}_{L^2}(\gamma_n) \leq 0$$

and $D_{\gamma_n, \xi} \gamma_n, \xi = |D_{\gamma_n, \xi}| \gamma_n, \xi$, we get

$$\begin{aligned} & \frac{l^3}{(2\pi)^2} \int_{Q_l^*} \text{Tr}_{L^2_\xi}((D_{\gamma_n, \xi} - \epsilon_F - 1/2\alpha V_{\gamma_n, \xi})\gamma_n, \xi) d\xi \\ &= \frac{l^3}{(2\pi)^2} \int_{Q_l^*} \text{Tr}_{L^2_\xi}((|D_{\gamma_n, \xi}| - \epsilon_F - 1/2\alpha V_{\gamma_n, \xi})\gamma_n, \xi) d\xi \\ &\geq \frac{l^3}{(2\pi)^2} \int_{Q_l^*} \text{Tr}_{L^2_\xi}(((1 - \kappa)|D_\xi| - \epsilon_F - 1/2\alpha V_{\gamma_n, \xi})\gamma_n, \xi) d\xi \\ &\geq (1 - \kappa)\|\gamma_n\|_X - 1/2\alpha C_{EE}\|\gamma_n\|_{\sigma_{1,1} \cap Y} \|\gamma_n\|_X - \epsilon_F \|\gamma_n\|_{\sigma_{1,1}} \\ &\geq (1 - \kappa - 1/2\alpha C_{EE}q^+)\|\gamma_n\|_X - \epsilon_F q \end{aligned}$$

Thus,

$$(1 - \kappa - 1/2\alpha C_{EE}q^+)\|\gamma_n\|_X - \epsilon_F q \leq 0.$$

As $1 - \kappa - 1/2\alpha C_{EE}q^+ > 0$,

$$\|\gamma_n\|_X \leq (1 - \kappa - 1/2\alpha C_{EE}q^+)^{-1}\epsilon_F q.$$

Thus,

$$\|\gamma_n\|_{X \cap Y} \leq \max\{(1 - \kappa - 1/2\alpha C_{EE}q^+)^{-1}\epsilon_F q, 1\}.$$

□

Corollary 4.9. *Assume that $\kappa < 1 - 1/2\alpha C_{EE}q^+$, and let A as above. And assume that*

$$A\sqrt{\max\{(1 - \kappa - 1/2\alpha C_{EE}q^+)^{-1}\epsilon_F q, 1\}q^+} < 1.$$

Then there are A, R as in Proposition 4.5 and $\rho > 0$ such that, if $\gamma \in \Gamma_{\leq q}^+$ satisfies $\mathcal{E}^{DF}(\gamma) - \epsilon_F \text{Tr}_{L^2}(\gamma) \leq 0$, then $B_{X \cap Y}(\gamma, \rho) \cap \Gamma_{\leq q}$ is a subset of F .

Proposition 4.10. *Assume that $\kappa < 1$. Let $\gamma, \gamma' \in \Gamma_{\leq q}$ such that $0 \leq \gamma'_\xi \leq \mathbb{1}_{[0, (1-\kappa)^{-1}c^*(q+1)]}(D_{\gamma, \xi})$. Then,*

$$\|\gamma'\|_{X \cap Y} \leq \max\{(1 - \kappa)^{-2}qc^*(q + 1), 1\}.$$

Proof. By Lemma 4.1, we have

$$\begin{aligned} & \frac{l^3}{(2\pi)^3} \int_{Q_i^*} d\xi \text{Tr}_{L_\xi^2}(D_{\gamma, \xi} \gamma'_\xi) \\ &= \frac{l^3}{(2\pi)^3} \int_{Q_i^*} d\xi \text{Tr}_{L_\xi^2}(|D_{\gamma, \xi}| \gamma'_\xi) \\ &\geq (1 - \kappa) \frac{l^3}{(2\pi)^3} \int_{Q_i^*} d\xi \text{Tr}_{L_\xi^2}(|D_\xi| \gamma'_\xi) \\ &= (1 - \kappa) \|\gamma'\|_X, \end{aligned}$$

And since $\gamma' \in \Gamma_{\leq q}$,

$$\frac{l^3}{(2\pi)^3} \int_{Q_i^*} d\xi \text{Tr}_{L_\xi^2}(D_{\gamma, \xi} \gamma'_\xi) \leq (1 - \kappa)^{-1}c^*(q+1) \frac{l^3}{(2\pi)^3} \int_{Q_i^*} d\xi \text{Tr}_{L_\xi^2} \gamma'_\xi \leq q(1 - \kappa)^{-1}c^*(q+1).$$

Now we have

$$\|\gamma'\|_X \leq (1 - \kappa)^{-2}qc^*(q + 1).$$

And by $\|\gamma\|_Y \leq 1$, we have

$$\|\gamma'\|_{X \cap Y} \leq \max\{(1 - \kappa)^{-2}qc^*(q + 1), 1\}.$$

□

5 Existence of minimizers

5.1 Spectral properties of periodic Dirac operators

Our result is based on the observation of the spectral properties of Dirac operators, which will be used several times:

Lemma 5.1. *Assume that $\kappa = \alpha(C'_H(z + q) + C'_W q^+) < 1$, and $\gamma \in \Gamma_{\leq q}$. Then there are constants $c^*(k), c_*(k) > 0$ independent of ξ , with $1 \leq c_*(k) \leq c^*(k)$ and $c_*(k) \rightarrow \infty$ when $k \rightarrow \infty$ such that the k -th eigenvalue (counted with multiplicity) of the mean-field operator $D_{\gamma, \xi}$ is situated in the interval $[c_*(k)(1 - \kappa), c^*(k)(1 - \kappa)^{-1}]$ independent of γ . Moreover, there is a constant $e > c^*(q + 2)(1 - \kappa)^{-1}$ and another constant $M > 0$, such that there are at most $q + M$ eigenvalues in $[0, e]$.*

Proof. Letting

$$\Lambda_\xi^+ := \mathbb{1}_{\mathbb{R}^+}(D_\xi) = \frac{1}{2} + \frac{D_\xi}{2|D_\xi|}$$

and

$$\Lambda_\xi^- := \mathbb{1}_{\mathbb{R}^-}(D_\xi) = \frac{1}{2} - \frac{D_\xi}{2|D_\xi|}.$$

By the formula in [12, Equation (64)], we know the positive eigenvalues (λ_k) of $D_{\gamma,\xi}$:

$$\lambda_k := \inf_{\substack{V \text{ subspace of } \Lambda_\xi^+ H_\xi^{1/2} \\ \dim V = k}} \sup_{u_\xi \in (V \oplus \Lambda_\xi^- H_\xi^{1/2}) \setminus \{0\}} \frac{(D_{\gamma,\xi} u_\xi, u_\xi)}{\|u_\xi\|_{L_\xi^2}^2} \quad (5.1)$$

For the lower bound, we have

$$\lambda_k \geq \inf_{\substack{V \text{ subspace of } \Lambda_\xi^+ H_\xi^{1/2} \\ \dim V = k}} \sup_{u_\xi \in V \setminus \{0\}} \frac{(D_{\gamma,\xi} u_\xi, u_\xi)}{\|u_\xi\|_{L_\xi^2}^2}.$$

By inequality (4.3), we know

$$(D_{\gamma,\xi} u_\xi, u_\xi) \geq (1 - \kappa) (|D_\xi| u_\xi, u_\xi).$$

Thus,

$$(1 - \kappa)^{-1} \lambda_k \geq \inf_{\substack{V \text{ subspace of } \Lambda_\xi^+ H_\xi^{1/2} \\ \dim V = k}} \sup_{u_\xi \in V \setminus \{0\}} \frac{(|D_\xi| u_\xi, u_\xi)}{\|u_\xi\|_{L_\xi^2}^2} \geq \inf_{\substack{V \text{ subspace of } H_\xi^{1/2} \\ \dim V = k}} \sup_{u_\xi \in V \setminus \{0\}} \frac{(|D_\xi| u_\xi, u_\xi)}{\|u_\xi\|_{L_\xi^2}^2}.$$

Denote $c_*(k)$ by

$$c_*(k) := \inf_{\xi \in Q_l^*} \inf_{\substack{V \text{ subspace of } H_\xi^{1/2} \\ \dim V = k}} \sup_{u_\xi \in V \setminus \{0\}} \frac{(|D_\xi| u_\xi, u_\xi)}{\|u_\xi\|_{L_\xi^2}^2} = \inf_{\xi \in Q_l^*} \inf_{\substack{\mathbb{Z}_k \text{ subspace of } \mathbb{Z}^3 \\ \dim \mathbb{Z}_k = k}} \sup_{j \in \mathbb{Z}_k} \sqrt{1 + |j/l - \xi|^2}.$$

Now, we know

$$\lambda_k \geq (1 - \kappa) c_*(k).$$

And obviously,

$$c_*(k) \rightarrow \infty \quad \text{when } k \rightarrow \infty.$$

For the upper bound, by Formula (5.1), we yield

$$\lambda_k \leq \sup_{\xi \in Q_l^*} \inf_{\substack{V \text{ subspace of } \Lambda^+ H_\xi^{1/2} \\ \dim V = k}} \sup_{u_\xi \in (V \oplus \Lambda_\xi^- H_\xi^{1/2}) \setminus \{0\}} \frac{(D_{\gamma,\xi} u_\xi, u_\xi)}{\|u_\xi\|_{L_\xi^2}^2}.$$

Taking $u_\xi \in (V \oplus \Lambda^- H_\xi^{1/2}) \setminus \{0\}$, then let

$$u_\xi^+ = \Lambda^+ u_\xi \in V, \quad u_\xi^- = \Lambda^- u_\xi \in \Lambda^- H_\xi^{1/2}.$$

Thus, we know

$$(D_\xi u_\xi^+, u_\xi^-) = 0.$$

Together with inequality (4.3), we have

$$\begin{aligned}
& (D_{\gamma,\xi}u_\xi, u_\xi) \\
&= \left(D_{\gamma,\xi}u_\xi^+, u_\xi^+ \right) + 2\Re \left(D_{\gamma,\xi}u_\xi^+, u_\xi^- \right) + \left(D_{\gamma,\xi}u_\xi^-, u_\xi^- \right) \\
&\leq \| |D_\xi|^{1/2}u_\xi^+ \|_{L_\xi^2}^2 - \| |D_\xi|^{1/2}u_\xi^- \|_{L_\xi^2}^2 + \| |D_{\gamma,\xi} - D_\xi|^{1/2}u_\xi^+ \|_{L_\xi^2}^2 \\
&\quad + \| |D_{\gamma,\xi} - D_\xi|^{1/2}u_\xi^- \|_{L_\xi^2}^2 + 2\| |D_{\gamma,\xi} - D_\xi|^{1/2}u_\xi^+ \|_{L_\xi^2} \| |D_{\gamma,\xi} - D_\xi|^{1/2}u_\xi^- \|_{L_\xi^2} \\
&\leq (1 + \kappa) \| |D_\xi|^{1/2}u_\xi^+ \|_{L_\xi^2}^2 + 2\kappa \| |D_\xi|^{1/2}u_\xi^+ \|_{L_\xi^2}^2 - (1 - \kappa) \| |D_\xi|^{1/2}u_\xi^- \|_{L_\xi^2}^2 \\
&\leq (1 - \kappa)^{-1} \| |D_\xi|^{1/2}u_\xi^+ \|_{L_\xi^2}^2.
\end{aligned}$$

Let

$$c^*(k) := \sup_{\xi \in Q_l^*} \sup_{V \text{ subspace of } \Lambda^+ H_\xi^{1/2}} \inf_{\dim V=k} \sup_{u_\xi^+ \in V} \frac{\| |D_\xi|^{1/2}u_\xi^+ \|_{L_\xi^2}^2}{\| u_\xi^+ \|_{L_\xi^2}^2}.$$

As $\| u_\xi^+ \|_{L_\xi^2} \leq \| u_\xi \|_{L_\xi^2}$, we know

$$\lambda_k \leq (1 - \kappa)^{-1} c^*(k).$$

And obviously, $c_*(k) \leq c^*(k)$. □

5.2 Proof of Theorem 2.13

Now, we embark on the study of the existence. The following assumptions are necessary:

Assumption 5.2. Let $q^+ = \max\{q, 1\}$, $\kappa := \alpha((C'_H(z + q) + C'_W q^+))$, $C_{EE} := C'_H + C'_W$ and $A > 1/4\alpha(1 - \kappa)^{-2}(1 + \kappa)C_{EE}$. We assume that

1. $\kappa < 1 - 1/2\alpha C_{EE}q^+$,
2. $\kappa' := \alpha(C'_G(z + q) + C'_W q^+) < 1$,
3. $A\sqrt{\max\{(1 - \kappa - 1/2\alpha C_{EE}q^+)^{-1}\epsilon_F q, 1\}}q^+ < 1$.

We have

Theorem 5.3. *Under Assumption 5.2, for some constant $c^*(q) > 0$ only dependent on q , if $\epsilon_F > (1 - \kappa)^{-1}c^*(q + 1)$ there exists $\gamma_* \in \Gamma_{\leq q}^+$ such that*

$$\mathcal{E}^{DF}(\gamma_*) - \epsilon_F \text{Tr}_{L^2}(\gamma_*) = I_{\leq} := \min_{\gamma \in \Gamma_{\leq q}^+} (\mathcal{E}^{DF}(\gamma) - \epsilon_F \text{Tr}_{L^2}(\gamma)). \quad (5.2)$$

Besides, γ_* solves the following nonlinear self-consistent equation:

$$\begin{cases} \gamma = \mathbb{1}_{[0,\nu)}(D_\gamma) + \delta \\ D_\gamma = \frac{l^3}{(2\pi)} \int_{Q_l^*}^\oplus d\xi D_{\gamma,\xi}, \end{cases} \quad (5.3)$$

where $0 \leq \delta \leq \mathbb{1}_{\{\nu\}}(D_\gamma)$ and $0 \leq \nu \leq (1 - \kappa)^{-1}c^*(q + 1)$ independent of ϵ_F .

Furthermore, $\frac{l^3}{(2\pi)^3} \int_{Q_l^*} d\xi \text{Tr}_{L_\xi^2} \gamma_{*,\xi} = q$, thus $\nu \in \mathbb{R}$ is a Lagrange multiplier due to the charge constraint $\frac{l^3}{(2\pi)^3} \int_{Q_l^*} d\xi \text{Tr}_{L_\xi^2} \gamma_{*,\xi} = q$.

We will prove this theorem in the subsection 5.4.

Proof of Theorem 2.13. By Theorem 5.3, for $\epsilon_F > (1 - \kappa)^{-1}c^*(q + 1)$, any minimizer γ_* of I_{\leq} satisfies that

$$\gamma_* \in \Gamma_q^+.$$

Then

$$\mathcal{E}^{DF}(\gamma_*) - \epsilon_F \operatorname{Tr}_{L^2}(\gamma_*) \geq \min_{\gamma \in \Gamma_q^+} (\mathcal{E}^{DF}(\gamma) - \epsilon_F \operatorname{Tr}_{L^2}(\gamma)).$$

As $I_{\leq} \leq \min_{\gamma \in \Gamma_q^+} (\mathcal{E}^{DF}(\gamma) - \epsilon_F \operatorname{Tr}_{L^2}(\gamma))$, we yield

$$\mathcal{E}^{DF}(\gamma_*) - \epsilon_F \operatorname{Tr}_{L^2}(\gamma_*) = \min_{\gamma \in \Gamma_q^+} (\mathcal{E}^{DF}(\gamma) - \epsilon_F \operatorname{Tr}_{L^2}(\gamma)),$$

namely,

$$\mathcal{E}^{DF}(\gamma_*) = \min_{\gamma \in \Gamma_q^+} \mathcal{E}^{DF}(\gamma) = I.$$

And for any q satisfies the Assumption 2.12, we have a $\epsilon_F > (1 - \kappa)^{-1}c^*(q + 1)$, thus that

$$A\sqrt{\max\{(1 - \kappa - 1/2\alpha C_{EE}q^+)^{-1}\epsilon_F q, 1\}q^+} < 1.$$

Now the minimizers of I_{\leq} are the minimizers of I . We get the conclusion. \square

5.3 Existence of minimizers for the linearized problem

The following lemma will be used in the next sections:

Lemma 5.4. *Let $g \in \Gamma_{\leq q}$, $B := \{\gamma \in X \cap Y; \|\gamma\|_{\sigma_{1,\infty}} \leq q + M\}$. Then the minimum problem*

$$\inf_{\substack{\gamma \in \Gamma_{\leq q}, \\ \gamma = P_g^+ \gamma}} \int_{Q_l^*} \operatorname{Tr}_{L^2_\xi}((D_{g,\xi} - \epsilon_F)\gamma_\xi) d\xi,$$

admits a minimizer. Every minimizer γ_ has the structure $\gamma_* = \frac{l^3}{(2\pi)^3} \int_{Q_l^*}^\oplus \mathbb{1}_{[0,\nu)}(D_{g,\xi}) d\xi + \delta$, with some $0 \leq \delta \leq \frac{l^3}{(2\pi)^3} \int_{Q_l^*}^\oplus \mathbb{1}_{\{\nu\}}(D_{g,\xi}) d\xi$ for some $\nu \in (0, \epsilon_F]$ independent of $\xi \in Q_l^*$.*

Furthermore, for every ϵ_F , we have that $\nu \leq (1 - \kappa)^{-1}c^(q + 1)$, and $\gamma_* \in B$. If $\epsilon_F \leq \nu$, every $\gamma_* \in \Gamma_{\leq q}$ with the structure $\gamma_* = \frac{l^3}{(2\pi)^3} \int_{Q_l^*}^\oplus \mathbb{1}_{[0,\epsilon_F)}(D_{g,\xi}) d\xi + \delta$ and $0 \leq \delta \leq \frac{l^3}{(2\pi)^3} \int_{Q_l^*}^\oplus \mathbb{1}_{\{\epsilon_F\}}(D_{g,\xi}) d\xi$ is a minimizer. And if $\epsilon_F > (1 - \kappa)^{-1}c^*(q + 1)$, the set of solutions γ_* is independent of ϵ_F , and $\frac{l^3}{(2\pi)^3} \int_{Q_l^*} d\xi \operatorname{Tr}_{L^2_\xi} \gamma_{*,\xi} = q$.*

Proof. For any $\xi \in Q_l^*$ we can choose $\{\psi_k(\xi, \cdot)\}_k$ a basis of eigenfunctions of $D_{g,\xi}$, such that

$$D_{g,\xi} = \sum_{k \geq 1} \lambda_k(\xi) |\psi_k(\xi)\rangle \langle \psi_k(\xi)|.$$

We know from Lemma 5.1 that each positive $\lambda_k(\xi)$ is bounded independent of ξ . Let us introduce like in [20, 5] the function

$$C : s \mapsto \frac{l^3}{(2\pi)^3} \sum_{1 \leq k} |\{\xi \in Q_l^* : 0 \leq \lambda_k(\xi) \leq s\}|.$$

This function $C(s)$ is nondecreasing on \mathbb{R} , and by Lemma 5.1, $C(0) = 0, C(\infty) = \infty$. Thus we deduce that there exists a $\nu_1 \in [0, \infty)$ and a periodic operator δ_ξ such that

$$\lim_{s \rightarrow \nu_1^-} C(s) \leq q \leq \lim_{s \rightarrow \nu_1^+} C(s). \quad (5.4)$$

We will prove that every minimizer $\gamma_* \in \Gamma_{\leq q}$ has the structure

$$\gamma_* = \frac{l^3}{(2\pi)^3} \int_{Q_l^*}^{\oplus} \mathbb{1}_{[0, \nu)}(D_g) d\xi + \delta$$

with some $0 \leq \delta \leq \frac{l^3}{(2\pi)^3} \int_{Q_l^*}^{\oplus} \mathbb{1}_{\{\nu\}}(D_{g, \xi}) d\xi$ and $\nu := \min\{\nu_1, \epsilon_F\}$. However, we prove firstly $\nu \leq (1 - \kappa)^{-1} c^*(q + 1)$, and as a result $\gamma_* \in B$.

Now, we prove that $(1 - \kappa)c_*(q - 1) \leq \nu_1 \leq (1 - \kappa)^{-1} c^*(q + 1)$. If not, we assume that $\nu_1 > (1 - \kappa)^{-1} c^*(q + 1)$ first. Then by Lemma 5.1,

$$\lim_{s \rightarrow \nu_1^-} C(s) \geq C((1 - \kappa)^{-1} c^*(q + 1)) \geq q + 1,$$

contradicts with formula (5.4). Similarly, for $\nu_1 < (1 - \kappa)c_*(q - 1)$, we have that

$$\lim_{s \rightarrow \nu_1^+} C(s) \leq C((1 - \kappa)c_*(q - 1)) \leq q - 1.$$

Thus, $\nu \leq (1 - \kappa)^{-1} c^*(q + 1)$. And if $\epsilon_F \geq (1 - \kappa)^{-1} c^*(q + 1)$, then the minimizer is independent of ϵ_F .

We have that

$$0 \leq \gamma_{*, \xi} \leq \mathbb{1}_{[0, (1 - \kappa)^{-1} c^*(q + 1)]}(D_{g, \xi}).$$

And by Lemma 5.1 since $(1 - \kappa)^{-1} c^*(q + 1) < e$, we know that

$$\|\gamma_*\|_{\sigma_{1, \infty}} \leq q + M.$$

Thus, $\gamma_* \in B$.

Now, we return back to say that the minimizer in $\Gamma_{\leq q}$ has the structure $\gamma_* = \frac{l^3}{(2\pi)^3} \int_{Q_l^*}^{\oplus} \mathbb{1}_{[0, \nu)}(D_g) d\xi + \delta$. The proof is similar to [5].

We consider $\nu = \nu_1 < \epsilon_F$ firstly. Notice that

$$\int_{Q_l^*} \text{Tr}_{L_\xi^2}((D_{g, \xi} - \epsilon_F)\gamma_{*, \xi}) = \int_{Q_l^*} \text{Tr}_{L_\xi^2}((D_{g, \xi} - \nu)\mathbb{1}_{[0, \nu)}(D_{g, \xi})) + (\nu - \epsilon_F) \int_{Q_l^*} \text{Tr}_{L_\xi^2} \gamma_{*, \xi} d\xi.$$

which means if γ_* is the minimizer, then

$$\frac{l^3}{(2\pi)^3} \int_{Q_l^*} \text{Tr}_{L_\xi^2} \gamma_{*, \xi} d\xi = q.$$

For any $\gamma \in \Gamma_{\leq q}$, we write

$$\begin{aligned}
& \int_{Q_l^*} \mathrm{Tr}_{L_\xi^2}((D_{g,\xi} - \epsilon_F)(\gamma_\xi - \gamma_{*,\xi}))d\xi \\
&= \int_{Q_l^*} \mathrm{Tr}_{L_\xi^2}((D_{g,\xi} - \nu)(\gamma_\xi - \gamma_{*,\xi}))d\xi + \int_{Q_l^*} \mathrm{Tr}_{L_\xi^2}(\nu - \epsilon_F)(\gamma_\xi - \gamma_{*,\xi})d\xi \\
&= \int_{Q_l^*} \mathrm{Tr}_{L_\xi^2}((D_{g,\xi} - \nu)(\gamma_\xi - \gamma_{*,\xi}))d\xi + |\nu - \epsilon_F| \left| \int_{Q_l^*} \mathrm{Tr}_{L_\xi^2}(\gamma_\xi - \gamma_{*,\xi})d\xi \right| \\
&\geq \int_{Q_l^*} \mathrm{Tr}_{L_\xi^2}((D_{g,\xi} - \nu)(\gamma_\xi - \gamma_{*,\xi}))d\xi
\end{aligned}$$

Since $0 \leq \gamma_\xi \leq \mathbb{1}_{L_\xi^2}$, we have that $\langle \gamma_\xi \psi_k(\xi), \psi_k(\xi) \rangle \in [0, 1]$, for almost every $\xi \in Q_l^*$. Hence,

$$\begin{aligned}
& \int_{Q_l^*} \mathrm{Tr}_{L_\xi^2}((D_{g,\xi} - \nu)(\gamma_\xi - \gamma_{*,\xi}))d\xi \\
&= \int_{Q_l^*} \sum_{\lambda_k(\xi) < \nu} \mathrm{Tr}_{L_\xi^2}(|\lambda_k(\xi) - \nu| |\langle \gamma_\xi \psi_k(\xi), \psi_k(\xi) \rangle - 1|) d\xi \\
&\quad + \int_{Q_l^*} \sum_{\lambda_k(\xi) > \nu} \mathrm{Tr}_{L_\xi^2}(|\lambda_k(\xi) - \nu| \langle \gamma_\xi \psi_k(\xi), \psi_k(\xi) \rangle) d\xi
\end{aligned} \tag{5.5}$$

Obviously, if γ is the minimizer, then γ must have the structure $\gamma = \frac{l^3}{(2\pi)^3} \int_{Q_l^*}^{\oplus} \mathbb{1}_{[0,\nu]}(D_g)d\xi + \delta$.

For the case $\nu = \epsilon_F \leq \nu_1$, we prove firstly that every minimizer γ_* satisfies $\gamma_* = \frac{l^3}{(2\pi)^3} \int_{Q_l^*}^{\oplus} \mathbb{1}_{[0,\epsilon_F]}(D_{g,\xi})d\xi + \delta$, with some $0 \leq \delta \leq \frac{l^3}{(2\pi)^3} \int_{Q_l^*}^{\oplus} \mathbb{1}_{\{\epsilon_F\}}(D_{g,\xi})d\xi$. If not, it means that there is a minimizer $\gamma := \gamma_1 + \gamma_2 + \delta$ with $0 \leq \gamma_{1,\xi} \leq \mathbb{1}_{[0,\epsilon_F]}(D_{g,\xi})$, $0 \leq \gamma_{2,\xi} \leq \mathbb{1}_{(\epsilon_F,\infty)}(D_{g,\xi})$. And there is a nonempty set $U \subset Q_l^*$, such that if $\gamma_2 = 0$ then for $\xi \in U$, $\gamma_{1,\xi} < \mathbb{1}_{[0,\epsilon_F]}(D_{g,\xi})$. Using formula (5.5) again, we get

$$\int_{Q_l^*} \mathrm{Tr}_{L_\xi^2}((D_{g,\xi} - \epsilon_F)(\gamma_\xi - \gamma_{*,\xi}))d\xi > 0$$

contradicts the fact that γ is the minimizer.

And for every $\gamma \in \Gamma_{\leq q}$ with $\gamma = \frac{l^3}{(2\pi)^3} \int_{Q_l^*}^{\oplus} \mathbb{1}_{[0,\epsilon_F]}(D_{g,\xi})d\xi + \delta$, obviously we have that

$$\int_{Q_l^*} \mathrm{Tr}_{L_\xi^2}((D_{g,\xi} - \epsilon_F)(\gamma_\xi - \gamma_{*,\xi}))d\xi = 0.$$

Thus γ is equally a minimizer. □

5.4 Proof of Theorem 5.3

However, because of the complexity of the potential, we can not prove the Theorem 5.3 directly. Thus, we confine the existence into the ball $B_R := \{\gamma \in X \cap Y; \|\gamma\|_{\sigma_{1,\infty}} \leq R\}$ with R large enough which will be used in Lemma 5.14. And global existence of minimizers (Theorem 5.3) will be a consequence of the following result:

Theorem 5.5. *Under Assumption 5.2, for a constant M large enough and a constant $c^*(q) > 0$ only dependent on q , if $\epsilon_F > (1 - \kappa)^{-1}c^*(q + 1)$ and $R \geq R_0 := q + M$, there exists a minimizer $\gamma_* \in \Gamma_{\leq q}^+ \cap B_R$ such that*

$$\mathcal{E}^{DF}(\gamma_*) - \epsilon_F \text{Tr}_{L^2}(\gamma_*) = I_{\leq, R} := \min_{\gamma \in \Gamma_{\leq q}^+ \cap B_R} (\mathcal{E}^{DF}(\gamma) - \epsilon_F \text{Tr}_{L^2}(\gamma)). \quad (5.6)$$

Besides, γ_* solves the following nonlinear self-consistent equation:

$$\begin{cases} \gamma = \mathbb{1}_{[0, \nu]}(D\gamma) + \delta \\ D\gamma = \frac{l^3}{(2\pi)^3} \int_{Q_l^*}^{\oplus} d\xi D_{\gamma, \xi}, \end{cases} \quad (5.7)$$

where $0 \leq \delta \leq \mathbb{1}_{\{\nu\}}(D\gamma)$ and $0 \leq \nu \leq (1 - \kappa)^{-1}c^*(q + 1)$ independent of ϵ_F .

Furthermore, $\gamma_* \in B_{R_0}$, and $\frac{l^3}{(2\pi)^3} \int_{Q_l^*} d\xi \text{Tr}_{L_\xi^2} \gamma_{*, \xi} = q$. Thus $\nu \in \mathbb{R}$ is a Lagrange multiplier due to the charge constraint $\frac{l^3}{(2\pi)^3} \int_{Q_l^*} d\xi \text{Tr}_{L_\xi^2} \gamma_{*, \xi} = q$. And

$$\|\gamma_*\|_X \leq (1 - \kappa)^{-2}qc^*(q + 1). \quad (5.8)$$

The following theorem indeed explains the relationship between I_{\leq} and $I_{\leq, R}$, and this theorem will cover the proof of Theorem 5.3:

Theorem 5.6. *The minimum problem $I_{\leq, R}$ with $R \geq R_0$ is equivalent to the minimum problem I_{\leq} in the following sense:*

- $I_{\leq, R} = I_{\leq}$;
- Any minimizer of I_{\leq} minimizes $I_{\leq, R}$, and vice versa.

Proof. We split the proof into two steps:

Step 1. Any minimizer of $I_{\leq, R}$ minimizes I_{\leq} :

By Theorem 5.5, for any minimizer γ_* of $I_{\leq, R}$ such that

$$\mathcal{E}^{DF}(\gamma_*) - \epsilon_F \text{Tr}_{L^2}(\gamma_*) := I_{\leq, R},$$

we have that

$$I_{\leq, R} \leq I_{\leq, R_0}.$$

As $\gamma_* \in \Gamma_{\leq q}^+ \cap B_{R_0}$, we yield

$$I_{\leq, R_0} \leq \mathcal{E}^{DF}(\gamma_*) - \epsilon_F \text{Tr}_{L^2}(\gamma_*) = I_{\leq, R}.$$

Thus for any $R \geq R_0$,

$$I_{\leq, R} = I_{\leq, R_0}.$$

As $\cup_{R \geq R_0} (\Gamma_{\leq q}^+ \cap B_R) = \Gamma_{\leq q}^+$, we know that

$$I_{\leq} = \lim_{R \rightarrow \infty} I_{\leq, R} = I_{\leq, R_0}.$$

Obviously this γ_* minimizes I_{\leq} .

Step 2. Any minimizer of I_{\leq} minimizes $I_{\leq, R}$:

Now for Theorem 5.6, it remains to prove that any minimizer γ_* of I_{\leq} is in B_{R_0} . We have the following linearized problem for the minimizer:

Lemma 5.7. *Under the Assumption 5.2, and assume that $\gamma_* \in \Gamma_{\leq q}^+$ is a minimizer of problem 5.2, then*

$$\int_{Q_l^*} \text{Tr}_{L_\xi^2}((D_{\gamma_*, \xi} - \epsilon_F)\gamma_{*, \xi})d\xi = \inf_{\substack{\gamma \in \Gamma_{\leq q}, \\ \gamma = P_{\gamma_*}^+ \gamma}} \int_{Q_l^*} \text{Tr}_{L_\xi^2}((D_{\gamma_*, \xi} - \epsilon_F)\gamma_\xi)d\xi \quad (5.9)$$

Proof. Let $F(\gamma) = (\mathcal{E}^{DF} - \epsilon_F \text{Tr}_{L^2})(\gamma)$.

By Lemma 5.4, there exists an operator $\gamma'_n \in \Gamma_{\leq q}$, $\gamma' = P_{\gamma_*}^+ \gamma'$ such that

$$\int_{Q_l^*} \text{Tr}_{L_\xi^2}((D_{\gamma_*, \xi} - \epsilon_F)\gamma'_\xi)d\xi = \inf_{\substack{\gamma \in \Gamma_{\leq q}, \\ \gamma = P_{\gamma_*}^+ \gamma}} \int_{Q_l^*} \text{Tr}_{L_\xi^2}((D_{\gamma_*, \xi} - \epsilon_F)\gamma_\xi)d\xi$$

Now, from Proposition 4.10 and Lemma 5.4, we have a bound on $\|\gamma'\|_{X \cap Y}$. So there is $\sigma > 0$ such that for any $s \in [0, \sigma]$, $(1-s)\gamma_* + s\gamma' \in \Gamma_{\leq q} \cap B_{X \cap Y}(\gamma_*, \rho) \subset F$. Then from Theorem 4.7, $\omega(s) := \theta[(1-s)\gamma_* + s\gamma'_n] \in \Gamma_{\leq q}^+$ for $s \in [0, \sigma]$, we have

$$0 \leq F(\omega(s)) - F(\gamma_*) = sDF(\gamma_*)(\gamma' - \gamma_*) + o(s),$$

and

$$DF(\gamma_*)(\gamma' - \gamma_*) := \frac{d}{ds}F(\omega(s))|_{s=0} = \frac{l^3}{(2\pi)^3} \int_{Q_l^*} \text{Tr}_{L_\xi^2}((D_{\gamma_*, \xi} - \epsilon_F)(\gamma' - \gamma_*))d\xi,$$

since by formula (4.10)

$$\frac{d}{ds}\omega_\xi(s)|_{s=0} = D\theta_\xi(\gamma_*)(\gamma' - \gamma_*) = P_{\gamma_*, \xi}^+(\gamma'_\xi - \gamma_{*, \xi})P_{\gamma_*, \xi}^+ + b_{\gamma_*, \xi}(\gamma' - \gamma_*)^* + b_{\gamma_*, \xi}(\gamma' - \gamma_*)$$

with

$$P_{\gamma_*, \xi}^+(\gamma' - \gamma_*)P_{\gamma_*, \xi}^+ = \gamma' - \gamma_*,$$

and

$$\text{Tr}_{L_\xi^2}((D_{\gamma_*, \xi} - \epsilon_F)b_{\gamma_*, \xi}(\gamma' - \gamma_*)) = \text{Tr}_{L_\xi^2}((D_{\gamma_*, \xi} - \epsilon_F)b_{\gamma_*, \xi}(\gamma' - \gamma_*)^*) = 0.$$

Thus, we know that

$$0 \leq DF(\gamma_*) = \inf_{\substack{\gamma \in \Gamma_{\leq q}, \\ \gamma = P_{\gamma_*}^+ \gamma}} \int_{Q_l^*} \text{Tr}_{L_\xi^2}((D_{\gamma_*, \xi} - \epsilon_F)\gamma_\xi)d\xi - \int_{Q_l^*} \text{Tr}_{L_\xi^2}((D_{\gamma_*, \xi} - \epsilon_F)\gamma_{*, \xi})d\xi \leq 0.$$

Now, we know that

$$\int_{Q_l^*} \text{Tr}_{L_\xi^2}((D_{\gamma_*, \xi} - \epsilon_F)\gamma_{*, \xi})d\xi = \inf_{\substack{\gamma \in \Gamma_{\leq q}, \\ \gamma = P_{\gamma_*}^+ \gamma}} \int_{Q_l^*} \text{Tr}_{L_\xi^2}((D_{\gamma_*, \xi} - \epsilon_F)\gamma_\xi)d\xi.$$

□

We only need to prove that any minimizer of (5.2) minimizes the problem (5.6). By Lemma 5.7 and Lemma (5.4), we know that if γ_* minimizes I_{\leq} , then $\gamma_* \in B_{R_0}$. Thus,

$$I_{\leq, R_0} = I_{\leq}.$$

Now we know that γ_* minimizes the problem (5.6). This ends the proof. \square

5.5 proof of Theorem 5.5

It remains to prove Theorem 5.5.

Proof of Theorem 5.5. We split the proof into 6 steps.

Step 1. Regularity of the eigenfunctions.

We will need some regularities in $H_{\xi}^1(Q_l)$ for Lemma 5.18 for almost every $\xi \in Q_l^*$ to pass to the limit in the kinetic term:

Lemma 5.8. *Assume that $\kappa' = \alpha(C_G(z+q) + C'_W q^+) < 1$, and $\gamma \in \Gamma_{\leq q}$. Then under the Assumption 5.2, for every $\xi \in Q_l^*$ and for every eigenfunction $u_{\xi}(x)$ of the operator $D_{\gamma, \xi}$ with the corresponding eigenvalue $0 \leq \lambda(\xi) \leq e$, we have that $u_{k, \xi} \in H_{\xi}^1(Q_l)$, with the following estimates independent of ξ*

$$\| |D_{\xi}| u_{\xi} \|_{L^{\infty}(Q_l^*; L_{\xi}^2(Q_l))} \leq (1 - \kappa')^{-1} e.$$

Proof. By Lemma 2.9 and Lemma 2.11, we have that

$$\| D_{\gamma, \xi} u_{\xi} \|_{L_{\xi}^2} \geq (1 - C_G(z+q) - C'_W q^+) \| D_{\xi} u_{\xi} \|_{L^{\infty}(Q_l^*; L_{\xi}^2(Q_l))} = (1 - \kappa') \| D_{\xi} u_{\xi} \|_{L_{\xi}^2}.$$

As u_{ξ} is the eigenfunction corresponding to eigenvalue $0 \leq \lambda(\xi) \leq e$, we have that

$$\| D_{\gamma, \xi} u_{\xi} \|_{L^{\infty}(Q_l^*; L_{\xi}^2(Q_l))} = \| \lambda(\xi) u_{\xi} \|_{L_{\xi}^2} \leq e \| u_{\xi} \|_{L_{\xi}^2} = e.$$

Thus,

$$\| D_{\xi} u_{\xi} \|_{L^{\infty}(Q_l^*; L_{\xi}^2(Q_l))} \leq (1 - \kappa')^{-1} e$$

\square

Step 2. The corresponding linearized problem.

Lemma 5.9. *Under the Assumption 5.2, and assume that $\gamma_n \in \Gamma_{\leq q}^+ \cap B_R$ is a minimizing sequence of 5.6. Then*

$$\int_{Q_l^*} \text{Tr}_{L_{\xi}^2}((D_{\gamma_n, \xi} - \epsilon_F) \gamma_{n, \xi}) d\xi - \inf_{\substack{\gamma \in \Gamma_{\leq q}^+ \\ \gamma = P_{\gamma_n}^+ \gamma}} \int_{Q_l^*} \text{Tr}_{L_{\xi}^2}((D_{\gamma, \xi} - \epsilon_F) \gamma) d\xi \rightarrow 0 \quad (5.10)$$

Proof. Otherwise, there would be a ϵ_0 such that, after extraction,

$$\frac{l^3}{(2\pi)^2} \int_{Q_i^*} \text{Tr}_{L_\xi^2}((D_{\gamma_n, \xi} - \epsilon_F)\gamma_{n, \xi})d\xi \geq \inf_{\substack{\gamma \in \Gamma_{\leq q}, \\ \gamma = P_{\gamma_n}^+ \gamma}} \frac{l^3}{(2\pi)^2} \int_{Q_i^*} \text{Tr}_{L_\xi^2}((D_{\gamma_n, \xi} - \epsilon_F)\gamma_\xi)d\xi + \epsilon_0,$$

By Lemma 5.4, there exists an operator $\gamma'_n \in \Gamma_{\leq q}$ such that $\gamma'_n \in \Gamma_{\leq q} \cap B_{R_0}$ minimizes the following problem

$$\frac{l^3}{(2\pi)^2} \int_{Q_i^*} \text{Tr}_{L_\xi^2}((D_{\gamma_n, \xi} - \epsilon_F)\gamma'_{n, \xi})d\xi := \inf_{\substack{\gamma \in \Gamma_{\leq q}, \\ \gamma = P_{\gamma_n}^+ \gamma}} \frac{l^3}{(2\pi)^2} \int_{Q_i^*} \text{Tr}_{L_\xi^2}((D_{\gamma_n, \xi} - \epsilon_F)\gamma_\xi)d\xi.$$

Now, from Proposition 4.10 and Lemma 5.4, we have a bound on $\|\gamma'_n\|_{X \cap Y}$ and $\gamma'_n \in B_R$. So there is $\sigma > 0$ such that for any n large enough and any $s \in [0, \sigma]$, $(1-s)\gamma_n + s\gamma'_n \in \Gamma_{\leq q} \cap B_X \cap Y(\gamma_n, \rho) \cap B_R \subset F \cap B_R$. Then from Theorem 4.7, the function $f_n : s \in [0, \sigma] \rightarrow (\mathcal{E}_{DF} - \epsilon_F \text{Tr}_{L^2})(\theta[(1-s)\gamma_n + s\gamma'_n])$ is of class C^1 and the sequence of derivatives (f'_n) is equicontinuous on $[0, \delta]$. By Formula (4.11),

$$f'_n(0) = \frac{l^3}{(2\pi)^2} \int_{Q_i^*} \text{Tr}_{L_\xi^2}((D_{\gamma_n, \xi} - \epsilon_F)(\gamma'_{n, \xi} - \gamma_{n, \xi})) \leq -\epsilon_0.$$

So there is $0 < s_0 < \sigma$ independent of n , such that $\forall s \in [0, s_0]$, $f'(s) \leq -\frac{\epsilon}{2}$. Hence,

$$\begin{aligned} (\mathcal{E}^{DF} - \epsilon_F \text{Tr}_{L^2})(\theta[(1-s_0)\gamma_n + s_0\gamma'_n]) &\leq f_n(0) - \frac{\epsilon_0 s_0}{2} \\ &= (\mathcal{E}^{DF} - \epsilon_F \text{Tr}_{L^2})(\gamma_n) - \frac{\epsilon_0 s_0}{2}. \end{aligned}$$

But $\theta[(1-s)\gamma_n + s\gamma'_n] \in \Gamma_{\leq q}^+ \cap B_R$ and $(\mathcal{E}^{DF} - \epsilon_F \text{Tr}_{L^2})(\gamma_n) \rightarrow \min_{\gamma \in \Gamma_{\leq q}^+ \cap B_R} (\mathcal{E}^{DF} - \epsilon_F \text{Tr}_{L^2})(\gamma)$. This is a contradiction. And we get the conclusion. \square

Step 3. The decomposition of minimizing sequence.

Lemma 5.10. *Under the Assumption 5.2 and the statement of Lemma 5.9, there is a minimizing sequence $\gamma_n \in \Gamma_{\leq q}^+ \cap B_R$ of (5.6). Then, for each n define $p_n := \frac{l^3}{(2\pi)^3} \int_{Q_i^*}^\oplus p_{n, \xi} d\xi$ with $p_{n, \xi} = \mathbb{1}_{[0, e]}(D_{\gamma_n, \xi})$ with e defined in Lemma 5.1. Then if $\epsilon_F > (1 - \kappa)^{-1}c^*(q + 1)$:*

$$\frac{l^3}{(2\pi)^3} \int_{Q_i^*} \text{Tr}_{L_\xi^2} \gamma_{n, \xi} d\xi \rightarrow q \quad \text{and} \quad \|\gamma_n - p_n \gamma_n p_n\|_X \rightarrow 0.$$

Proof. By Lemma 5.4, for some $\nu_n \in [0, (1-\kappa)^{-1}c^*(q+1)]$, then $\frac{l^3}{(2\pi)^3} \int_{Q_i^*}^\oplus d\xi \mathbb{1}_{[0, \nu_n]}(D_{\gamma_n, \xi})d\xi + \delta$ with $0 \leq \delta \leq \frac{l^3}{(2\pi)^3} \int_{Q_i^*}^\oplus \mathbb{1}_{\nu_n}(D_{\gamma_n, \xi})d\xi$ is the minimizer of the problem

$$\inf_{\substack{\gamma \in \Gamma_{\leq q}, \\ \gamma = P_{\gamma_n}^+ \gamma}} \frac{l^3}{(2\pi)^3} \int_{Q_i^*} \text{Tr}_{L_\xi^2}((D_{\gamma_n, \xi} - \epsilon_F)\gamma_\xi)d\xi = \frac{l^3}{(2\pi)^3} \int_{Q_i^*} d\xi \text{Tr}_{L_\xi^2}(D_{\gamma_n, \xi} \mathbb{1}_{\nu_n}(D_{\gamma_n, \xi})) + (\nu_n - \epsilon_F)q.$$

We denote $\pi_n := \frac{l^3}{(2\pi)^3} \int_{Q_l^*}^{\oplus} d\xi \mathbb{1}_{(e,\infty)}(D_{\gamma_n,\xi})$, $\pi'_n := \frac{l^3}{(2\pi)^3} \int_{Q_l^*}^{\oplus} d\xi \mathbb{1}_{(\nu_n,e]}(D_{\gamma_n,\xi})$, and $\pi''_n := \frac{l^3}{(2\pi)^3} \int_{Q_l^*}^{\oplus} d\xi \mathbb{1}_{[0,\nu_n)}(D_{\gamma_n,\xi})$. Then we may write

$$\begin{aligned} & \frac{l^3}{(2\pi)^3} \int_{Q_l^*} d\xi \operatorname{Tr}_{L_\xi^2}((D_{\gamma_n,\xi} - \epsilon_F)\gamma_{n,\xi}) - \inf_{\substack{\gamma \in \Gamma \leq q, \\ \gamma = P_{\gamma_n}^+ \gamma}} \frac{l^3}{(2\pi)^3} \int_{Q_l^*} \operatorname{Tr}_{L_\xi^2}((D_{\gamma_n,\xi} - \epsilon_F)\gamma_\xi) d\xi \\ &= \frac{l^3}{(2\pi)^3} \int_{Q_l^*} d\xi \operatorname{Tr}_{L_\xi^2}((D_{\gamma_n,\xi} - \nu_n)\pi_{n,\xi}\gamma_{n,\xi}\pi_{n,\xi}) + \frac{l^3}{(2\pi)^3} \int_{Q_l^*} d\xi \operatorname{Tr}_{L_\xi^2}((D_{\gamma_n,\xi} - \nu_n)\pi'_{n,\xi}\gamma_{n,\xi}\pi'_{n,\xi}) \\ & \quad + \frac{l^3}{(2\pi)^3} \int_{Q_l^*} d\xi \operatorname{Tr}_{L_\xi^2}((D_{\gamma_n,\xi} - \nu_n)(\pi''_{n,\xi}\gamma_{n,\xi}\pi''_{n,\xi} - \mathbb{1}_{[0,\nu_n]}(D_{\gamma_n,\xi}))) \\ & \quad + (\epsilon_F - \nu_n) \left(q - \frac{l^3}{(2\pi)^3} \int_{Q_l^*} d\xi \operatorname{Tr}_{L_\xi^2}(\gamma_{n,\xi}) \right). \end{aligned}$$

But the four terms in the right hand of the above equation are non-negative.

So Lemma 5.9 implies that $\frac{l^3}{(2\pi)^3} \int_{Q_l^*} d\xi \operatorname{Tr}_{L_\xi^2} \gamma_{n,\xi} \rightarrow q$ and $\frac{l^3}{(2\pi)^3} \int_{Q_l^*} d\xi \operatorname{Tr}_{L_\xi^2}((D_{\gamma_n,\xi} - \nu_n)\pi_{n,\xi}\gamma_{n,\xi}\pi_{n,\xi}) \rightarrow 0$.

But $\pi_{n,\xi}(D_{\gamma_n,\xi} - \nu_n)\pi_{n,\xi} \geq (c^*(q+2) - c^*(q+1))(1-\kappa)^{-1}\pi_{n,\xi}$ and $\pi_{n,\xi}(D_{\gamma_n,\xi} - \nu_n)\pi_{n,\xi} \geq \pi_{n,\xi}(|D_{\gamma_n,\xi}| - (1-\kappa)^{-1}c^*(q+1))\pi_{n,\xi}$, so that, taking a convex combination of these two estimates:

$$\frac{c^*(q+2)}{c^*(q+2) - c^*(q+1)} \pi_{n,\xi}(D_{\gamma_n,\xi} - \nu_n)\pi_{n,\xi} \geq \pi_{n,\xi}|D_{\gamma_n,\xi}|\pi_{n,\xi}.$$

Hence

$$\begin{aligned} \|\pi_n \gamma_n \pi_n\|_X &= \frac{l^3}{(2\pi)^3} \int_{Q_l^*} d\xi \operatorname{Tr}_{L_\xi^2}(\pi_{n,\xi}|D_\xi|\pi_{n,\xi}\gamma_{n,\xi}) \\ &\leq (1-\kappa)^{-1} \frac{l^3}{(2\pi)^3} \int_{Q_l^*} d\xi (\pi_{n,\xi}|D_{\gamma_n,\xi}|\pi_{n,\xi}\gamma_{n,\xi}) \operatorname{Tr}_{L_\xi^2} \rightarrow 0. \end{aligned}$$

It remains to study the limit of $u_n := \pi_n \gamma_n p_n$ as n goes to infinity. Since $(\gamma_n)^2 \leq \gamma_n$, we have

$$(\pi_n \gamma_n \pi_n)^2 + u_n u_n^* = \pi_n (\gamma_n)^2 \pi_n \leq \pi_n \gamma_n \pi_n.$$

Hence

$$\frac{l^3}{(2\pi)^3} \int_{Q_l^*} d\xi \operatorname{Tr}_{L_\xi^2}(|D_{\gamma_n,\xi}|^{1/2} u_{n,\xi} u_{n,\xi}^* |D_{\gamma_n,\xi}|^{1/2}) \rightarrow 0.$$

Now, take any operator A , such that $\|A\|_Y < \infty$. By the Cauchy-Schwartz inequality,

$$\begin{aligned} & \frac{l^3}{(2\pi)^3} \int_{Q_l^*} d\xi \operatorname{Tr}_{L_\xi^2}(A_\xi |D_{\gamma_n,\xi}|^{1/2} u_{n,\xi}^* |D_{\gamma_n,\xi}|^{1/2}) \\ & \leq \frac{l^3}{(2\pi)^3} \left\| \operatorname{Tr}_{L_\xi^2}(|D_{\gamma_n,\xi}|^{1/2} p_{n,\xi} A_\xi^* A_\xi p_{n,\xi} |D_{\gamma_n,\xi}|^{1/2}) \right\|_{L^\infty}^{1/2} \\ & \quad \times \left(\int_{Q_l^*} d\xi \operatorname{Tr}_{L_\xi^2}(|D_{\gamma_n,\xi}|^{1/2} u_{n,\xi} u_{n,\xi}^* |D_{\gamma_n,\xi}|^{1/2}) \right)^{1/2} \end{aligned}$$

But by Lemma 5.1, there is a $M > 0$, such that $p_{n,\xi}$ has at most $q + M$ eigenfunctions, which means that $p_{n,\xi}$ has rank at most $q + M$ and $\|p_n |D_{\gamma_n}|^{1/2}\|_Y \leq e^{1/2}$. As a consequence,

$$\|\mathrm{Tr}_{L_\xi^2}(|D_{\gamma_n,\xi}|^{1/2} p_{n,\xi} A_\xi^* A_\xi p_{n,\xi} |D_{\gamma_n,\xi}|^{1/2})\|_{L^\infty} \leq (q + M)e \|A\|_Y^2.$$

So we have

$$\left\| |D_{\gamma_n}|^{1/2} u_n |D_{\gamma_n}|^{1/2} \right\|_{\sigma_{1,1}} \rightarrow 0.$$

Hence, $\|u_n\|_X \rightarrow 0$.

$$\text{Finally, } \|\gamma_n - p_n \gamma_n p_n\|_X \leq \|\pi_n \gamma_n \pi_n\|_X + 2\|u_n\|_X \rightarrow 0.$$

□

Now, we have that $\|\gamma_n - p_n \gamma_n p_n\|_X \rightarrow 0$. Thus, we only need to study the convergence of $p_n \gamma_n p_n$. Before it, we give some statements of regularity about $p_n \gamma_n p_n$.

From now on, let

$$h_n := p_n \gamma_n p_n.$$

Lemma 5.11. *Assume that $\kappa' = \alpha(C_G(z + q) + C'_W q^+) < 1$, then*

$$h_n \in X_\infty^2.$$

Let $h_{n,\xi}(x, y)$ be the kernel of $h_{n,\xi}$, then we have that $h_{n,\xi} \in L^\infty(Q_l^*; H_\xi^1(Q_l^2))$.

Proof. We prove that $\|p_{n,\xi}\|_{X_\infty^2}$ is bounded first of all. Let $(u_{n,k,\xi})_{k \geq 1}$ be the eigenfunctions for the operator $D_{\gamma_n,\xi}$ with the corresponding eigenvalues $\lambda_{n,k}(\xi)$. We know that

$$p_{n,\xi} = \sum_{1 \leq k} \delta_{n,k}(\xi) |u_{n,k,\xi}\rangle \langle u_{n,k,\xi}|$$

with $\delta_{n,k} = 1$ if $0 \leq \lambda_{n,k}(\xi) \leq e$ and if not $\delta_{n,k} = 0$.

By Lemma 5.1, we know $|\{k; \delta_{n,k}(\xi) = 1\}| \leq q + M$. And by Lemma 5.8, for any eigenfunction $u_{n,k,\xi}$, we have that $\|\delta_{n,k}(\xi) u_{n,k,\xi}\|_{L^\infty(H_\xi^1)} \leq (1 - \kappa')^{-1} e$. Now,

$$\|p_{n,\xi}\|_{X^2(\xi)} = \sum_k \delta_{n,k}(\xi) \|u_{n,k,\xi}\|_{H_\xi^1}^2 \leq (q + M) \sup_k \|\delta_{n,k}(\xi) u_{n,k,\xi}\|_{H_\xi^1}^2,$$

hence

$$\|p_n\|_{X_\infty^2} \leq (q + M)(1 - \kappa')^{-2} e^2.$$

For h_n , notice that $p_{n,\xi} = p_{n,\xi}^2$ and $h_{n,\xi} = p_{n,\xi} h_{n,\xi} p_{n,\xi}$, thus we have

$$\begin{aligned} \|h_{n,\xi}\|_{X_\infty^2} &= \| |D_\xi| h_{n,\xi} |D_\xi| \|_{\sigma_{1,\infty}} \\ &= \| |D_\xi| p_{n,\xi} h_{n,\xi} p_{n,\xi} |D_\xi| \|_{\sigma_{1,\infty}} \\ &\leq \|h_{n,\xi}\|_Y \| |D_\xi| p_{n,\xi} \|_{\sigma_{2,\infty}}^2 \\ &\leq \|p_n\|_{X_\infty^2} \\ &\leq (q + M)(1 - \kappa')^{-2} e^2. \end{aligned}$$

For the kernel,

$$\| |D_{\xi,x}| h_{n,\xi}(x,y) \|_{L^2_\xi(Q_l^2)} = \| |D_\xi| h_{n,\xi} \|_{\sigma_2(\xi)} \leq \| h_{n,\xi} \|_{X^2(\xi)} \leq (q+M)(1-\kappa')^{-2} e^2,$$

and same for $|D_{\xi,y}| h_{n,\xi}(x,y)$. Thus, $h_{n,\xi}(x,y) \in L^\infty(Q_l^*; H_\xi^1(Q_l^2))$, and

$$\| h_{n,\xi} \|_{L^\infty(Q_l^*; H_\xi^1(Q_l^2))} \leq 2(q+M)(1-\kappa')^{-2} e^2.$$

□

Step 4. The convergent subsequences.

After extraction, by Lemma 5.11 there is a γ_* , such that

$$h_n \xrightarrow{*} \gamma_* \quad \text{in} \quad X_\infty^2 \cap Y. \quad (5.11)$$

since $\sigma_{1,\infty}$ is the dual space of $L^1(Q_l^*; \mathcal{K}_\xi(Q_l))$ with \mathcal{K}_ξ the functional space of compact operators on $L^2_\xi(Q_l)$, and Y is the dual space of $\sigma_{1,1}$.

Now, we prove that there are some strong convergences for h_n .

Lemma 5.12. *Defining that $\mathcal{S}_\xi(\gamma_\xi)(x,y) = \frac{l^3}{(2\pi)^3} \int_{Q_l^*} \gamma_\xi(x,y) d\xi$, then we have the following estimates:*

- $\rho_{h_n}^{1/2}$ is uniformly bounded in $H^1(Q_l)$.
- For $0 \leq s \leq 1$, if $f(\xi, x, y) \in W^{\alpha,1}(Q_l^*; H^{s+t}(Q_l^2))$ with $t > 3$, then $\mathcal{S}_{\xi'}(f(\xi - \xi')h_{n,\xi'})(x,y)$ is uniformly bounded in $W^{\alpha,\infty}(Q_l^*; H_\xi^s(Q_l^2))$.
- If $f(\xi, x, y) \in W^{1,1}(Q_l^*; L^\infty(Q_l^2))$, then $\mathcal{S}_{\xi'}(f(\xi - \xi')h_{n,\xi'})(x,y)$ is uniformly bounded in $W^{1,\infty}(Q_l^*; L_\xi^2(Q_l^2))$.

Consequently, after extraction,

•

$$\rho_{h_n}^{1/2}(x) \rightarrow \rho_{\gamma_*}^{1/2}(x) \quad \text{in} \quad H^{1/2}(Q_l),$$

- for any $\epsilon > 0$ and $\alpha > 0$,

$$\mathcal{S}_{\xi'}(f(\xi - \xi')h_{n,\xi'})(x,y) \rightarrow \mathcal{S}_{\xi'}(f(\xi - \xi')\gamma_{*,\xi'})(x,y) \quad \text{in} \quad L^\infty(Q_l^*; H_\xi^{s-\epsilon}(Q_l^2)).$$

•

$$\begin{aligned} & |D_{\xi,x}|^{-1/2} |D_{\xi,y}|^{-1/2} \mathcal{S}_{\xi'}(f(\xi - \xi')h_{n,\xi'})(x,y) \\ & \rightarrow |D_{\xi,x}|^{-1/2} |D_{\xi,y}|^{-1/2} \mathcal{S}_{\xi'}(f(\xi - \xi')\gamma_{*,\xi'})(x,y) \quad \text{in} \quad L^\infty(Q_l^*; L_\xi^2(Q_l^2)). \end{aligned}$$

Proof. The first estimate has been studied in [7, p. 730]. Combining with Lemma 5.11 we just use their estimate:

$$\int_Q |\nabla \sqrt{\rho_{h_n}}(x, x)|^2 dx \leq \frac{l^3}{(2\pi)^3} \int_{Q_l^*} \text{Tr}_{L_\xi^2}[-\Delta_\xi h_{n,\xi}] d\xi \leq (q + M)(1 - \kappa')^{-2} e^2.$$

The second estimate is based on Lemma B.1 and Lemma 5.11:

$$\begin{aligned} \|\nabla_\xi |^\beta f(\xi - \xi', x, y) h_{n,\xi'}(x, y)\|_{H_\xi^s} &\leq C \|\nabla_\xi |^\beta f(\xi - \xi')\|_{H_{\xi-\xi'}^s} \|h_{n,\xi'}\|_{H_{\xi'}^s} \\ &\leq 2C(q + M)(1 - \kappa')^{-2} e^2 \|\nabla_\xi |^\beta f(\xi - \xi')\|_{H_{\xi-\xi'}^{s+t}} \end{aligned}$$

Then

$$\begin{aligned} &\|\nabla_\xi |^\beta \mathcal{S}_{\xi'}(f(\xi - \xi', x, y) h_{n,\xi'})(x, y)\|_{H_\xi^s} \\ &\leq \frac{l^3}{(2\pi)^3} \int_{Q_l^*} \|\nabla_\xi |^\beta f(\xi - \cdot, x, y) h_{n,\xi'}(x, y)\|_{H_\xi^s} d\xi' \\ &\leq \frac{2l^3 C}{(2\pi)^3} (q + M)(1 - \kappa')^{-2} e^2 \|\nabla_\xi |^\beta f(\xi)\|_{L^1(Q_l^*; H_\xi^{s+t}(Q_l^2))} \end{aligned}$$

Let $\beta = 0, \alpha$. Hence, we have that

$$\|\mathcal{S}_\xi(f(\xi - \xi') h_{n,\xi'})(x, y)\|_{W^{\alpha,\infty}(Q_l^*; H_\xi^s(Q_l^2))} \leq \frac{2l^3 C}{(2\pi)^3} (q + M)(1 - \kappa')^{-2} e^2 \|f\|_{W^{\alpha,1}(Q_l^*; H_\xi^{s+t}(Q_l^2))}.$$

Similarly, for the last estimate

$$\|\mathcal{S}_\xi(f(\xi - \xi') h_{n,\xi'})(x, y)\|_{W^{1,\infty}(Q_l^*; L_\xi^2(Q_l))} \leq \frac{2l^3}{(2\pi)^3} (q + M)(1 - \kappa')^{-2} e^2 \|f\|_{W^{1,1}(Q_l^*; L_\xi^\infty(Q_l^2))}.$$

For every estimate, we have a weak(-star) convergence subsequence. And by Rellich–Kondrachov Theorem, we get the strong convergence.

Now, we say that the limits are $\rho_{\gamma_*}^{1/2}$ and $\mathcal{S}_{\xi'}(f(\xi - \xi') \gamma_{*,\xi'})(x, y)$ respectively. For the first term, the proof is same with [7, p. 734]. Hence, we only deal with the last two convergences. Obviously, we also have that

$$h_n \xrightarrow{*} h_* \quad \text{in } \sigma_{2,\infty}.$$

And we only need prove that $\mathcal{S}_{\xi'}(f(\xi - \xi') h_{n,\xi}) \xrightarrow{*} \mathcal{S}_{\xi'}(f(\xi - \xi') h_{*,\xi})$ in $L^\infty(Q_l^*; L_\xi^2(Q_l^2))$. For any operator $g \in \sigma_{2,1}$ with the kernel $g_\xi(x, y) \in L^1(Q_l^*; L_\xi^2(Q_l^2))$, we have that

$$\begin{aligned} &\frac{l^3}{(2\pi)^3} \int_{Q_l^*} \int_{Q_l^2} \mathcal{S}_{\xi'}(f(\xi - \xi') h_{n,\xi}) g_\xi dx dy d\xi \\ &= \frac{l^3}{(2\pi)^3} \int_{Q_l^*} \int_{Q_l^2} h_{n,\xi'} \mathcal{S}_\xi(f(\xi - \xi') g_\xi) dx dy d\xi' \\ &= \frac{l^3}{(2\pi)^3} \int_{Q_l^*} \text{Tr}_{L_\xi^2}(h_{n,\xi'} \mathcal{S}_\xi(f(\xi - \xi') g_\xi)) d\xi' \\ &\rightarrow \frac{l^3}{(2\pi)^3} \int_{Q_l^*} \text{Tr}_{L_\xi^2}(h_{*,\xi'} \mathcal{S}_\xi(f(\xi - \xi') g_\xi)) d\xi' \\ &= \frac{l^3}{(2\pi)^3} \int_{Q_l^*} \int_{Q_l^2} \mathcal{S}_{\xi'}(f(\xi - \xi') \gamma_{*,\xi'}) g_\xi dx dy d\xi \end{aligned}$$

since by Young's convolution inequality

$$\begin{aligned}\|\mathcal{S}_\xi(f(\xi - \xi')g_\xi)\|_{\sigma_{2,1}} &= \|\mathcal{S}_\xi(f(\xi - \xi')g_\xi)(x, y)\|_{L^1(Q_l^*; L_{\xi'}^2(Q_l^2))} \\ &\leq \frac{l^3}{(2\pi)^3} \|f(\xi, x, y)\|_{L^1(Q_l^*; L_\xi^\infty(Q_l^2))} \|g_{\xi'}(x, y)\|_{L^1(Q_l^*; L_{\xi'}^2(Q_l^2))} \\ &< C \|g\|_{\sigma_{2,1}}.\end{aligned}$$

□

Step 5. Passing to the limit in the energy and in the constraints.

Lemma 5.13. *As n goes to infinity, then*

$$\| |D_0|^{-1/2} G_l * (\rho_{\gamma_n} - \rho_{\gamma_*}) |D_0|^{-1/2} \|_Y \rightarrow 0.$$

Proof. For the first one, notice that

$$\|G_l * (\rho_{\gamma_n} - \rho_{\gamma_*})\|_Y \leq \|G_l * (\rho_{\gamma_n} - \rho_{h_n})\|_Y + \|G_l * (\rho_{h_n} - \rho_{\gamma_*})\|_Y.$$

By inequality (3.5), we get that

$$\|G_l * (\rho_{\gamma_n} - \rho_{h_n})\|_Y \leq C'_H \|\gamma_n - h_n\|_X \rightarrow 0.$$

For the other term,

$$G_l * (\rho_{h_n} - \rho_{\gamma_*}) = G_l * \left(\rho_{h_n}^{1/2} (\rho_{h_n}^{1/2} - \rho_{\gamma_*}^{1/2}) + (\rho_{h_n}^{1/2} - \rho_{\gamma_*}^{1/2})^{1/2} \rho_{\gamma_*}^{1/2} \right).$$

By Hölder's inequality and Lemma 5.12, we have

$$\begin{aligned}& \| |D_\xi|^{-1/2} G_l * (\rho_{h_n}^{1/2} (\rho_{h_n}^{1/2} - \rho_{\gamma_*}^{1/2})) |D_\xi|^{-1/2} u_\xi \|_{L_\xi^2} \\ & \leq \int_{Q_l} |\rho_{h_n}^{1/2} (\rho_{h_n}^{1/2} - \rho_{\gamma_*}^{1/2})| dy \left(\sup_{y \in Q_l} \| |D_\xi|^{-1/2} G_l(\cdot - y) |D_\xi|^{-1/2} u_\xi \|_{L_\xi^2} \right) \\ & \leq \| |D_\xi|^{-1/2} |G_l|^{1/2} \|_{Y^2} \| \rho_{h_n} \|_{L^1}^{1/2} \| \rho_{h_n}^{1/2} - \rho_{\gamma_*}^{1/2} \|_{L^2} \| u_\xi \|_{L_\xi^2} \\ & \leq G_{H'}^2 \| \rho_{h_n} \|_{L^1}^{1/2} \| \rho_{h_n}^{1/2} - \rho_{\gamma_*}^{1/2} \|_{L^2} \| u_\xi \|_{L_\xi^2} \\ & \rightarrow 0.\end{aligned}$$

Finally,

$$\| |D_\xi|^{-1/2} G_l * (\rho_{h_n} - \rho_{\gamma_*}) |D_\xi|^{-1/2} \|_Y \rightarrow 0.$$

Now, we get the conclusion. □

Lemma 5.14. *As n goes to infinity, then*

$$\| |D_0|^{-1/2} (W_{\gamma_n, \xi} - W_{\gamma_*, \xi}) |D_0|^{-1/2} \|_Y \rightarrow 0.$$

Proof. Similar to Lemma 5.13, we divided it into two part:

$$\begin{aligned} & \| |D_0|^{-1/2}(W_{\gamma_n} - W_{\gamma_*}) |D_0|^{-1/2} \|_Y \\ & \leq \|W_{\gamma_n} - W_{h_n}\|_Y + \| |D_0|^{-1/2}(W_{h_n} - W_{\gamma_*}) |D_0|^{-1/2} \|_Y. \end{aligned}$$

By inequality 3.8, we know that

$$\|W_{\gamma_n} - W_{h_n}\|_Y \leq C_W'' \|\gamma_n - h_n\|_{X \cap \sigma_{1,4}}.$$

As $\gamma_n \in B_R$, then $\|h_n\|_{\sigma_{1,\infty}} \leq \|\gamma_n\|_{\sigma_{1,\infty}} \leq R$. Now

$$\|\gamma_n - h_n\|_{\sigma_{1,4}}^4 \leq (\|\gamma_n\|_{\sigma_{1,\infty}} + \|h_n\|_{\sigma_{1,\infty}})^3 \|\gamma_n - h_n\|_X \leq 8R^3 \|\gamma_n - h_n\|_X.$$

Thus,

$$\|W_{\gamma_n, \xi} - W_{h_n, \xi}\|_Y \rightarrow 0,$$

independent of $\xi \in Q_l^*$.

For the other term, we split it into three part. For convenience, let $f_n(\xi, x, y) := \mathcal{S}_{\xi'}(f(\xi - \xi')h_{n, \xi'})(x, y)$ and $f_*(\xi, x, y) := \mathcal{S}_{\xi'}(f(\xi - \xi')\gamma_{*, \xi'})(x, y)$.

For the term with all singularity in z , let $f(\xi, x, y) = e^{-i\xi(x-y)}$. Obviously, $f \in W^{1,1}(Q_l^*; H^5(Q_l^2))$, thus by Lemma 5.12, $f_n \rightarrow f_*$ in $L^\infty(Q_l^*; H_\xi^{1/2}(Q_l^2))$. Then by integration by parts

$$\begin{aligned} & \left\| |D_{\xi, x}|^{-1/2} \int_{Q_l^*} d\xi' \int_{Q_l} e^{-i(\xi - \xi')(x-y)} G(x-y)(h_{n, \xi'} - \gamma_{*, \xi'})(x, y) [|D_{\xi, y}|^{-1/2} \psi_\xi(y)] dy \right\|_{L_\xi^2(Q_l)} \\ & = \left\| \int_{Q_l} \left[|D_{\xi, x}|^{-1/2} |D_{\xi, y}|^{-1/2} (G_l(x-y)(f_n - f_*)(\xi, x, y)) \right] \psi_\xi(y) dy \right\|_{L_\xi^2(Q_l)} \\ & \leq \int_{Q_l} \| |D_{\xi, x}|^{-1/2} |D_{\xi, y}|^{-1/2} G_l(\cdot - y)(f_n - f_*)(\xi, \cdot, y) \|_{L_\xi^2(Q_l)} |\psi_\xi(y)| dy \\ & \leq \| |D_{\xi, x}|^{-1/2} |D_{\xi, y}|^{-1/2} G_l(x-y)(f_n - f_*) \|_{L^\infty(L_\xi^2(Q_l^2))} \|\psi_\xi\|_{L_\xi^2(Q_l)} \\ & \leq \| |D_{\xi, x}|^{-1/2} |D_{\xi, y}|^{-1/2} G_l(x-y) \|_Y \| (f_n - f_*) \|_{L^\infty(L_\xi^2(Q_l^2))} \|\psi_\xi\|_{L_\xi^2(Q_l)} \\ & \leq 1/2 (\| |D_{\xi, x}|^{-1} G_l(x-y) \|_Y + \| |D_{\xi, y}|^{-1} G_l(x-y) \|_Y) \|f_n - f_*\|_{L^\infty(L_\xi^2(Q_l^2))} \|\psi_\xi\|_{L_\xi^2(Q_l)} \\ & \leq C_G \|f_n - f_*\|_{L^\infty(L_\xi^2(Q_l^2))} \|\psi_\xi\|_{L_\xi^2(Q_l)} \\ & \rightarrow 0. \end{aligned}$$

For the second term, let

$$f(\xi, x, y) = \sum_{|m|_\infty \leq 1} \frac{e^{i(\xi + 2\pi m/l)(x-y)}}{|\xi - 2\pi m/l|^2}.$$

For $\alpha < 1$, $f(\xi, x, y) \in W^{\alpha,1}(Q_l^*; H^5(Q_l^2))$, we know that $f_n \rightarrow f_*$ in $L^\infty(Q_l^*; L_\xi^2(Q_l^2))$.

Thus, similarly, we have that

$$\begin{aligned}
& \left\| \int_{Q_l} (f_n - f_*)(\xi, x, y) \psi_\xi(y) dy \right\|_{L_\xi^2(Q_l)} \\
& \leq \int_{Q_l} \|(f_n - f_*)(\xi, \cdot, y)\|_{L_\xi^2(Q_l)} |\psi_\xi(y)| dy \\
& \leq \|f_n - f_*\|_{L^\infty(Q_l^*; L_\xi^2(Q_l^2))} \|\psi_\xi\|_{L_\xi^2(Q_l)} \\
& \rightarrow 0.
\end{aligned}$$

And for the last term, taking $f(\xi, x, y) = g_l(\xi, x - y) \in W^{1, \infty}(Q_l^*; L_\xi^\infty(Q_l^2))$, since by equation (2.16), $g_l(\xi, x) \in W^{1, \infty}(Q_l^*; L_\xi^\infty(Q_l))$. Thus, $|D_{\xi, x}|^{-1/2} |D_{\xi, y}|^{-1/2} f_n \rightarrow |D_{\xi, x}|^{-1/2} |D_{\xi, y}|^{-1/2} f_*$ in $L^\infty(Q_l^*; L_\xi^2(Q_l^2))$. Then, by integration by parts

$$\begin{aligned}
& \left\| |D_{\xi, x}|^{-1/2} \int_{Q_l} (f_n - f_*)(\xi, x, y) [|D_{\xi, y}|^{-1/2} \psi_\xi(y)] dy \right\|_{L_\xi^2} \\
& = \left\| \int_{Q_l} [|D_{\xi, x}|^{-1/2} |D_{\xi, y}|^{-1/2} (f_n - f_*)](\xi, x, y) \psi_\xi(y) dy \right\|_{L_\xi^2} \\
& \leq \| |D_{\xi, x}|^{-1/2} |D_{\xi, y}|^{-1/2} (f_n - f_*) \|_{L^\infty(Q_l^*; L_\xi^2(Q_l^2))} \|\psi_\xi\|_{L_\xi^2} \rightarrow 0.
\end{aligned}$$

Consequently,

$$\| |D_\xi|^{-1/2} (W_{h_n, \xi} - W_{\gamma_*, \xi}) |D_\xi|^{-1/2} \|_Y \rightarrow 0.$$

Thus,

$$\| |D_\xi|^{-1/2} (W_{\gamma_n, \xi} - W_{\gamma_*, \xi}) |D_\xi|^{-1/2} \|_Y \rightarrow 0.$$

□

Now we know that

Corollary 5.15. *As n goes to infinity,*

$$\| |D_0|^{-1/2} (V_{\gamma_n - \gamma_*}) |D_0|^{-1/2} \|_Y \rightarrow 0.$$

As a result, we have that following lemma

Lemma 5.16. *As n goes to infinity,*

$$\| P_{\gamma_*}^+ - P_{\gamma_n}^+ \|_Y \rightarrow 0.$$

Proof. Given

$$P_{\gamma_*, \xi}^+ - P_{\gamma_n, \xi}^+ = \frac{1}{2\pi} \int_{-\infty}^{+\infty} (D_{\gamma_*, \xi} - iz)^{-1} V_{\gamma_n - \gamma_*, \xi} (D_{\gamma_n, \xi} - iz)^{-1} dz,$$

by Corollary 5.15, we have

$$\begin{aligned}
& \|P_{\gamma_*,\xi}^+ - P_{\gamma_n,\xi}^+\|_{\mathcal{B}(L_\xi^2)} \\
& \leq \frac{1}{2\pi} \int_{-\infty}^{+\infty} \|(D_{\gamma_*,\xi} - iz)^{-1} V_{\gamma_n - \gamma_*,\xi} (D_{\gamma_n,\xi} - iz)^{-1}\|_{\mathcal{B}(L_\xi^2)} dz \\
& \leq \frac{1}{2\pi} \|D_0\|^{-1/2} (V_{\gamma_n - \gamma_*}) \|D_0\|^{-1/2} \|Y\| \\
& \quad \times \int_{-\infty}^{+\infty} \|(D_{\gamma_*,\xi} - iz)^{-1} D_\xi\|_{\mathcal{B}(L_\xi^2)}^{1/2} \|D_\xi\|_{\mathcal{B}(L_\xi^2)}^{1/2} (D_{\gamma_n,\xi} - iz)^{-1} \|_{\mathcal{B}(L_\xi^2)} dz \\
& \leq \frac{1}{4} (1 - \kappa)^{-1} \|D_0\|^{-1/2} (V_{\gamma_n - \gamma_*}) \|D_0\|^{-1/2} \|Y\|, \\
& \rightarrow 0.
\end{aligned}$$

□

Now, we begin to study the limit in the constraint and in the energy.

Lemma 5.17. $\gamma_* \in \Gamma_{\leq q}^+ \cap B_R$.

Proof. As

$$h_n \xrightarrow{*} \gamma_* \quad \text{in } X_\infty^2 \cap Y,$$

then

$$\|\gamma_*\|_{\sigma_{1,\infty}} \leq \inf \lim_{n \rightarrow \infty} \|h_n\|_{\sigma_{1,\infty}} \leq R,$$

and

$$\|\gamma_*\|_{X_\infty^2} \leq \inf \lim_{n \rightarrow \infty} \|h_n\|_{X_\infty^2} \leq (q + M)(1 - \kappa')^{-2} e^2,$$

as well as

$$\|\gamma_*\|_Y \leq \inf \lim_{n \rightarrow \infty} \|h_n\|_Y \leq 1$$

Thus, $\gamma_* \in \mathcal{T}$ and $\gamma_* \in X \cap Y \cap B_R$.

Besides, as $\|\gamma_n - h_n\|_X \rightarrow 0$, and $\|\rho_{h_n}^{1/2} - \rho_{\gamma_*}^{1/2}\|_{L^2} \rightarrow 0$. We know that

$$\frac{l^3}{(2\pi)^3} \int_{Q_l^*} \text{Tr}_{L_\xi^2} \gamma_{n,\xi} d\xi \rightarrow \frac{l^3}{(2\pi)^3} \int_{Q_l^*} \text{Tr}_{L_\xi^2} \hat{\gamma}_{*,\xi} d\xi.$$

Especially, if $\epsilon_F > (1 - \kappa)^{-1} c^*(q + 1)$, $\frac{l^3}{(2\pi)^2} \int_{Q_l^*} \text{Tr}_{L_\xi^2} \hat{\gamma}_{*,\xi} d\xi = q$ by Lemma 5.10.

Now, we only need to prove that $P_{\gamma_*,\xi}^+ \gamma_{*,\xi} = \gamma_{*,\xi}$, in the sense that for every $g \in L^1(Q_l^*; \mathcal{K}_\xi(Q_l))$,

$$\int_{Q_l^*} \text{Tr}_{L_\xi^2} [(P_{\gamma_*,\xi}^+ \gamma_{*,\xi} - \gamma_{*,\xi}) g_\xi] d\xi = 0.$$

Notice that

$$\begin{aligned}
& \left| \int_{Q_l^*} \text{Tr}_{L_\xi^2} [(P_{\gamma_*,\xi}^+ \gamma_{*,\xi} - \gamma_{*,\xi}) g_\xi] d\xi \right| \\
& \leq \left| \int_{Q_l^*} \text{Tr}_{L_\xi^2} [(P_{\gamma_*,\xi}^+ - P_{\gamma_n,\xi}^+) h_{n,\xi} g_\xi] d\xi \right| + \left| \int_{Q_l^*} \text{Tr}_{L_\xi^2} [P_{\gamma_*,\xi}^+ (\gamma_{*,\xi} - h_{n,\xi}) g_\xi] d\xi \right| \\
& \quad + \left| \int_{Q_l^*} \text{Tr}_{L_\xi^2} [(h_{n,\xi} - \gamma_{*,\xi}) g_\xi] d\xi \right|.
\end{aligned}$$

As $gP_{\gamma_*}^+ \in \mathcal{K}(Q_l)$, we know that

$$\int_{Q_l^*} \mathrm{Tr}_{L_\xi^2} [P_{\gamma_*, \xi}^+ (\gamma_{*, \xi} - h_{n, \xi}) g_\xi] d\xi \rightarrow 0,$$

and

$$\int_{Q_l^*} \mathrm{Tr}_{L_\xi^2} [(h_{n, \xi} - \gamma_{*, \xi}) g_\xi] d\xi \rightarrow 0.$$

For the first term in the right side, by Lemma 5.16, we have that

$$\left| \int_{Q_l^*} \mathrm{Tr}_{L_\xi^2} [(P_{\gamma_*, \xi}^+ - P_{\gamma_n, \xi}^+) h_{n, \xi} g_\xi] d\xi \right| \leq \|P_{\gamma_*}^+ - P_{\gamma_n}^+\|_Y \|h_n\|_{\sigma_{1,1}} \|g\|_Y \rightarrow 0.$$

Consequently, let $n \rightarrow \infty$,

$$\left| \int_{Q_l^*} \mathrm{Tr}_{L_\xi^2} [(P_{\gamma_*, \xi}^+ \gamma_{*, \xi} - \gamma_{*, \xi}) g_\xi] d\xi \right| = 0.$$

Now, we know that $\gamma_* \in \Gamma_{\leq q}^+$.

□

We only need to check that γ_* is the minimizer.

Lemma 5.18. $\mathcal{E}^{DF}(\gamma_*) - \epsilon_F \mathrm{Tr}_{L^2}(\gamma_*) = \min_{\gamma \in \Gamma_{\leq q}^+} (\mathcal{E}^{DF}(\gamma) - \epsilon_F \mathrm{Tr}_{L^2}(\gamma)).$

Proof. For the kinetic energy, we have that

$$\int_{Q_l^*} \mathrm{Tr}_{L_\xi^2} [D_\xi(\gamma_{n, \xi} - \gamma_{*, \xi})] d\xi = \int_{Q_l^*} \mathrm{Tr}_{L_\xi^2} [D_\xi(\gamma_{n, \xi} - h_{n, \xi})] d\xi + \int_{Q_l^*} \mathrm{Tr}_{L_\xi^2} [D_\xi(h_{n, \xi} - \gamma_{*, \xi})] d\xi.$$

By Formula 5.11, we know that

$$\int_{Q_l^*} \mathrm{Tr}_{L_\xi^2} [D_\xi(h_{n, \xi} - \gamma_{*, \xi})] d\xi = \int_{Q_l^*} \mathrm{Tr}_{L_\xi^2} [|D_\xi|(h_{n, \xi} - \gamma_{*, \xi}) |D_\xi| |D_\xi|^{-1} D_\xi |D_\xi|^{-1}] d\xi \rightarrow 0,$$

since $|D_\xi|^{-1} D_\xi |D_\xi|^{-1} \in L^1(Q_l^*; \mathcal{K}_\xi(Q_l))$. And since $\|\gamma_n - h_n\|_X \rightarrow 0$,

$$\int_{Q_l^*} \mathrm{Tr}_{L_\xi^2} [D_\xi(\gamma_{n, \xi} - h_{n, \xi})] d\xi \rightarrow 0$$

For the attractive potential, it is similar:

$$\int_{Q_l^*} \mathrm{Tr}_{L_\xi^2} (G(\cdot)(\gamma_{n, \xi} - \gamma_{*, \xi})) = \int_{Q_l^*} \mathrm{Tr}_{L_\xi^2} (G(\cdot)(\gamma_{n, \xi} - h_{n, \xi})) d\xi + \int_{Q_l^*} \mathrm{Tr}_{L_\xi^2} (G(\cdot)(h_{n, \xi} - \gamma_{*, \xi})) d\xi.$$

And

$$\left| \int_{Q_l^*} \mathrm{Tr}_{L_\xi^2} (G(\cdot)(\gamma_{n, \xi} - h_{n, \xi})) d\xi \right| \leq C'_H \|\gamma_n - h_n\|_X \rightarrow 0.$$

As $\||D_0|^{-1} G(\cdot) |D_0|^{-1}\|_{\sigma_{4,\infty}} \leq C_H \||D_0|^{-1}\|_{\sigma_{4,\infty}} < \infty$, we know that $|D_0|^{-1} G(\cdot) |D_0|^{-1} \in L^1(Q_l^*; \mathcal{K}_\xi(Q_l))$ and

$$\int_{Q_l^*} \mathrm{Tr}_{L_\xi^2} [G(\cdot)(h_{n, \xi} - \gamma_{*, \xi})] d\xi = \int_{Q_l^*} \mathrm{Tr}_{L_\xi^2} [|D_\xi|(h_{n, \xi} - \gamma_{*, \xi}) |D_\xi| |D_\xi|^{-1} G(\cdot) |D_\xi|^{-1}] d\xi \rightarrow 0,$$

For the repulsive potential, we have that

$$\begin{aligned}
& \int_{Q_l^*} \mathrm{Tr}_{L^2} [V_{\gamma_n, \xi} \gamma_{n, \xi} - V_{\gamma_*, \xi} \gamma_{*, \xi}] \\
&= \int_{Q_l^*} \mathrm{Tr}_{L^2} [V_{\gamma_n - \gamma_*, \xi} \gamma_{n, \xi} + V_{\gamma_n - \gamma_*, \xi} \gamma_*] \\
&= \int_{Q_l^*} \mathrm{Tr}_{L^2} [|D_\xi|^{-1/2} V_{\gamma_n - \gamma_*, \xi} |D_\xi|^{-1/2} |D_\xi|^{1/2} \gamma_{n, \xi} |D_\xi|^{1/2} \\
&\quad + |D_\xi|^{-1/2} V_{\gamma_n - \gamma_*, \xi} |D_\xi|^{-1/2} |D_\xi|^{1/2} \gamma_* |D_\xi|^{1/2}] \\
&\leq \| |D_0|^{-1/2} (V_{\gamma_n - \gamma_*}) |D_0|^{-1/2} \|_Y (\|\gamma_n\|_X + \|\gamma_*\|_X) \\
&\rightarrow 0.
\end{aligned}$$

We get the conclusion. \square

Step 6. The conclusion.

Now, we could say that γ_* is the minimizer under the condition $\gamma_* \in \Gamma_{\leq q}^+ \cap B_R$. Applying Lemma 5.9, we get

$$\int_{Q_l^*} \mathrm{Tr}_{L_\xi^2} ((D_{\gamma_*, \xi} - \epsilon_F) \gamma_{*, \xi}) d\xi = \inf_{\gamma \in \Gamma_{\leq q}, \gamma = P_{\gamma_*}^+ \gamma} \int_{Q_l^*} \mathrm{Tr}_{L_\xi^2} ((D_{\gamma_*, \xi} - \epsilon_F) \gamma_\xi) d\xi.$$

Then, by Lemma 5.4, we get $\gamma_* = \frac{l^3}{(2\pi)^3} \int_{Q_l^*}^\oplus \mathbb{1}_{[0, \nu)}(D_{\gamma_*, \xi}) d\xi + \delta$ with some $0 \leq \delta \leq \frac{l^3}{(2\pi)^3} \int_{Q_l^*}^\oplus \mathbb{1}_\nu(D_{\gamma_*, \xi}) d\xi$ for $\nu \in (0, \epsilon_F]$ independent of ξ . If $\epsilon_F \geq (1 - \kappa)^{-1} c^*(q + 1)$, the solution γ_* is independent of ϵ_F , and $\frac{l^3}{(2\pi)^3} \int_{Q_l^*} d\xi \mathrm{Tr}_{L_\xi^2} \gamma_{*, \xi} = q$.

Besides, $\|\gamma_*\|_{\sigma_{1, \infty}} \in B_{R_0}$ for any minimizers in $\Gamma_{\leq q}^+ \cap B_R$ if $R \geq R_0 := q + M$. \square

A Séré's retraction

At the end of this article, we state the Séré's retraction for reader's convenience.

Theorem A.1. *Let $(X, \|\cdot\|_X)$ be a Banach space and \mathcal{U} an open subset of X . Let $T : \mathcal{U} \rightarrow \mathcal{U}$ a continuous map. We assume:*

1. \mathcal{U} has a nonempty subset F which is closed in X and such that $T(F) \subset F$;
2. $\exists k \in (0, 1), \forall x \in T^{-1}(\mathcal{U}), \|T^2(x) - T(x)\|_X \leq k\|T(x) - x\|_X$.

Then there exists an open neighborhood \mathcal{V} of F in X with $\mathrm{Fix}(T) \subset \mathcal{V} \subset \mathcal{U}$, $T(\mathcal{V}) \subset \mathcal{V}$ and such that for any $x \in \mathcal{V}$, the sequence $(T^p(x))_{p \geq 0}$ has a limit $\theta(x) \in \mathcal{V}$ for the norm $\|\cdot\|_X$, with the estimate

$$\forall x \in \mathcal{V}, \|\theta(x) - T^p(x)\|_X \leq \frac{k^p}{1 - k} \|T(x) - x\|_X.$$

In this way we obtain a retraction θ of \mathcal{V} onto $\text{Fix}(T) \subset \mathcal{V}$ whose restriction to F is a retraction of F onto $F \cap \text{Fix}(T)$

Assume, moreover, that T is of class $C^{1,1}$ on \mathcal{U} and that:

3. The function $x \rightarrow \|DT(x)\|_{\mathcal{B}(X)}$ and $x \rightarrow \|T(x) - x\|_X$ are bounded on \mathcal{U} ;
4. $\exists L > 0, \forall x, y \in \mathcal{U}, \|DT(x) - DT(y)\|_{\mathcal{B}(X)} \leq L\|x - y\|_X$.

Then T^p converges uniformly to θ on \mathcal{V} and for each $x \in \mathcal{V}$, the sequence $(D(T^p)(x))_{p \geq 0}$ has a limit $l(x) \in \mathcal{B}(X)$ for the norm $\|\cdot\|_{\mathcal{B}(X)}$, this convergence being uniform in $x \in \mathcal{V}$. As a consequence, θ is of class C^1 on \mathcal{V} and $D\theta = l$ is uniformly continuous on \mathcal{V} .

B Product inequality in Sobolev space

In this section, we discuss the the following inequality in $H_\xi^s(Q_l^2)$:

Lemma B.1. *Suppose that $s > 0$ and $t > 3$. Then there is a continuous multiplication map*

$$\begin{aligned} H_\xi^s(Q_l^2) \times H_{\xi'}^{s+t}(Q_l^2) &\rightarrow H_{\xi+\xi'}^s(Q_l^2) \\ (u_\xi, v_{\xi'}) &\rightarrow u_\xi v_{\xi'}, \end{aligned}$$

and satisfies the estimate

$$\|u_\xi v_{\xi'}\|_{H_{\xi+\xi'}^s(Q_l^2)} \leq C \|u_\xi\|_{H_\xi^s(Q_l^2)} \|v_{\xi'}\|_{H_{\xi'}^{s+t}(Q_l^2)}$$

Remark B.2. This kind of inequality is a periodic case of the product inequality for Sobolev inequality:

$$\|uv\|_{H^s(\mathbb{R}^d)} \leq C \|u\|_{H^{s_1}(\mathbb{R}^d)} \|v\|_{H^{s_2}(\mathbb{R}^d)},$$

with $s_1, s_2 \geq s$ and $s_1 + s_2 > s + d/2$. And the proof is similar.

Proof. Obviously, we have

$$\begin{aligned} (1 + |k + k' - \xi' - \xi|)^2 &\leq (1 + |k - \xi|)(1 + |k' - \xi'|) \\ &\quad \times (1 + |k + k' - p - \xi|)(1 + |p - \xi'|). \end{aligned}$$

Then, applying the above inequality,

$$\begin{aligned} &\|u_\xi v_{\xi'}\|_{H^s}^2 \\ &= \sum_{k, k', p \in \mathbb{Z}^6} (1 + |k + k' - \xi - \xi'|)^{2s} \hat{u}_\xi(k) \hat{u}_\xi^*(k + k' - p) \hat{v}_{\xi'}(k') \hat{v}_{\xi'}^*(p) \\ &\leq \sum_{k', p \in \mathbb{Z}^6} (1 + |k' - \xi'|)^s |\hat{v}_{\xi'}(k')| (1 + |p - \xi'|)^s |\hat{v}_{\xi'}^*(p)| \\ &\quad \times \sum_{k \in \mathbb{Z}^6} (1 + |k - \xi|)^s |\hat{u}_\xi(k)| (1 + |k + k' - p - \xi|)^s |\hat{u}_\xi^*(k + k' - p)|. \end{aligned}$$

For the third line of the above inequality, there is a constant $C > 0$ such that

$$\begin{aligned}
& \sum_{k', p \in \mathbb{Z}^6} (1 + |k' - \xi'|)^s |\widehat{v}_{\xi'}(k')| (1 + |p - \xi'|)^s |\widehat{v}_{\xi'}^*(p)| \\
& \leq \sum_{k', p \in \mathbb{Z}^6} (1 + |k' - \xi'|)^{-t} (1 + |k' - \xi'|)^{s+t} |\widehat{v}_{\xi'}(k')| |(k + k' - p)| \\
& \quad \times (1 + |p - \xi'|)^{-t} (1 + |p - \xi'|)^{s+t} |\widehat{v}_{\xi'}^*(p)| \\
& \leq C \|v_{\xi'}\|_{H_{\xi'}^{s+t}}^2
\end{aligned}$$

if $t > 3$. And for the last line, by Chauchy-Schwartz's inequality, we have that

$$\begin{aligned}
& \sum_{k \in \mathbb{Z}^6} (1 + |k - \xi|)^s |\widehat{u}_{\xi}(k)| (1 + |k + k' - p - \xi|)^s |\widehat{u}_{\xi}^*(k + k' - p)| \\
& \leq \left(\sum_{k \in \mathbb{Z}^6} (1 + |k - \xi|)^{2s} |\widehat{u}_{\xi}(k)|^2 \right)^{1/2} \left(\sum_{k \in \mathbb{Z}^6} (1 + |k + k' - p - \xi|)^{2s} |\widehat{u}_{\xi}(k + k' - p)|^2 \right)^{1/2} \\
& = \|u_{\xi}\|_{H_{\xi}^s}^2
\end{aligned}$$

Now, we deduce that if $t > 3$

$$\|u_{\xi} v_{\xi'}\|_{H_{\xi+\xi'}^s(Q_i^2)} \leq C \|u_{\xi}\|_{H_{\xi}^s(Q_i^2)} \|v_{\xi'}\|_{H_{\xi'}^{s+t}(Q_i^2)}.$$

□

C Some singular integrals

In this part, we study the following type of singular integrals, which have been studied in [46] and [19].

Let $\mathcal{F}(u)(\xi) = \int e^{2\pi i x \cdot \xi} u(x) dx$ be the Fourier transform, then we have that in the sense of distribution for $0 < \alpha < d$

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

Hence, if $0 < \alpha < d$, the operator $|\nabla|^{\alpha}$ can be written as

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

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

$$|\nabla|^{-\alpha} |x|^{-\beta} = \frac{b_{\beta-\alpha} b_{d-\beta}}{(2\pi)^{\alpha} b_{d+\alpha-\beta} b_{\beta}} |x|^{\alpha-\beta}.$$

Thus, we know that in the sense of distribution

$$\int_{\mathbb{R}^3} |x-y|^{-d+\alpha} |y|^{\beta} dy = \frac{b_{\alpha} b_{\beta-\alpha} b_{d-\beta}}{b_{d-\alpha} b_{d+\alpha-\beta} b_{\beta}} |x|^{\alpha-\beta}.$$

Now, we know that in the sense of distribution

$$f(y) = \int_{\mathbb{R}^3} |x - y|^2 |x|^2 dx = \pi^3 |y|^{-1}.$$

As $f(y)$ and $\frac{1}{|y|}$ are continuous and bounded in $B_{1+r}(0) \setminus B_{1-r}(0)$ with any $0 < r < 1$ and $B_s(p) := \{x \in \mathbb{R}^3 : |x - p| \leq s\}$, we know that for $y \in B_{1+r}(0) \setminus B_{1-r}(0)$ with $r = 1/2$,

$$f(y) = \pi^3 \frac{1}{|y|}.$$

Thus, $f(e) = \pi^3$ with $|e| = 1$.

Similarly, we know that for $|e| = 1$,

$$\int_{\mathbb{R}^3} |x - e|^2 |x|^{1.5} dx = 4\pi^2,$$

and $e_{l,k} = \frac{l}{|k|}$ with $l, k \in \mathbb{Z}^3 \setminus \{0\}$

$$\int_{\mathbb{R}^3} |x - e_{l,k}|^2 |x|^{2.5} dx = 4\pi^2 |e_{l,k}|^{-1.5}.$$

D Estimates about the summations

D.1 Inequality 3.2

Now, we study the summation

$$T = \sum_{\substack{p, k \in \mathbb{Z}^3 \\ p \neq 0, k \\ k \neq 0}} \frac{1}{|k|^3} \frac{1}{\left| \frac{p}{|k|} - \frac{k}{|k|} \right|^2 \left| \frac{p}{|k|} \right|^2}$$

We consider the function

$$f_k(x) = \frac{1}{|x - e|^2 |x|^2},$$

with

$$e = \frac{k}{|k|}.$$

Now, we have that

$$\Delta f = \frac{12|x - \frac{1}{2}e|^2 - 1}{|x|^4 |x - e|^4}.$$

Thus,

$$\Delta f \geq 0 \quad \text{for } x \in B\left(\frac{1}{2}e, \frac{\sqrt{3}}{6}\right),$$

and let $r = |x - \frac{1}{2}e|$,

$$\Delta f \geq \frac{12r^2 - 1}{|\frac{1}{4} - r^2|^4} \geq -\frac{3^7}{2^3}.$$

Let $E_k = \left(\mathbb{Z}^3 \cap B\left(\frac{k}{2}, \frac{\sqrt{3}|k|}{6} + \frac{1}{2}\right)\right) \setminus \{0, k\}$ and $F_k = \mathbb{Z}^3 \setminus (E_k \cup \{0, k\})$.

For $p \in F_k$, $\Delta f \geq 0$ on $B\left(\frac{p}{|k|}, \frac{1}{2|k|}\right)$ by virtue of the mean value inequality of sub-harmonic function, we yield that

$$\frac{1}{|k|^3} f_k \left(\frac{p}{|k|} \right) \leq \frac{6}{\pi} \int_{B\left(\frac{p}{|k|}, \frac{1}{2|k|}\right)} f_k dx.$$

Thus,

$$\sum_{p \in F_k} \frac{1}{|k|^3} f_k \left(\frac{p}{|k|} \right) \leq \frac{6}{\pi} \int_{\cup_{p \in F_k} B\left(\frac{p}{|k|}, \frac{1}{2|k|}\right)} f_k dx.$$

Now, we only need to estimate the term of E_k . If $p \in E_k$, then $p + [-\frac{1}{2}, \frac{1}{2}]^3 \in B\left(\frac{k}{2}, \frac{\sqrt{3}}{6}|l| + \frac{1}{2} + \frac{\sqrt{3}}{2}\right)$, thus

$$|E_k| \leq \frac{4\pi}{3} \left(\frac{\sqrt{3}}{6}|l| + \frac{1}{2} + \frac{\sqrt{3}}{2} \right)^3.$$

For $0 < r \leq \frac{1}{2|k|}$, by Divergence Theorem, we have that

$$\begin{aligned} \frac{d}{dr} \left(\frac{1}{4\pi r^2} \int_{\partial B\left(\frac{p}{|k|}, r\right)} f_k ds \right) &= \frac{1}{4\pi r^2} \int_{\partial B\left(\frac{p}{|k|}, r\right)} \frac{\partial}{\partial n} f_k ds \\ &= \frac{1}{4\pi r^2} \int_{B\left(\frac{p}{|k|}, r\right)} \Delta f_k dy \\ &\geq -\frac{3^6}{2^3} r. \end{aligned}$$

Thus, we have that

$$\frac{1}{4\pi} \int_{\partial B\left(\frac{p}{|k|}, r\right)} f_k ds \geq r^2 f_k \left(\frac{p}{|k|} \right) - \frac{3^6}{2^4} r^4.$$

And by the integration over $[0, \frac{1}{2|k|}]$, we get that

$$\frac{1}{|k|^3} f_k \left(\frac{p}{|k|} \right) \leq \frac{6}{\pi} \int_{B\left(\frac{p}{|k|}, \frac{1}{2|k|}\right)} f_{l,k} dy + \frac{3^7}{2^6 \times 5|k|^5},$$

and

$$\sum_{p \in E_k} \frac{1}{|k|^3} f_k \left(\frac{p}{|k|} \right) \leq \frac{6}{\pi} \int_{\cup_{p \in E_k} B\left(\frac{p}{|k|}, \frac{1}{2|k|}\right)} f_k dy + \frac{3^7}{2^6 \times 5|k|^5} |E_{l,k}|.$$

Besides, after calculation, we know that for $|k| \leq 10$

$$\sum_{p \in E_k} \frac{1}{|k|^3} f_k \leq 5.258.$$

As a consequence, we deduce that for $|k| \geq 11$,

$$\begin{aligned} &\sum_{p \neq 0, k; k \neq 0} \frac{1}{|k|^3} f_k \left(\frac{p}{|k|} \right) \\ &\leq \frac{6}{\pi} \int_{\cup_{p \in \mathbb{Z}^3 \setminus \{0, l\}} f_k dy + \frac{3^7}{2^6 \times 5|k|^5} \frac{4\pi}{3} \left(\frac{\sqrt{3}|k|}{6} + \frac{1}{2} + \frac{\sqrt{3}}{2} \right)^3 \\ &\leq \frac{6}{\pi} \int_{\mathbb{R}^3} f_k dx + 0.017 \\ &\leq 59.235. \end{aligned}$$

D.2 Inequality 3.3

We are going to estimate the summation:

$$T := \sum_{\substack{l,p,k \in \mathbb{Z}^3 \\ p,k \neq 0 \\ l \neq k,p}} \frac{1}{|k|^6} \frac{1}{\left| \frac{l}{|k|} - \frac{k}{|k|} \right|^2 \left| \frac{l}{|k|} - \frac{p}{|k|} \right|^2 \left| \frac{p}{|k|} \right|^{2.5}}.$$

Let

$$T_1 := \sum_{\substack{l,p,k \in \mathbb{Z}^3 \\ l,p,k \neq 0 \\ l \neq k,p}} \frac{1}{|k|^6} \frac{1}{\left| \frac{l}{|k|} - \frac{k}{|k|} \right|^2 \left| \frac{l}{|k|} - \frac{p}{|k|} \right|^2 \left| \frac{p}{|k|} \right|^{2.5}}.$$

Now, we have that

$$T = T_1 + \sum_{p,k \neq 0} \frac{1}{|k|^6} \frac{1}{\left| \frac{p}{|k|} \right|^{4.5}} \leq T_1 + \sum_{p \neq 0} \frac{1}{|p|^{4.5}}.$$

We consider first the term

$$\sum_{p \neq 0, l} \frac{1}{|k|^3} \frac{1}{\left| \frac{l}{|k|} - \frac{p}{|k|} \right|^2 \left| \frac{p}{|k|} \right|^{2.5}},$$

and the function

$$f_{l,k}(y) = \frac{1}{|y - e_{l,k}|^2 |y|^{2.5}},$$

with

$$e_{l,k} = \frac{l}{|k|}.$$

Now, we have that

$$\begin{aligned} \Delta f_{l,k}(y) &= \frac{63|y|^2 - 70e_{l,k} \cdot y + 15|e_{l,k}|^2}{4|y - e_{l,k}|^4 |y|^{4.5}} \\ &= \frac{63}{4} \frac{|y - \frac{5}{9}e_{l,k}|^2 - \frac{40}{567}|e_{l,k}|^2}{|y - e_{l,k}|^4 |y|^{4.5}} \end{aligned}$$

Thus,

$$\Delta f_{l,k} \geq 0 \quad \text{for } y \in \mathbb{R}^3 \setminus B\left(\frac{5}{9}e_{l,k}, \frac{\sqrt{280}}{63}|e_{l,k}|\right).$$

Besides, we yield numerically that

$$\Delta f_{l,k} \geq -490|e_{l,k}|^{-6.5}.$$

Let $E_{l,k} = \left(\mathbb{Z}^3 \cap B\left(\frac{35}{63}l, \frac{\sqrt{380}}{63}|l| + \frac{1}{2}\right)\right) \setminus \{0, k\}$, and $F_{l,k} = \mathbb{Z}^3 \setminus (E_{l,k} \cup \{0, k\})$.

For $p \in F_{l,k}$, we have that $\Delta f_{l,k} \geq 0$ on $B\left(\frac{p}{|k|}, \frac{1}{2|k|}\right)$. Thus

$$|k|^{-3} f_{l,k}\left(\frac{p}{|k|}\right) \leq \frac{6}{\pi} \int_{B\left(\frac{p}{|k|}, \frac{1}{2|k|}\right)} f_{l,k}.$$

And we yield

$$\sum_{p \in F_{l,k}} |k|^{-3} f_{l,k} \left(\frac{p}{|k|} \right) \leq \frac{6}{\pi} \int_{\cup_{p \in F_{l,k}} B\left(\frac{p}{|k|}, \frac{1}{2|k|}\right)} \frac{1}{|y - e_{l,k}|^2 |y|^{2.5}} dy.$$

Now, we only need to estimate the term of $E_{l,k}$. If $p \in E_{l,k}$, then $p + [-\frac{1}{2}, \frac{1}{2}]^3 \in B\left(\frac{5}{9}l, \frac{\sqrt{280}}{63}|l| + \frac{1}{2} + \frac{\sqrt{3}}{2}\right)$. Thus,

$$|E_{l,k}| \leq \frac{4\pi}{3} \left(\frac{\sqrt{280}}{63}|l| + \frac{1}{2} + \frac{\sqrt{3}}{2} \right)^3.$$

For $0 < r \leq \frac{1}{2|k|}$, we have that

$$\begin{aligned} \frac{d}{dr} \left(\frac{1}{4\pi r^2} \int_{\partial B\left(\frac{p}{|k|}, r\right)} f_{l,k} ds \right) &= \frac{1}{4\pi r^2} \int_{\partial B\left(\frac{p}{|k|}, r\right)} \frac{\partial}{\partial n} f_{l,k} ds \\ &= \frac{1}{4\pi r^2} \int_{B\left(\frac{p}{|k|}, r\right)} \Delta f_{l,k} dy \\ &\geq -\frac{490|k|^{6.5}}{3|l|^{6.5}} r. \end{aligned}$$

Thus, we have that

$$\frac{1}{4\pi} \int_{\partial B\left(\frac{p}{|k|}, r\right)} f_{l,k} ds \geq r^2 f_{l,k} \left(\frac{p}{|k|} \right) - \frac{245|k|^{6.5}}{3|l|^{6.5}} r^4.$$

And by the integration again over $[0, \frac{1}{2|k|}]$, we get that

$$\frac{1}{|k|^3} f_{l,k} \left(\frac{p}{|k|} \right) \leq \frac{6}{\pi} \int_{B\left(\frac{p}{|k|}, \frac{1}{2|k|}\right)} f_{l,k} dy + \frac{49|k|^{1.5}}{4|l|^{6.5}},$$

and

$$\sum_{p \in E_k} \frac{1}{|k|^3} f_{l,k} \left(\frac{p}{|k|} \right) \leq \frac{6}{\pi} \int_{\cup_{p \in E_k} B\left(\frac{p}{|k|}, \frac{1}{2|k|}\right)} f_{l,k} dy + \frac{49|k|^{1.5}}{4|l|^{6.5}} |E_{l,k}|.$$

Thus, we get that

$$\begin{aligned} &\sum_{p \neq 0, l; k \neq 0} \frac{1}{|k|^3} f_{l,k} \left(\frac{p}{|k|} \right) \\ &\leq \frac{6}{\pi} \int_{\cup_{p \in \mathbb{Z}^3 \setminus \{0, l\}} B\left(\frac{p}{|k|}, \frac{1}{2|k|}\right)} f_{l,k} dy + \frac{49\pi|k|^{1.5}}{3|l|^{6.5}} \left(\frac{\sqrt{280}}{63}|l| + \frac{1}{2} + \frac{\sqrt{3}}{2} \right)^3 \\ &\leq \frac{6}{\pi} \int_{\mathbb{R}^3} f_{l,k} dy + \frac{49\pi|k|^{1.5}}{3|l|^{6.5}} \left(\frac{\sqrt{280}}{63}|l| + \frac{1}{2} + \frac{\sqrt{3}}{2} \right)^3 \\ &\leq 24\pi |e_{l,k}|^{-1.5} + \frac{49\pi}{3} \left(\frac{\sqrt{280}}{63} + \frac{1}{2} + \frac{\sqrt{3}}{2} \right)^3 |l|^{-2} |e_{l,k}|^{-1.5} |l|^{-2} \\ &\leq 298.289 |e_{l,k}|^{-1.5}. \end{aligned}$$

Now, we yield that

$$T_1 \leq 298.289 \sum_{l \neq 0; k \neq 0} \frac{1}{|k|^3} \frac{1}{\left| \frac{l}{|k|} - \frac{k}{|k|} \right|^2 \left| \frac{l}{|k|} \right|^{1.5}}.$$

Now, we consider the function

$$f_k(x) = \frac{1}{|x - e|^2 |x|^{1.5}},$$

with $e = \frac{k}{|k|}$. Similarly, we know that

$$\Delta f_k(x) = \frac{35}{4} \frac{|x - \frac{3}{7}e|^2 - \frac{24}{245}}{|x|^{3.5} |x - e|^4}.$$

Now, we know that

$$\Delta f_k \geq 0 \quad \text{for } x \in \mathbb{R}^3 \setminus B\left(\frac{3}{7}e, \frac{\sqrt{120}}{35}\right)$$

and

$$-\Delta f_k \geq -284.$$

Let $E_k = \left(\mathbb{Z}^3 \cap B\left(\frac{3}{7}k, \frac{\sqrt{120}}{35}|k| + \frac{1}{2}\right)\right) \setminus \{0, k\}$, and $F_k = \mathbb{Z}^3 \setminus (E_k \cup \{0, k\})$. And

$$|E_k| \leq \frac{4\pi}{3} \left(\frac{\sqrt{120}}{35}|k| + \frac{1}{2} + \frac{\sqrt{3}}{2}\right)^3.$$

Now, we know that

$$\sum_{l \in F_k} \frac{1}{|k|^3} f_k\left(\frac{l}{|k|}\right) \leq \frac{6}{\pi} \int_{\cup_{p \in F_k} B\left(\frac{p}{|k|}, \frac{1}{2|k|}\right)} f_k(x) dx.$$

And for the term of E_k , we have analogously that

$$\frac{1}{|k|^3} f_k\left(\frac{l}{|k|}\right) \leq \frac{6}{\pi} \int_{B\left(\frac{p}{|x|}, \frac{1}{2|k|}\right)} f_k dx + 7.1|k|^{-5}.$$

Besides, after direct calculation, we now get that for $|k| \leq 10$

$$\sum_{l \in E_k} \frac{1}{|k|^3} f_k\left(\frac{l}{|k|}\right) \leq 4.3217.$$

Thus, for $|k| \leq 10$, we have that

$$\sum_{l \neq 0, k; k \neq 0} \frac{1}{|k|^3} f_k\left(\frac{l}{|k|}\right) \leq 4.3217 + 24\pi.$$

And for the term $|k| > 10$, we have that

$$\begin{aligned} & \sum_{l \neq 0, k; k \neq 0} \frac{1}{|k|^3} f_k\left(\frac{l}{|k|}\right) \\ & \leq \frac{6}{\pi} \int_{\cup_{p \in \mathbb{Z}^3 \setminus \{0, k\}} B\left(\frac{p}{|x|}, \frac{1}{2|k|}\right)} f_k dx + 7.1 \times 10^{-5} \frac{4\pi}{3} \left(\frac{\sqrt{120}}{35}|k| + \frac{1}{2} + \frac{\sqrt{3}}{2}\right)^3 \\ & \leq 75.426. \end{aligned}$$

Now, we get conclusion that

$$T \leq 22498.747 + \sum_{p \neq 0} \frac{1}{|p|^{4.5}}.$$

E Numerical results about constants

In this section, we will show the numerical results about the constants used in Remark 2.14 under the condition $l = 1000$, and then we show that the Assumption 2.12 is satisfied for $q \leq 4$ for the neutral systems.

First, we compute numerically the infimum of the potential G_l ,

$$C_0 \approx 0.802.$$

And as

$$\sum_{k \neq 0} \frac{1}{|k|^5} \approx 10.378,$$

we know that

$$C_H \approx 3.199,$$

thus

$$C'_H = C_H + 2C_0/l \approx 3.201.$$

Similarly,

$$\sum_{k \neq 0} \frac{1}{|k|^4} \approx 16.512,$$

and

$$\sum_{k \neq 0} \frac{1}{|k|^{4.5}} \approx 12.403,$$

and

$$\sum_{\substack{p \neq k \\ k, p \neq 0}} \frac{1}{|p-k|^4 |p|^4 |k|^2} \approx 55.488.$$

Thus,

$$C_G \approx 7.688.$$

For the potential W_l ,

$$\|g_1\|_{L^\infty} \approx 0.188\pi,$$

and for the constant C_l , we have that

$$\begin{aligned} C_l &= \sup_{\xi' \in Q_i^*} \sum_{m \in \mathbb{Z}^3, |m|_\infty \leq 1} \int_{Q_i^*} d\xi \frac{4\pi}{|\xi - \xi' - 2\pi m/l|^2} \\ &= \sup_{\xi' \in Q_i^*} \sum_{m \in \mathbb{Z}^3, |m|_\infty \leq 1} \int_{Q_i^* + 2\pi m/l} \frac{4\pi}{|\xi - \xi'|^2} d\xi. \end{aligned}$$

As $Q_i^* = [-\frac{\pi}{l}, \frac{\pi}{l}]^3$, we have that if $m_1, m_2 \in \mathbb{Z}^3$ and $m_1 \neq m_2$,

$$(Q_i^* + 2\pi m_1/l) \cap (Q_i^* + 2\pi m_2/l) = \emptyset,$$

and let $Q = [-3, 3]^3$, then we have that

$$C_l = \sup_{\xi' \in Q_i^*} \int_{3Q_i^*} \frac{4\pi}{|\xi - \xi'|^2} d\xi = \frac{4\pi^2}{l} \int_Q \frac{1}{|\xi|^2} d\xi \approx 1.818.$$

Thus, we get

$$C_W = C'_H + \|g_l\|_{L^\infty} + C_l = C'_H + \frac{1}{l}\|g_1\|_{L^\infty} + C_l \approx 5.019,$$

and

$$C'_W = C_G + \|g_l\|_{L^\infty} + C_l = C_G + \frac{1}{l}\|g_1\|_{L^\infty} + C_l \approx 9.506.$$

Thus

$$C_{EE} \approx 8.220.$$

Finally, we estimate $c^*(q)$. Recall that

$$c^*(q) := \sup_{\xi \in Q_l^*} \inf_{\substack{V \text{ subspace of } \Lambda^+ H_\xi^{1/2} \\ \dim V = q}} \sup_{u_\xi^+ \in V} \frac{\| |D_\xi|^{1/2} u_\xi^+ \|_{L_\xi^2}^2}{\|u_\xi^+\|_{L_\xi^2}^2}.$$

Let $u_{p,\xi}(x) = e^{(2i\pi p/l + i\xi) \cdot x}$ with $p \in \mathbb{Z}^3$. Then $(u_{p,\xi})_{p \in \mathbb{Z}^3}$ is an orthogonal basis on $L_\xi^2(Q_l)$.

And

$$\Lambda^+ u_{p,\xi} = \left(\frac{1}{2} + \frac{(2\pi p + l\xi) \cdot \alpha + l\beta}{2\sqrt{l^2 + |2\pi p + l\xi|^2}} \right) e^{(2i\pi p/l + i\xi) \cdot x},$$

and

$$|D_\xi|^{1/2} \Lambda^+ u_{p,\xi} = (1 + |2\pi p/l + \xi|^2)^{1/4} \Lambda^+ u_{p,\xi}.$$

Obviously, $(\Lambda^+ u_{p,\xi})_p$ is equally an orthogonal basis on $L_\xi^2(Q_l)$. Let

$$V_q = \{\Lambda^+ u_{p,\xi}(x); p = \{1, \dots, q\} \times \{0\} \times \{0\}\},$$

then

$$c^*(q) \leq \sup_{\xi \in Q_l^*} \sup_{u_\xi^+ \in V_q} \frac{\| |D_\xi|^{1/2} u_\xi^+ \|_{L_\xi^2}^2}{\|u_\xi^+\|_{L_\xi^2}^2} \leq \sqrt{1 + |2\pi(q+1)/l|^2}.$$

Now we can check the Assumption 2.12 for $z = q = 4$ and $z = q = 5$. For $z = q = 5$,

- $\kappa \approx 0.581$,
- $\kappa + 1/2\alpha C_{EE} q^+ \approx 0.731 < 1$
- $A > \frac{1}{4}\alpha(1 - \kappa)^{-2}(1 + \kappa)C_{EE} > 0.134$,
- $\kappa' = \alpha(C_G(z + q) + C'_W q^+) \approx 0.908$,
- $c^*(6) > 1$,
- $A\sqrt{\max\{(1 - \kappa - 1/2\alpha C_{EE} q^+)^{-1}(1 - \kappa)^{-1}c^*(q+1)q, 1\}} q^+ > 1.993 > 1$.

And for $z = q = 4$,

- $\kappa \approx 0.465$,
- $\kappa + 1/2\alpha C_{EE} q^+ \approx 0.585 < 1$

- $A = 0.078 > \frac{1}{4}\alpha(1 - \kappa)^{-2}(1 + \kappa)C_{EE} \approx 0.077$,
- $\kappa' = \alpha(C_G(z + q) + C'_W q^+) \approx 0.727$,
- $c^*(5) < 1.001$,
- $A\sqrt{\max\{(1 - \kappa - 1/2\alpha C_{EE}q^+)^{-1}(1 - \kappa)^{-1}c^*(q + 1)q, 1\}q^+} \approx 0.662 < 1$.

Consequently, we know that the Assumption 2.12 is satisfied for $q \leq 4$ in solid state physics.

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RÉSUMÉ

Cette thèse est une étude rigoureuse du problème à N corps en interaction coulombienne et de certaines de ses approximations en chimie quantique non relativiste et relativiste. Pour le problème de Schrödinger à N corps stationnaire ou dépendant du temps, nous généralisons des résultats théoriques de régularité mixte introduits par H. Yserentant, qui ont des conséquences directes sur la complexité des calculs numériques. Dans le cadre relativiste, l'équation de Dirac remplace l'équation de Schrödinger et l'étude rigoureuse du problème exact à N corps semble hors de portée. En conséquence, nous étudions seulement une approximation, le modèle de Dirac-Fock. Nous donnons le premier résultat d'existence de solutions stationnaires des équations de Dirac-Fock dans les cristaux.

MOTS CLÉS

Mécanique quantique ; N corps; Schrödinger; régularité; analyse numérique; Dirac-Fock; cristaux; quasi-périodique; existence; théorie spectrale.

ABSTRACT

This thesis is a rigorous study of the N-body problem in Coulomb interaction and some of its approximations in non-relativistic and relativistic quantum chemistry. For the N-body stationary or time-dependent Schrödinger problem, we generalize theoretical results of mixed regularity due to H. Yserentant, which have direct consequences on the complexity of numerical calculations. In the relativistic framework, the Dirac equation replaces the Schrödinger equation and a rigorous study of the exact N-body problem seems out of reach. Consequently, we only study an approximation, the Dirac-Fock model. We give the first existence result for stationary solutions of the Dirac-Fock equations in crystals.

KEYWORDS

Quantum mechanics; many-body; Schrödinger; regularity; numerical analysis; Dirac-Fock; crystal; quasi-periodic; existence; spectral theory.