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Existence of minimizers for the Dirac–Fock Model of Crystals

Isabelle Catto* Long Meng† Eric Paturel‡ Eric Séré§

Abstract

Whereas many different models exist in the mathematical and physics literature for ground-states of non-relativistic crystals, the relativistic case has been much less studied and we are not aware of any mathematical result on a relativistic treatment of crystals. In this paper, we introduce a mean-field relativistic energy for crystals in terms of periodic density matrices. This model is inspired both from a recent definition of the Dirac–Fock ground state for atoms and molecules, due to one of us, and from the non-relativistic Hartree–Fock model for crystals. We prove existence of a ground-state when the number of electrons per cell is not too large.

1 Introduction

For solids with heavy atoms, relativistic shifts may affect the bonding properties and the optical properties. It is shown in [27] that the fact that gold is yellow is a result of relativistic effects. Furthermore, by studying the relativistic band structure in solids, it is shown in [7, 8] that the relativistic shifts of the $5d$ bands relative to the $s - p$ bands in gold change the main interband edge more than $1eV$.

A natural way to build quantum models for the crystal 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 an (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 applied successfully by different authors for different well-known models from quantum chemistry [6, 5, 3, 23] – see also [4] for a review – but always for non-relativistic crystals.

Among relativistic models, the atomic and molecular Dirac–Fock model (DF) is the most attractive one since it has been formally justified by Mittleman [25]. It gives numerical results in excellent agreement with experimental data [9, 15, 21]. To our knowledge this model has not been extended to crystals: there exist fully relativistic treatments of crystals in the physics literature, but they use the Kohn–Sham approach (see [11, 19] and the references therein).

The mathematical study of the atomic and molecular Dirac–Fock model has been done in [12, 26]. Compared to the non-relativistic models, the situation is different: Existence of bound-states only holds if the total positive charge Z is not too large (with physical units, $Z \leq 124$). Moreover, the Dirac–Fock energy functional is strongly indefinite and the notion of ground-state has to be handled very carefully [12]. These difficulties exclude a thermodynamic limit approach to derive the Dirac–Fock model for crystals.

Esteban and Séré [13] showed that certain solutions of the (relativistic) 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 validates *a posteriori* the notions of ground-state solutions and ground-state energy for the Dirac–Fock equations. In Esteban and Séré’s approach, the ground state is modelled by the electrons’ wavefunction. On the other hand, Huber and Siedentop

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introduced a density matrix formulation of the Dirac–Fock model [18]. Recently, one of us proved the existence of the ground-state for the Dirac–Fock model in atoms and molecules in terms of density matrix using a retraction technique [29]. This approach guarantees that we exhibit the ground-state energy of a relativistic crystal, not only a bound-state. Inspired by this work and by the analysis of the periodic Hartree–Fock model due to Le Bris, Lions and one of us [5], we propose a definition for the ground state of Dirac–Fock model for crystals which is a relativistic analogue of Lieb’s variational principle for Hartree–Fock model [1, 22], and we prove the existence of minimizers. In addition, our result shows that these minimizers solve a self-consistent equation, as established by Ghimenti and Lewin in [14] for the periodic Hartree–Fock model. Our method can be used to calculate the ground-state of neutral crystals with at most 17 electrons per cell. However, some estimates used in this paper are not optimal, and we strongly believe that this limiting bound can be improved.

The minimization problem under consideration in this paper combines several difficulties related to compactness issues. Obviously, the Dirac operator is not bounded from below and the kinetic energy term order is of the same order as the Coulomb-type potential energy terms, a standard feature of Coulomb–Dirac–Fock type models. Nevertheless, our proof of existence of minimizers for crystals is neither a straight adaptation of the one for atoms and molecules in [29] or of the one for crystals in Hartree–Fock theory in [5]: A major issue arises from the regularity in the momentum variable ξ resulting from the Bloch decomposition of the space, the density matrices and the self-consistent operator. Compactness in the momentum variable is crucial to deal with the periodic exchange term and with the nonlinear constraint that ensures that the electrons lie in the positive spectral subspace of the self-consistent periodic Dirac–Fock operator. Our results rely on a careful analysis of the periodic exchange potential. (In passing, we have corrected some false estimates on the exchange term in [5] and improved the regularity results therein.) Furthermore, we provide an asymptotically optimal constant for the Hardy inequality associated with periodic Coulomb potential that is new in the literature, as far as we know.

In addition, compared with existing results for crystals, such as the Hartree–Fock one [5], we provide a new general method to prove the existence of minimizers for crystals: Based on the spectral analysis of the self-consistent operator, we can describe the behaviour of the minimizing sequences with respect to the momentum ξ and rely on it to improve the regularity, hence the compactness of subsequences.

2 General setting of the model and main result

2.1 Preliminaries – Functional framework

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. For the sake of simplicity, we only consider the case of a cubic crystal with a single point-like nucleus per unit cell, that is located at the centre of the cell. The reader should however keep in mind that the general case could be handled as well. Let $\ell > 0$ denote the length of the elementary cell $Q_\ell = (-\frac{\ell}{2}, \frac{\ell}{2}]^3$. The nuclei with positive charge z are treated as classical particles with infinite mass that are located at each point of the lattice $\ell\mathbb{Z}^3$. The electrons are treated quantum mechanically through a periodic density matrix. The electronic density is modelled by a Q_ℓ -periodic function whose L^1 norm over the elementary cell equals the “number of electrons” q – the electrons’ charge per cell being equal to $-q$. Especially, when $q = z$, electrical neutrality per cell is ensured.

In this periodic setting, the Q_ℓ -periodic Coulomb potential G_ℓ resulting from a distribution of point particles of charge 1 that are periodically located at the centers of the cubic cells of the lattice is defined, up to a constant, by

$$-\Delta G_\ell = 4\pi \left[-\frac{1}{\ell^3} + \sum_{k \in \mathbb{Z}^3} \delta_{\ell k} \right]. \quad (2.1)$$

By convention, we choose G_ℓ such that

$$\int_{Q_\ell} G_\ell dx = 0. \quad (2.2)$$

The function G_ℓ is actually the Green function of the periodic Laplace operator on Q_ℓ . The Fourier

series of G_ℓ writes

$$G_\ell(x) = \frac{1}{\pi\ell} \sum_{p \in \mathbb{Z}^3 \setminus \{0\}} \frac{e^{\frac{2i\pi}{\ell} p \cdot x}}{|p|^2}, \quad \text{for every } x \in \mathbb{R}^3. \quad (2.3)$$

Remark 2.1. *The size of the unit cell ℓ does not play a specific role here. It is however involved in the study of the Hardy-type inequalities for the periodic Coulomb potential (see Section 4.1). When ℓ goes to infinity, one expects to recover the Dirac–Fock model for atoms.*

The free Dirac operator is defined by $D^0 = -i \sum_{k=1}^3 \alpha_k \partial_k + \beta$, with 4×4 complex matrices $\alpha_1, \alpha_2, \alpha_3$ and β , whose standard forms are $\beta = \begin{pmatrix} 1_2 & 0 \\ 0 & -1_2 \end{pmatrix}$, $\alpha_k = \begin{pmatrix} 0 & \sigma_k \\ \sigma_k & 0 \end{pmatrix}$ where 1_2 is the 2×2 identity matrix and the σ_k 's, for $k \in \{1, 2, 3\}$, 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 . 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 $H^{1/2}(\mathbb{R}^3; \mathbb{C}^4)$ (denoted by L^2 , H^1 and $H^{1/2}$ in the following, when there is no ambiguity). Its spectrum is $\sigma(D^0) = (-\infty, -1] \cup [+1, +\infty)$. Following the notation in [12, 26], we denote by Λ^+ and $\Lambda^- = 1_{L^2} - \Lambda^+$ respectively the two orthogonal projectors on $L^2(\mathbb{R}^3; \mathbb{C}^4)$ corresponding to the positive and negative eigenspaces of D^0 ; that is

$$\begin{cases} D^0 \Lambda^+ = \Lambda^+ D^0 = \Lambda^+ \sqrt{1 - \Delta} = \sqrt{1 - \Delta} \Lambda^+; \\ D^0 \Lambda^- = \Lambda^- D^0 = -\Lambda^- \sqrt{1 - \Delta} = -\sqrt{1 - \Delta} \Lambda^-. \end{cases}$$

According to the Floquet theory [28], the underlying Hilbert space $L^2(\mathbb{R}^3; \mathbb{C}^4)$ is unitarily equivalent to $L^2(Q_\ell^*) \otimes L^2(Q_\ell; \mathbb{C}^4)$, where $Q_\ell^* = [-\frac{\pi}{\ell}, \frac{\pi}{\ell}]^3$ is the so-called reciprocal cell of the lattice, with volume $|Q_\ell^*| = (2\pi)^3/\ell^3$. (In the Physics literature Q_ℓ^* is known as the first Brillouin zone.) The Floquet unitary transform $U : L^2(\mathbb{R}^3; \mathbb{C}^4) \rightarrow L^2(Q_\ell^*) \otimes L^2(Q_\ell; \mathbb{C}^4)$ is given by

$$(U\phi)_\xi = \sum_{k \in \mathbb{Z}^3} e^{-i\ell k \cdot \xi} \phi(\cdot + \ell k) \quad (2.4)$$

for every $\xi \in Q_\ell^*$ and ϕ in $L^2(\mathbb{R}^3; \mathbb{C}^4)$. For every $\xi \in Q_\ell^*$, the function $(U\phi)_\xi$ belongs to the space

$$L_\xi^2(Q_\ell; \mathbb{C}^4) = \{\psi \in L_{\text{loc}}^2(\mathbb{R}^3; \mathbb{C}^4) \mid e^{-i\xi \cdot x} \psi \text{ is } Q_\ell\text{-periodic}\},$$

which will be denoted by L_ξ^2 in the sequel. Functions ψ of this form are called Bloch waves or Q_ℓ -quasi-periodic functions with quasi-momentum $\xi \in Q_\ell^*$. They satisfy

$$\psi(\cdot + \ell k) = e^{i\ell k \cdot \xi} \psi(\cdot), \quad \text{for every } k \in \mathbb{Z}^3.$$

For any function $\phi_\xi \in L_\xi^2$, using the definition of Fourier series expansion for Q_ℓ -periodic functions, we write

$$\phi_\xi(x) = \sum_{k \in \mathbb{Z}^3} \hat{\phi}_\xi(k) e^{(2i\pi k/\ell + i\xi) \cdot x}, \quad \text{a.e. } x \in \mathbb{R}^3, \quad (2.5)$$

with coefficients

$$\hat{\phi}_\xi(k) = \frac{1}{\ell^3} \int_{Q_\ell} \phi_\xi(y) e^{-(2i\pi k/\ell + i\xi) \cdot y} dy \in \mathbb{C}^4.$$

The Hilbert space L_ξ^2 is endowed with the norm

$$\|\phi\|_{L_\xi^2} := \left(\ell^3 \sum_{k \in \mathbb{Z}^3} |\hat{\phi}_\xi(k)|^2 \right)^{1/2} = \left(\int_{Q_\ell} |\phi_\xi(x)|^2 dx \right)^{1/2} = \|\phi_\xi\|_{L^2(Q_\ell)}.$$

Here, and in the whole paper, we use the same notation $|\cdot|$ for the canonical Euclidian norm in \mathbb{R}^n , \mathbb{C}^n or $\mathcal{M}_n(\mathbb{C})$. When applied to self-adjoint operators, $|T|$ means the absolute value of T .

We also define

$$H_\xi^s(Q_\ell; \mathbb{C}^4) := L_\xi^2(Q_\ell; \mathbb{C}^4) \cap H_{\text{loc}}^s(\mathbb{R}^3; \mathbb{C}^4)$$

for every real number s , endowed with the norm

$$\|\phi_\xi\|_{H_\xi^s} = \left(\ell^3 \sum_{k \in \mathbb{Z}^3} (1 + |2\pi k/\ell + \xi|^2)^s |\widehat{\phi}_\xi(k)|^2 \right)^{1/2}.$$

To simplify the notation, we simply write here and below H_ξ^s when there is no ambiguity.

Operators \mathcal{L} on $L^2(\mathbb{R}^3; \mathbb{C}^4)$ that commute with the translations of $\ell\mathbb{Z}^3$ can be decomposed accordingly into a direct integral of operators \mathcal{L}_ξ acting on L_ξ^2 and defined by

$$\mathcal{L}_\xi(U\phi)_\xi = (U\mathcal{L}\phi)_\xi \text{ for every } \phi \in L^2(\mathbb{R}^3; \mathbb{C}^4), \text{ a.e. } \xi \in Q_\ell^* \quad (2.6)$$

(see [28] for more details). We use the notation $\mathcal{L} = \int_{Q_\ell^*}^\oplus \mathcal{L}_\xi d\xi$, with the shorthand \int_Ω for $\frac{1}{|\Omega|} \int_\Omega$, to refer to this decomposition. In particular, for the free Dirac operator D^0 we have

$$D^0 = \int_{Q_\ell^*}^\oplus D_\xi d\xi. \quad (2.7)$$

where the D_ξ 's are self-adjoint operators on L_ξ^2 with domains H_ξ^1 and form-domains $H_\xi^{1/2}$. Note that $D_\xi^2 = 1 - \Delta_\xi$, where $-\Delta = \int_{Q_\ell^*}^\oplus -\Delta_\xi d\xi$. For every function $\phi_\xi \in H_\xi^1$, the operator D_ξ is also defined by

$$D_\xi \phi_\xi(x) = \sum_{k \in \mathbb{Z}^3} \left[\sum_{j=1}^3 \left(\frac{2\pi}{\ell} k_j + \xi_j \right) \cdot \alpha_j + \beta \right] \widehat{\phi}_\xi(k) e^{i\left(\frac{2\pi k}{\ell} + \xi\right) \cdot x}.$$

In particular,

$$(\phi_\xi, |D_\xi| \phi_\xi)_{L_\xi^2} = \ell^3 \sum_{k \in \mathbb{Z}^3} \sqrt{1 + \left| \xi + \frac{2\pi}{\ell} k \right|^2} |\widehat{\phi}_\xi(k)|^2. \quad (2.8)$$

For almost every $\xi \in Q_\ell^*$, the positive spectrum of D_ξ is composed of a non-decreasing sequence of real eigenvalues $(d_n^+(\xi))_{n \geq 1}$ counted with multiplicity such that

$$d_n^+(\xi) \geq 1, \quad \lim_{n \rightarrow \infty} d_n^+(\xi) = +\infty.$$

In the same manner, the negative spectrum of D_ξ is $(d_n^-(\xi))_{n \geq 1}$ is composed of the non-increasing sequence of real eigenvalues $d_n^-(\xi) = -d_n^+(\xi)$. Finally, one has

$$\bigcup_{\xi \in Q_\ell^*} \sigma(D_\xi) = \bigcup_{\xi \in Q_\ell^*} \bigcup_{n \geq 1} \{d_n^-(\xi), d_n^+(\xi)\} = \sigma(D^0) = (-\infty, -1] \cup [+1, +\infty). \quad (2.9)$$

As in the Hartree–Fock model for crystals [5], the electrons will be modelled by an operator on $L^2(\mathbb{R}^3; \mathbb{C}^4)$, called the one-particle density matrix, that reflects their periodic distribution in the nuclei lattice.

We now introduce various functional spaces for linear operators onto $L^2(Q_\ell; \mathbb{C}^4)$ and for operators onto $L^2(\mathbb{R}^3; \mathbb{C}^4)$ that commute with translations. Let $\mathcal{B}(E)$ be the set of bounded operators on a Banach space E to itself. We use the shorthand $\mathcal{B}(L_\xi^2)$ for $\mathcal{B}(L_\xi^2(Q_\ell; \mathbb{C}^4))$. The space of bounded operators on $\int_{Q_\ell^*}^\oplus L_\xi^2 d\xi = L^2(Q_\ell^*) \otimes L^2(Q_\ell; \mathbb{C}^4)$ which commute with the translations of $\ell\mathbb{Z}^3$ is denoted by Y . It is isomorphic to $L^\infty(Q_\ell^*; \mathcal{B}(L_\xi^2))$. Moreover, for every $h = \int_{Q_\ell^*}^\oplus h_\xi d\xi \in Y$,

$$\|h\|_Y := \text{ess sup}_{\xi \in Q_\ell^*} \|h_\xi\|_{\mathcal{B}(L_\xi^2)} = \|h\|_{\mathcal{B}(L^2(\mathbb{R}^3; \mathbb{C}^4))}$$

(see [28, Theorem XIII.83]). For $s \in [1, \infty)$ and $\xi \in Q_\ell^*$, we define

$$\mathfrak{S}_s(\xi) := \left\{ h_\xi \in \mathcal{B}(L_\xi^2) \mid \text{Tr}_{L_\xi^2}(|h_\xi|^s) < \infty \right\}$$

endowed with the norm

$$\|h_\xi\|_{\mathfrak{S}_s(\xi)} = \left(\text{Tr}_{L_\xi^2}(|h_\xi|^s) \right)^{1/s}.$$

We denote by $\mathfrak{S}_\infty(\xi)$ the subspace of compact operators in $\mathcal{B}(L_\xi^2)$, endowed with the operator norm $\|\cdot\|_{\mathcal{B}(L_\xi^2)}$. Similarly, for $t \in [1, +\infty]$, we define

$$\mathfrak{S}_{s,t} := \left\{ h = \int_{Q_\ell^*}^\oplus h_\xi d\xi \mid h_\xi \in \mathfrak{S}_s(\xi) \text{ a.e. } \xi \in Q_\ell^*, \|h_\xi\|_{\mathfrak{S}_s(\xi)} \in L^t(Q_\ell^*) \right\}$$

endowed with the usual norm of $L^t(Q_\ell^*; \mathfrak{S}_s(\xi))$:

$$\|h\|_{\mathfrak{S}_{s,t}} = \left(\int_{Q_\ell^*} \|h_\xi\|_{\mathfrak{S}_s(\xi)}^t d\xi \right)^{1/t}.$$

In particular $\mathfrak{S}_{\infty,\infty} = L^\infty(Q_\ell^*; \mathfrak{S}_\infty(L_\xi^2)) \subset Y$. We also define

$$X^\alpha(\xi) = \left\{ h \in \mathcal{B}(L_\xi^2) \mid |D_\xi|^{\alpha/2} h_\xi |D_\xi|^{\alpha/2} \in \mathfrak{S}_1(\xi) \right\}$$

endowed with the norm

$$\|h_\xi\|_{X^\alpha(\xi)} = \left\| |D_\xi|^{\alpha/2} h_\xi |D_\xi|^{\alpha/2} \right\|_{\mathfrak{S}_1(\xi)}$$

and

$$X_s^\alpha := \left\{ h = \int_{Q_\ell^*}^\oplus h_\xi d\xi \mid h_\xi \in \mathfrak{S}_1(\xi) \text{ a.e. } \xi \in Q_\ell^*, \int_{Q_\ell^*} \| |D_\xi|^{\alpha/2} h_\xi |D_\xi|^{\alpha/2} \|_{\mathfrak{S}_1(\xi)}^s d\xi < \infty \right\}$$

endowed with the norm

$$\|h\|_{X_s^\alpha} = \left(\int_{Q_\ell^*} \| |D_\xi|^{\alpha/2} h_\xi |D_\xi|^{\alpha/2} \|_{\mathfrak{S}_1(\xi)}^s d\xi \right)^{1/s} = \| |D^0|^{\alpha/2} h |D^0|^{\alpha/2} \|_{\mathfrak{S}_{1,s}}.$$

For any two functional spaces A and B the norm of the intersected space is defined by

$$\|\gamma\|_{A \cap B} = \max\{\|\gamma\|_A, \|\gamma\|_B\}.$$

For future convenience, we use the notation $X(\xi)$ for $X^1(\xi)$, and we set $X := X_1^1$. The functional spaces $\mathfrak{S}_{1,1}$, X and Y will play an essential role in the whole paper, while the functional space $\mathfrak{S}_{1,\infty}$ and its subspace X_∞^2 are mainly used in Section 6. In addition, we will also use the functional space $\mathfrak{S}_{\infty,1}$ in Section 6 since $\mathfrak{S}_{1,\infty}$ is its dual space.

Definition 2.2 (Periodic one-particle density matrices). *We denote by \mathcal{T} the set of Q_ℓ -periodic one-particle density matrices*

$$\mathcal{T} := \{ \gamma \in X \mid \gamma^* = \gamma, 0 \leq \gamma \leq 1_{L^2(\mathbb{R}^3)} \} \subset X \cap Y.$$

Remark 2.3 (Projectors). *According to [1, 14, 22] any minimizer of the Hartree–Fock model (both for the molecules and crystals) is a projector. However we do not know whether minimizers of Dirac–Fock models are projectors in general.*

Remark 2.4. *For $\gamma \in \mathcal{T}$ and for almost every ξ in Q_ℓ^* , the operator γ_ξ is compact on L_ξ^2 and admits a complete set of eigenfunctions $(u_n(\xi, \cdot))_{n \geq 1}$ in L_ξ^2 (actually lying in $H_\xi^{1/2}$), corresponding to a non-decreasing sequence of eigenvalues $0 \leq \lambda_n(\xi) \leq 1$ (counted with their multiplicity). This is expressed as*

$$\gamma_\xi = \sum_{n \geq 1} \lambda_n(\xi) |u_n(\xi, \cdot)\rangle \langle u_n(\xi, \cdot)|, \quad (u_n(\xi, \cdot), u_m(\xi, \cdot))_{L_\xi^2} = \delta_{n,m} \quad (2.10)$$

where $|u\rangle \langle u|$ denotes the projector onto the vector space spanned by the function u . Equivalently, for almost every ξ in Q_ℓ^* and for any $(x, y) \in \mathbb{R}^3 \times \mathbb{R}^3$, the Hilbert–Schmidt kernel writes

$$\gamma_\xi(x, y) = \sum_{n \geq 1} \lambda_n(\xi) u_n(\xi, x) u_n^*(\xi, y). \quad (2.11)$$

In the above equation, the superscript $*$ refers to the duality in L^2_ξ . In particular $\gamma_\xi(\cdot, \cdot)$ is a 4×4 complex matrix in $\mathcal{M}_4(\mathbb{C})$, and for every function $\varphi \in L^2_\xi$,

$$(\gamma_\xi \varphi)(x) = \int_{Q_\ell} \gamma_\xi(x, y) \varphi(y) dy = \sum_{n \geq 1} \lambda_n(\xi) u_n(\xi, x) \int_{Q_\ell} u_n^*(\xi, y) \varphi(y) dy.$$

By definition of the trace of an operator,

$$\mathrm{Tr}_{L^2_\xi}(\gamma_\xi) = \sum_{n \geq 1} \lambda_n(\xi).$$

This allows us to define the trace per unit cell as

$$\widetilde{\mathrm{Tr}}_{L^2}(\gamma) := \int_{Q_\ell^*} \mathrm{Tr}_{L^2_\xi}(\gamma_\xi) d\xi,$$

where the \sim reminds us that γ is not trace-class on $L^2(\mathbb{R}^3)$.

Definition 2.5 (Integral kernel and electronic density). *Let γ belong to \mathcal{T} . Then we can define in a unique way an integral kernel $\gamma(\cdot, \cdot) \in L^2(Q_\ell \times \mathbb{R}^3) \cap L^2(\mathbb{R}^3 \times Q_\ell)$ with $\gamma(\cdot + k, \cdot + k) = \gamma(\cdot, \cdot)$ for any $k \in \mathbb{Z}^3$ and a Q_ℓ -periodic density ρ_γ associated to γ by*

$$\gamma(x, y) = \int_{Q_\ell^*} \gamma_\xi(x, y) d\xi \quad (2.12)$$

and

$$\rho_\gamma(x) = \int_{Q_\ell^*} \mathrm{Tr}_4 \gamma_\xi(x, x) d\xi, \quad (2.13)$$

where the notation Tr_4 stands for the trace of a 4×4 matrix. The function ρ_γ is non-negative and belongs to $L^1(Q_\ell; \mathbb{R})$. Indeed, using the decomposition (2.11), we have

$$\rho_\gamma(x) = \int_{Q_\ell^*} \sum_{n=1}^{\infty} \lambda_n(\xi) |u_n(\xi, x)|^2 d\xi \quad (2.14)$$

and

$$\int_{Q_\ell} \rho_\gamma(x) dx = \int_{Q_\ell^*} \sum_{n=1}^{\infty} \lambda_n(\xi) d\xi = \int_{Q_\ell^*} \mathrm{Tr}_{L^2_\xi}(\gamma_\xi) d\xi.$$

In the physical setting we are interested in, the value of the above integral is the number of electrons per cell q .

By the Cauchy–Schwarz inequality, it is easily checked that

$$|\gamma(x, y)|^2 \leq \rho_\gamma(x) \rho_\gamma(y), \quad \text{a.e. } x, y \in \mathbb{R}^3. \quad (2.15)$$

Note that, when h is a Q_ℓ -periodic trace-class operator but is not necessarily a positive operator, we still may define ρ_h with the help of (2.13), but (2.15) becomes $|h(x, y)|^2 \leq \rho_{|h|}(x) \rho_{|h|}(y)$ where $|h| = \sqrt{h^* h}$.

We can now introduce the periodic Dirac–Fock functional.

2.2 The periodic Dirac–Fock model

We introduce the following set of periodic density matrices :

$$\Gamma_q := \{ \gamma \in \mathcal{T} \mid \|\gamma\|_{\mathfrak{S}_{1,1}} = q \}$$

and

$$\Gamma_{\leq q} := \{ \gamma \in \mathcal{T} \mid \|\gamma\|_{\mathfrak{S}_{1,1}} \leq q \}.$$

When q is an integer, Γ_q and $\Gamma_{\leq q}$ are the sets of all Dirac–Fock states of a system of exactly q , respectively at most q , electrons per unit cell.

For $\gamma \in \Gamma_{\leq q}$, we define the periodic Dirac–Fock functional

$$\begin{aligned} \mathcal{E}^{DF}(\gamma) &= \int_{Q_\ell^*} \text{Tr}_{L_\xi^2} [D_\xi \gamma_\xi] d\xi - \alpha z \int_{Q_\ell} G_\ell(x) \rho_\gamma(x) dx \\ &\quad + \frac{\alpha}{2} \iint_{Q_\ell \times Q_\ell} \rho_\gamma(x) G_\ell(x-y) \rho_\gamma(y) dx dy \\ &\quad - \frac{\alpha}{2} \iint_{Q_\ell^* \times Q_\ell^*} d\xi d\xi' \iint_{Q_\ell \times Q_\ell} \text{Tr}_4[\gamma_\xi(x, y) \gamma_{\xi'}(y, x)] W_\ell^\infty(\xi - \xi', x - y) dx dy. \end{aligned} \quad (2.16)$$

In the above definition of the energy functional, the so-called fine structure constant α is a dimensionless positive constant (the physical value is approximately $1/137$). Note that $D_\xi \gamma_\xi$ is not a trace-class operator, so $\text{Tr}_{L_\xi^2} [D_\xi \gamma_\xi]$ is not really a trace, it is just a notation for the rigorous mathematical object $\text{Tr}_{L_\xi^2} [|D_\xi|^{1/2} \gamma_\xi |D_\xi|^{1/2} \text{sign}(D_\xi)]$. We will make this abuse of notation throughout the paper.

The last term in (2.16) is called the “exchange term”. The potential W_ℓ^∞ that enters its definition is defined by

$$W_\ell^\infty(\eta, x) = \sum_{k \in \mathbb{Z}^3} \frac{e^{i\ell k \cdot \eta}}{|x + \ell k|} = \frac{4\pi}{\ell^3} \sum_{k \in \mathbb{Z}^3} \frac{1}{|\frac{2\pi k}{\ell} - \eta|^2} e^{i(\frac{2\pi k}{\ell} - \eta) \cdot x} \quad (2.17)$$

(see [5] for a formal derivation of the 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 . For every $\gamma \in \Gamma_{\leq q}$, we now define the mean-field periodic Dirac operator

$$D_\gamma = \int_{Q_\ell^*}^\oplus D_{\gamma, \xi} d\xi \quad \text{with} \quad D_{\gamma, \xi} := D_\xi - \alpha z G_\ell + \alpha V_{\gamma, \xi}$$

where

$$V_{\gamma, \xi} = \rho_\gamma * G_\ell - W_{\gamma, \xi} \quad (2.18)$$

with

$$\rho_\gamma * G_\ell(x) = \int_{Q_\ell} G_\ell(y-x) \rho_\gamma(y) dy = \widetilde{\text{Tr}}_{L^2} [G_\ell(\cdot - x) \gamma] \quad (2.19)$$

and

$$W_{\gamma, \xi} \psi_\xi(x) = \int_{Q_\ell^*} d\xi' \int_{Q_\ell} W_\ell^\infty(\xi' - \xi, x - y) \gamma_{\xi'}(x, y) \psi_\xi(y) dy.$$

(In (2.19) we keep the notation $\cdot * \cdot$ for the convolution of periodic functions on Q_ℓ .)

The relation between \mathcal{E}^{DF} and D_γ is the following : If γ and $\gamma + h$ are in $\Gamma_{\leq q}$ with h in \mathcal{T} , then the right derivative of $t \mapsto \mathcal{E}^{DF}(\gamma + th)$ at $t = 0$ is $\int_{Q_\ell^*} \text{Tr}_{L_\xi^2} (D_{\gamma, \xi} h_\xi) d\xi$.

Our goal is to define the ground-state despite the fact that this functional is strongly indefinite on $\Gamma_{\leq q}$, due to the unboundedness of the Dirac operator D^0 .

2.3 Ground-state energy and main result

We follow Dirac’s interpretation of the negative energy states of Dirac–Fock models: such states are supposed to be occupied by virtual electrons that form the Dirac sea. Therefore, by the Pauli exclusion principle, the states of physical electrons are orthogonal to all the negative energy states. The ground-energy and state should thus be defined on the positive spectral subspaces of the corresponding Dirac–Fock operator. Let

$$P_\gamma^\pm = \int_{Q_\ell^*}^\oplus P_{\gamma, \xi}^\pm d\xi \quad \text{with} \quad P_{\gamma, \xi}^\pm := 1_{\mathbb{R}_\pm}(D_{\gamma, \xi}).$$

Note that by definition $P_{0, \xi}^\pm = 1_{\mathbb{R}_\pm}(D_\xi - \alpha z G_\ell)$. We define the set

$$\Gamma_q^+ := \{ \gamma \in \Gamma_q \mid \gamma = P_\gamma^+ \gamma P_\gamma^+ \} \quad (2.20)$$

and the ground-state energy

$$I_q := \inf_{\gamma \in \Gamma_q^+} \mathcal{E}^{DF}(\gamma). \quad (2.21)$$

We need the following assumption.

Assumption 2.6. Let $q^+ := \max\{q, 1\}$, $\kappa := \alpha(C_{Gz} + C'_{EE}q^+)$ and $A := \frac{\alpha}{2}C_{EE}(1 - \kappa)^{-1/2}\lambda_0^{-1/2}$. We demand that

1. $\kappa < 1 - \frac{\alpha}{2}C_{EE}q^+$;
2. $2A\sqrt{\max\{(1 - \kappa - \frac{\alpha}{2}C_{EE}q^+)^{-1}(1 - \kappa)^{-1}c^*(q + 1)q, 1\}}q^+ < 1$.

The positive constants C_G , C_{EE} , C'_{EE} and λ_0 are defined respectively in Lemmas 4.1, 4.7 and 4.10 below.

Our main result is the following.

Theorem 2.7 (Existence of a minimizer). *When α , q , z and ℓ satisfy Assumption 2.6, there exists $\gamma_* \in \Gamma_q^+$ such that*

$$\mathcal{E}^{DF}(\gamma_*) = I_q = \min_{\gamma \in \Gamma_q^+} \mathcal{E}^{DF}(\gamma). \quad (2.22)$$

Besides, γ_* solves the following nonlinear self-consistent equation

$$\gamma = 1_{[0, \nu)}(D_\gamma) + \delta \quad (2.23)$$

where $0 \leq \delta \leq 1_{\{\nu\}}(D_\gamma)$ and $0 \leq \nu \leq (1 - \kappa)^{-1}c^*(q + 1)$, with $\kappa = \kappa(z, q, \ell, \alpha) > 0$ being defined in Assumption 2.6 below and

$$c^*(k) := \sup_{\xi \in Q_\ell^*} d_k^+(\xi) \quad (2.24)$$

with the $d_k^+(\xi)$'s appearing in (2.9).

Remark 2.8. *In Solid State Physics, the length of the unit cell is about a few Ångströms. In our system of units, $\hbar = m = c = 1$, thus $\alpha \approx \frac{1}{137}$ and $\ell \approx 1000$. Under the condition $q = z$ for electrical neutrality, Assumption 2.6 is satisfied for $q \leq 17$. The proof is detailed in Appendix D. Our estimates are far from optimal : The ideas of this paper are expected to apply to higher values of q .*

3 Sketch of proof

We are convinced that the constraint set Γ_q^+ is not convex, and we are not able to prove that it is closed for the weak-* topology, and this is the source of considerable difficulties. Mimicking [29], we shall use a retraction technique as for the Dirac–Fock model for atoms and molecules. This imposes to search the ground-state in the set $\Gamma_{\leq q}^+$ defined by

$$\Gamma_{\leq q}^+ := \{\gamma \in \Gamma_{\leq q} \mid \gamma = P_\gamma^+ \gamma P_\gamma^+\}.$$

However, under above constraint, the minimizers may not be situated in Γ_q^+ . To overcome this problem, we next subtract a penalization term $\epsilon_P \widetilde{\text{Tr}}_{L^2}(\gamma)$, for some parameter $\epsilon_P > 0$ to be chosen later, and first study the minimization problem for the penalized functional with relaxed constraint :

$$I_{\leq q} := \min_{\gamma \in \Gamma_{\leq q}^+} \left[\mathcal{E}^{DF}(\gamma) - \epsilon_P \widetilde{\text{Tr}}_{L^2}(\gamma) \right].$$

We prove below that, when ϵ_P is sufficiently large, every minimizer of problem $I_{\leq q}$ is indeed in Γ_q^+ , thus is a minimizer of I_q (Corollary 3.3).

For the penalized problem, the analogues to Assumption 2.6 and Theorem 2.7 read as follows.

Assumption 3.1. Let $q^+ = \max\{q, 1\}$, $\kappa := \alpha(C_{Gz} + C'_{EE}q^+)$ and $A := \frac{\alpha}{2}C_{EE}(1 - \kappa)^{-1/2}\lambda_0^{-1/2}$. We assume that

1. $\kappa < 1 - \frac{\alpha}{2} C_{EE} q^+$;
2. $2A\sqrt{\max\{(1 - \kappa - \frac{\alpha}{2} C_{EE} q^+)^{-1} \epsilon_P q, 1\}} q^+ < 1$.

Theorem 3.2 (Existence of a minimizer for the penalized problem). *We assume that Assumption 3.1 on q, z, ϵ_P holds. If $\epsilon_P > (1 - \kappa)^{-1} c^*(q + 1)$, then there exists $\gamma_* \in \Gamma_{\leq q}^+$ such that*

$$\mathcal{E}^{DF}(\gamma_*) - \epsilon_P \widetilde{\text{Tr}}_{L^2}(\gamma_*) = I_{\leq q}. \quad (3.1)$$

Besides, $\widetilde{\text{Tr}}_{L^2}(\gamma_*) = \int_{Q_\ell^*} \text{Tr}_{L_\xi^2}(\gamma_{*,\xi}) d\xi = q$ and γ_* solves the following nonlinear self-consistent equation

$$\gamma = 1_{[0,\nu]}(D_\gamma) + \delta \quad (3.2)$$

where $0 \leq \delta \leq 1_{\{\nu\}}(D_\gamma)$ and ν is the Lagrange multiplier due to the charge constraint $\text{Tr}_{L^2}(\gamma) \leq q$ satisfying $0 \leq \nu \leq (1 - \kappa)^{-1} c^*(q + 1)$.

Corollary 3.3 (Existence of a minimizer for the original problem). *We assume that Assumption 2.6 on q, z holds. Then, there is a constant $\epsilon_P > (1 - \kappa)^{-1} c^*(q + 1)$ such that Assumption 3.1 is satisfied. Therefore I_q is achieved and the minimizer γ_* solves (2.23).*

Proof of Corollary 3.3. The first claim is obvious: Under Assumption 2.6 on q, z , there is a small constant $\epsilon > 0$ such that q, z and $\epsilon_P = (1 - \kappa)^{-1} c^*(q + 1) + \epsilon$ satisfy Assumption 3.1. By Theorem 3.2, since $\epsilon_P > (1 - \kappa)^{-1} c^*(q + 1)$, any minimizer γ_* of $I_{\leq q}$ lies in Γ_q^+ . Thus,

$$\begin{aligned} \mathcal{E}^{DF}(\gamma_*) - \epsilon_P q &= \mathcal{E}^{DF}(\gamma_*) - \epsilon_P \widetilde{\text{Tr}}_{L^2}(\gamma_*) \geq \min_{\gamma \in \Gamma_q^+} \left[\mathcal{E}^{DF}(\gamma) - \epsilon_P \widetilde{\text{Tr}}_{L^2}(\gamma) \right] \\ &= \min_{\gamma \in \Gamma_q^+} [\mathcal{E}^{DF}(\gamma)] - \epsilon_P q \geq I_{\leq q} = \mathcal{E}^{DF}(\gamma_*) - \epsilon_P q. \end{aligned}$$

Therefore, all inequalities in the above string of inequalities are equalities, and

$$\mathcal{E}^{DF}(\gamma_*) = \min_{\gamma \in \Gamma_q^+} \mathcal{E}^{DF}(\gamma) = I_q. \quad \square$$

We therefore focus on the proof of Theorem 3.2. Before going further, we explain our difficulties and method by comparing with the Hartree–Fock ones [5]. Indeed, the method used in [5] is based on some properties of the Schrödinger operator $-\Delta$:

1. This operator is non-negative. Hence the Hartree–Fock model for crystals is well-defined and the kinetic energy is weakly lower semi-continuous w.r.t. the density matrix ;
2. The exchange potential W_ℓ^∞ is rather easily controlled by the Schrödinger operator $-\Delta$.

In [5], these properties allow to deduce bounds on the minimizing sequence of density matrices w.r.t. the ξ, x and y variables, and to pass to the limit in the different terms of the energy functional, in particular in the exchange term which is the most intricate one. In the proof, the strong convergence of the density matrix kernels $\gamma_n(x, y) = \int_{Q_\ell^*} \gamma_{n,\xi}(x, y) d\xi$ plays an important role. In addition, the charge constraint in the periodic Hartree–Fock model is linear with respect to the density, and there is no possible loss of charge in passing to the limit.

In the Dirac–Fock model for crystals, two additional difficulties occur. First of all, the Dirac operator does not control the potential energy terms, which are of the same order. Secondly, the convergence of the nonlinear constraint $\int_{Q_\ell^*} P_{\gamma,\xi}^+ \gamma_\xi d\xi = \int_{Q_\ell^*} \gamma_\xi d\xi$ requires stronger compactness properties of the sequence of density matrices with respect to the ξ variable. Therefore the proof of existence of minimizers in the periodic Hartree–Fock setting cannot be applied *mutatis mutandis*. On the other hand, compared to the Dirac–Fock model for atoms and molecules, we suffer from a serious compactness issue in the ξ -variable. The functional space $\mathfrak{S}_{1,1}$ is natural to give a sense to the energy functional and to the constraints, but the weak-convergence of minimizing sequences in $\mathfrak{S}_{1,1}$ is not strong enough to deal with exchange term and the non-linear constraints. The whole paper (except Section 5 about the retraction) is devoted to solving the difficulties arising from the integration w.r.t. the ξ variable.

Our strategy rather relies on the spectral analysis of the periodic Dirac-Fock operator, which is totally new for the proof of existence of minimizers in the periodic case. In Lemma 4.12 together with Lemma 5.1 (see also Remark 4.13), we can prove that any minimizer of $I_{\leq q}$ actually lies in $\mathfrak{S}_{1,\infty}$, and is situated in \overline{B}_{R_0} where we have defined

$$B_R := \{\gamma \in X \cap Y \mid \|\gamma\|_{\mathfrak{S}_{1,\infty}} < R\} \quad (3.3)$$

and

$$R_0 := q + M \quad \text{with } M \text{ being defined in Lemma 4.11 below.} \quad (3.4)$$

In particular, any minimizer γ_* satisfies $q_*(\xi) := \text{Tr}_{L^2_\xi}(\gamma_{*,\xi}) \leq R_0$ for every $\xi \in Q_\ell^*$. We may therefore assume that, for any minimizing sequence, if $q_n(\xi) = \text{Tr}_{L^2_\xi}(\gamma_{n,\xi})$, then $\gamma_{n,\xi}, |q_n(\xi)| \leq R$ for any $R > R_0$ independent of n and ξ , at least for n large enough. In particular, by dominated convergence theorem, $q_n(\xi) \rightarrow q_*(\xi)$ strongly in $L^1(Q_\ell^*)$ (up to subsequences).

The main idea in the proof of the existence of minimizers of $I_{\leq q}$ is therefore to use the fact that any minimizer will be situated in \overline{B}_{R_0} , and then in any set B_R with $R > R_0$. Then, thanks to Lemma 6.2, for any minimizing sequence γ_n of $I_{\leq q}$, we can find another minimizing sequence $\tilde{\gamma}_n$ with better regularity ; that is $\tilde{\gamma}_n \in \overline{B}_{R_0}$. Setting an equivalent minimization problem in a ball B_R with $R > R_0$ helps considerably to overcome the difficulty in passing to the limit in the constraint $f_{Q_\ell^*}^\oplus P_{\gamma,\xi}^+ \gamma_\xi d\xi = f_{Q_\ell^*}^\oplus \gamma_\xi d\xi$. In addition, the exchange term is well-controlled for density matrices in this set. Moreover, it turns out that the minimizers in this set do not saturate the constraint $\|\gamma\|_{\mathfrak{S}_{1,\infty}} < R$.

More precisely, existence of minimizers for the penalized problem will be a consequence of the followings.

Proposition 3.4 (Existence of a minimizer in the set B_R). *Let $R_0 := q + M$ where M is defined in Lemma 4.11 below. Under Assumption 3.1, if $\epsilon_P > (1 - \kappa)^{-1}c^*(q + 1)$ and for any $R > R_0$, there exists γ_* in $\Gamma_{\leq q}^+ \cap B_R$ such that*

$$I_{\leq q,R} := \min_{\gamma \in \Gamma_{\leq q}^+ \cap B_R} \left[\mathcal{E}^{DF}(\gamma) - \epsilon_P \widetilde{\text{Tr}}_{L^2}(\gamma) \right] = \mathcal{E}^{DF}(\gamma_*) - \epsilon_P \widetilde{\text{Tr}}_{L^2}(\gamma_*). \quad (3.5)$$

Besides, $\gamma_* \in \overline{B}_{R_0}$ and $\widetilde{\text{Tr}}_{L^2}(\gamma_*) = q$. Furthermore, γ_* solves the following nonlinear self-consistent equation

$$\gamma = 1_{[0,\nu]}(D_\gamma) + \delta \quad (3.6)$$

where $0 \leq \delta \leq 1_{\{\nu\}}(D_\gamma)$ and ν is the Lagrange multiplier due to the charge constraint $\widetilde{\text{Tr}}_{L^2}(\gamma) \leq q$ satisfying $0 \leq \nu \leq (1 - \kappa)^{-1}c^*(q + 1)$.

Theorem 3.2 is a direct consequence of the following.

Corollary 3.5 (Existence of a minimizer for the penalized problem). *We assume that $\epsilon_P > (1 - \kappa)^{-1}c^*(q + 1)$ and that Assumption 3.1 holds. Then $I_{\leq q}$ is achieved. Any minimizer γ_* of (3.5) is a minimizer of $I_{\leq q}$. It satisfies $\widetilde{\text{Tr}}_{L^2}(\gamma_*) = q$ and γ_* lies in $\mathfrak{S}_{1,\infty}$.*

Proof of Corollary 3.5. First of all, since $I_{\leq q} \leq I_{\leq q,R}$ for any $R > R_0$, we have

$$I_{\leq q} \leq \inf_{R > R_0} I_{\leq q,R}. \quad (3.7)$$

As $R \mapsto I_{\leq q,R}$ is non-increasing, we have $\inf_{R > R_0} I_{\leq q,R} = \lim_{R \rightarrow +\infty} I_{\leq q,R}$. Let $(\gamma_n)_n$ in $\Gamma_{\leq q}^+$ be a minimizing sequence of $I_{\leq q}$. It is easy to see that $\gamma_n \in \bigcup_{R > R_0} (\Gamma_{\leq q}^+ \cap B_R)$ since $\Gamma_{\leq q}^+ = \bigcup_{R > R_0} (\Gamma_{\leq q}^+ \cap B_R)$. Thus,

$$\inf_{R > R_0} I_{\leq q,R} \leq \mathcal{E}^{DF}(\gamma_n) - \epsilon_P \widetilde{\text{Tr}}_{L^2}(\gamma_n).$$

Taking $n \rightarrow \infty$ and using (3.7), we have

$$I_{\leq q} = \inf_{R > R_0} I_{\leq q,R} = \lim_{R \rightarrow +\infty} I_{\leq q,R}.$$

According to Proposition 3.4, for any $R > R_0$, any minimizer $\gamma_{R,*}$ of $I_{\leq q,R}$ is actually located in \overline{B}_{R_0} . Therefore, $I_{\leq q,R} = I_{\leq q,R'}$ for any $R, R' > R_0$. Thus $I_{\leq q} = \lim_{R' > R_0} I_{\leq q,R'} = I_{\leq q,R}$ for any $R > R_0$. This implies that any minimizer of $I_{\leq q,R}$, for $R > R_0$, is a minimizer of $I_{\leq q}$. This ends the proof. \square

Organisation of the paper. Next sections are devoted to the proof of Proposition 3.4. Our paper is organized as follows.

In Section 4, we collect some fundamental estimates on the potentials G_ℓ and W_ℓ^∞ . In Subsection 4.2, we study the spectral properties of the Dirac–Fock operators $D_{\gamma,\xi}$ for every $\xi \in Q_\ell^*$. Relying on them, we study in Subsection 4.3 the properties of minimizers of a linear Dirac–Fock problem. Finally, we collect the first estimates on minimizing sequences.

In Section 5, we study the linearization problem associated to (3.5). We conclude that the minimizers of (3.5) are in $B_{R_0} \cap \Gamma_q^+$ and solve a self-consistent equation. In Hartree–Fock type models for molecules [24] or crystals [14], it is a standard fact that the approximate minimizers are also approximate ground states of their mean-field Hamiltonian. The proof relies on the convexity of the constraint set. However, in Dirac–Fock model (both for molecules and crystals), the constraint set $\Gamma_{\leq q}^+$ is more sophisticated. By using a retraction technique, a similar result has been recently proved by one of us in the Dirac–Fock model for molecules [29]. Adapting the technique in [29], we build a regular map $\theta : \mathcal{V} \rightarrow \mathcal{V}$ on a relatively open neighborhood \mathcal{V} of the minimizing sequence of (3.5) in $\Gamma_{\leq q}$ such that $\theta(\gamma) = P_{\theta(\gamma)}^+ \theta(\gamma) P_{\theta(\gamma)}^+$. Next, we consider an equivalent minimization problem with locally convex constraint; namely

$$\min_{\gamma \in \mathcal{V} \cap B_R} \mathcal{E}^{DF}(\theta(\gamma)) - \epsilon_P \widetilde{\text{Tr}}_{L^2}[\theta(\gamma)].$$

In Section 6, we build an approximate minimizing sequence with better regularity and convergence properties. Finally, we conclude on the convergence of a minimizing sequence on the set B_R and the existence of minimizer; that is, the proof of Proposition 3.4.

Assumption 2.6 involves optimal constants in Hardy-type inequalities introduced in Subsection 4.1. Therefore, in Appendix A–C, we prove Lemma 4.1, Lemma 4.5 and Lemma 4.7 respectively. Finally, in Appendix D, we calculate the maximum number of electrons per cell allowed by the model, relying on approximate values of the constants obtained in Appendices A–C.

4 Fundamental estimates

In this section, we give Hardy-type inequalities for the periodic Coulomb potential and provide estimates on the interaction potential between electrons in crystals. Then we study the spectrum of the periodic self-consistent Dirac–Fock operators. Finally, we derive properties of minimizing sequences of the linearized and the penalized problem from the spectral analysis.

4.1 Hardy-type estimates on the periodic Coulomb potential

First of all, and this is a major difference with the usual Coulomb potential $\frac{1}{|x|}$ in \mathbb{R}^3 , the periodic Coulomb potential G_ℓ may not be positive, since it is defined up to constant, but it is bounded from below (see Lemma A.1). Nevertheless, it is the kernel of a positive operator on $L^2(Q_\ell)$ in virtue of (2.3). Moreover, we have the following Hardy-type estimates concerning the periodic potential G_ℓ .

Lemma 4.1 (Hardy-type inequalities for the periodic Coulomb potential). *There exist positive constants $C_H = C_H(\ell) > 0$ that only depends on ℓ and such that*

$$G_\ell \leq |G_\ell| \leq C_H |D^0| \tag{4.1}$$

in the sense of operators on $L^2(Q_\ell^*) \otimes L^2(Q_\ell; \mathbb{C}^4)$.

Moreover, there exists a positive constant $C_G = C_G(\ell)$ with $C_G \geq C_H$ that only depends on ℓ and such that

$$\|G_\ell |D^0|^{-1}\|_Y = C_G. \tag{4.2}$$

Remark 4.2. In (4.1), the inequality $A \leq B$ is equivalent to : For almost every $\xi \in Q_\ell^*$, $A_\xi \leq B_\xi$ in the sense of operators on L_ξ^2 .

Remark 4.3. The constant $C_G(\ell)$ is estimated in (A.4) in Appendix A below. While it is far from optimal when ℓ is small, it converges to 2 when ℓ goes to infinity; that is, to the value of the optimal constant for the Coulomb potential on the whole space. By interpolation,

$$C_H \leq C_G. \tag{4.3}$$

Therefore, (4.1) holds with C_H being replaced by C_G . However, C_H is expected to converge to $\pi/2$ as ℓ goes to infinity; that is, to the best constant in the Kato–Herbst Inequality on the whole space [17, 20].

A by-product of Lemma 4.1 is the following.

Corollary 4.4 (Estimates on the direct term). *For any $\gamma \in X$, we have*

$$\|\rho_\gamma * G_\ell\|_Y \leq C_H \|\gamma\|_X \quad (4.4)$$

and

$$\|(\rho_\gamma * G_\ell) |D^0|^{-1}\|_Y \leq C_G \|\gamma\|_{\mathfrak{S}_{1,1}}. \quad (4.5)$$

Proof. For every $x \in \mathbb{R}^3$ and $\gamma \in X$

$$\begin{aligned} |\rho_\gamma * G_\ell(x)| &= \left| \int_{Q_\ell^*} \text{Tr}_{L_\xi^2} [G_\ell(x - \cdot) \gamma_\xi(\cdot)] d\xi \right| \\ &\leq \int_{Q_\ell^*} \left| \text{Tr}_{L_\xi^2} [|D_\xi|^{-1/2} |G_\ell(x - \cdot)| |D_\xi|^{-1/2} |D_\xi|^{1/2} \gamma_\xi |D_\xi|^{1/2}] \right| d\xi \\ &\leq \int_{Q_\ell^*} \left\| |D_\xi|^{-1/2} |G_\ell(x - \cdot)| |D_\xi|^{-1/2} \right\|_{\mathcal{B}(L_\xi^2)} \left\| |D_\xi|^{1/2} \gamma_\xi |D_\xi|^{1/2} \right\|_{\mathfrak{S}_1(\xi)} d\xi \leq C_H \|\gamma\|_X. \end{aligned}$$

Indeed, the bound (4.1) in Lemma 4.1 yields

$$\left\| |G_\ell(\cdot - x)|^{1/2} |D_\xi|^{-1/2} \right\|_Y \leq (C_H)^{1/2}$$

uniformly in x . We now turn to the proof of (4.5). For every $\xi \in Q_\ell^*$ and $\varphi_\xi \in L_\xi^2$, we have

$$\begin{aligned} \|(\rho * G_\ell) |D_\xi|^{-1} \varphi_\xi\|_{L_\xi^2} &\leq \int_{Q_\ell} |\rho(x)| \|G_\ell(\cdot - x) |D_\xi|^{-1} \varphi_\xi\|_{L_\xi^2} dx \\ &\leq \sup_{x \in \mathbb{R}^3} \|G_\ell(\cdot - x) |D_\xi|^{-1} \varphi_\xi\|_{L_\xi^2} \int_{Q_\ell} |\rho(x)| dx \leq C_G \|\gamma\|_{\mathfrak{S}_{1,1}} \|\varphi_\xi\|_{L_\xi^2}. \end{aligned} \quad (4.6)$$

In (4.6), we have used the bound (4.2) in Lemma 4.1 and the obvious fact that it remains true for $G_\ell(\cdot - x)$ for any $x \in \mathbb{R}^3$. \square

Now, we consider the exchange term. We can separate the singularities of W_ℓ^∞ with respect to $\eta \in 2Q_\ell^*$ and $x \in 2Q_\ell$ as follows

$$W_\ell^\infty(\eta, x) = W_{\geq m, \ell}(\eta, x) + W_{< m, \ell}(\eta, x), \quad \forall m \in \mathbb{N}, m \geq 2, \quad (4.7)$$

with

$$W_{\geq m, \ell}(\eta, x) = \frac{4\pi}{\ell^3} \sum_{\substack{|k|_\infty \geq m \\ k \in \mathbb{Z}^3}} \frac{1}{|\frac{2\pi k}{\ell} - \eta|^2} e^{i(\frac{2\pi k}{\ell} - \eta) \cdot x}$$

and

$$W_{< m, \ell}(\eta, x) = \frac{4\pi}{\ell^3} \sum_{\substack{|k|_\infty < m \\ k \in \mathbb{Z}^3}} \frac{1}{|\frac{2\pi k}{\ell} - \eta|^2} e^{i(\frac{2\pi k}{\ell} - \eta) \cdot x}$$

where $|k|_\infty := \max\{|k_1|, |k_2|, |k_3|\}$. It is easy to see that the singularity of $W_{< m, \ell}$ behaves like $\frac{1}{|\eta|^2}$, and we will show in Appendix B that the singularity of $W_{\geq m, \ell}(\eta, x)$ behaves like $\frac{1}{|x|}$ or equivalently $G_\ell(x)$. Then we have the following estimates.

Lemma 4.5 (Estimates on $W_{\gamma, \xi}$). *There exist positive constants $C_W = C_W(\ell)$, $C'_W = C'_W(\ell)$ and $C''_W = C''_W(\ell)$ that only depend on ℓ such that*

$$\|W_\gamma\|_Y \leq C_W \|\gamma\|_{X \cap Y} \quad \text{if } \gamma \in X \cap Y, \quad (4.8)$$

$$\|W_\gamma\|_Y \leq C''_W (\|\gamma\|_X + \|\gamma\|_{\mathfrak{S}_{1, \infty}}^{3/4} \|\gamma\|_{\mathfrak{S}_{1,1}}^{1/4}) \quad \text{if } \gamma \in X \cap \mathfrak{S}_{1, \infty}, \quad (4.9)$$

$$\|W_\gamma |D^0|^{-1}\|_Y \leq C'_W \|\gamma\|_{\mathfrak{S}_{1,1} \cap Y} \quad \text{if } \gamma \in \mathfrak{S}_{1,1} \cap Y. \quad (4.10)$$

Remark 4.6. The constants C_W , C'_W and C''_W are estimated in (B.15).

Gathering together Lemma 4.1, Corollary 4.4 and Lemma 4.5 we can get some rough estimates on the self-consistent potential $V_{\gamma,\xi}$ defined in (2.18). We can obtain much better estimates by a careful study of the structure of $V_{\gamma,\xi}$.

Lemma 4.7 (Estimates on $V_{\gamma,\xi}$). *There exist positive constants $C_{EE} = C_{EE}(\ell) > 0$ and $C'_{EE} = C'_{EE}(\ell) > 0$ that only depend on ℓ and such that*

$$\|V_{\gamma,\xi}\|_Y \leq C_{EE} \|\gamma\|_{X \cap Y} \quad (4.11)$$

and

$$\|V_{\gamma,\xi} |D_\xi|^{-1}\|_Y \leq C'_{EE} \|\gamma\|_{\mathfrak{S}_{1,1} \cap Y}. \quad (4.12)$$

For any $\psi_\xi \in H_\xi^{1/2}$,

$$\left| (\psi_\xi, V_{\gamma,\xi} \psi_\xi)_{L_\xi^2} \right| \leq C_{EE} \|\gamma\|_{\mathfrak{S}_{1,1} \cap Y} \|\psi_\xi\|_{H_\xi^{1/2}}^2 \quad (4.13)$$

Furthermore, if $\gamma \geq 0$, for any $\psi \in L_\xi^2$,

$$-C''_{EE} \|\gamma\|_{\mathfrak{S}_{1,1} \cap Y} \|\psi\|_{L_\xi^2}^2 \leq (\psi, V_{\gamma,\xi} \psi)_{L_\xi^2}. \quad (4.14)$$

Remark 4.8. The constants C_{EE} , C'_{EE} and C''_{EE} are estimated in (C.7), (C.5) and (C.8) in Appendix C respectively.

4.2 Spectral properties of the mean-field Dirac–Fock operator

Recall that $\kappa := \alpha (C_G z + C'_{EE} q^+)$. We start with the following.

Lemma 4.9. *Let $\gamma \in \mathfrak{S}_{1,1} \cap Y$. We assume that $C_G z + C'_{EE} \|\gamma\|_{\mathfrak{S}_{1,1} \cap Y} < 1/\alpha$, then $D_{\gamma,\xi}$ is a self-adjoint operator on L_ξ^2 with domain H_ξ^1 and form-domain $H_\xi^{1/2}$. In addition, the following holds*

$$\left\| |D_\gamma|^{1/2} |D^0|^{-1/2} \right\|_Y \leq (1 + \alpha (C_G z + C'_{EE} \|\gamma\|_{\mathfrak{S}_{1,1} \cap Y}))^{1/2} \quad (4.15)$$

and

$$\left\| |D^0|^{1/2} |D_\gamma|^{-1/2} \right\|_Y \leq (1 - \alpha (C_G z + C'_{EE} \|\gamma\|_{\mathfrak{S}_{1,1} \cap Y}))^{-1/2}. \quad (4.16)$$

In particular, if $\gamma \in \Gamma_{\leq q}$, we have

$$(1 - \kappa) |D^0| \leq |D_\gamma| \leq (1 + \kappa) |D^0|. \quad (4.17)$$

Proof. Recall $q^+ = \max\{1, q\}$. By Lemma 4.1 and Lemma 4.7, we obtain

$$\|(-\alpha z G_\ell + \alpha V_\gamma) |D^0|^{-1}\|_Y \leq \alpha (C_G z + C'_{EE} \|\gamma\|_{\mathfrak{S}_{1,1} \cap Y}). \quad (4.18)$$

In particular, D_γ is self-adjoint on $f_{Q_\ell^*}^\oplus H_\xi^1 d\xi$ by the Rellich-Kato theorem if $C_G z + C'_{EE} \|\gamma\|_{\mathfrak{S}_{1,1} \cap Y} < 1/\alpha$ (see [28, Theorem XIII-85]). Let now $\xi \in Q_\ell^*$ and $u_\xi \in H_\xi^1(Q_\ell)$. We have

$$\|D_{\gamma,\xi} u_\xi\|_{L_\xi^2} \leq (1 + \alpha C_G z + \alpha C'_{EE} \|\gamma\|_{\mathfrak{S}_{1,1} \cap Y}) \|D_\xi u_\xi\|_{L_\xi^2}, \quad (4.19)$$

which implies (4.15). On the other hand,

$$\begin{aligned} \|D_\xi u_\xi\|_{L_\xi^2} &\leq \|(D_{\gamma,\xi} - D_\xi) u_\xi\|_{L_\xi^2} + \|D_{\gamma,\xi} u_\xi\|_{L_\xi^2} \\ &\leq \alpha (C_G z + C'_{EE} q^+) \|D_\xi u_\xi\|_{L_\xi^2} + \|D_{\gamma,\xi} u_\xi\|_{L_\xi^2}, \end{aligned}$$

Hence,

$$\|D_\xi u_\xi\|_{L_\xi^2} \leq (1 - \alpha (C_G z + C'_{EE} \|\gamma\|_{\mathfrak{S}_{1,1} \cap Y}))^{-1} \|D_{\gamma,\xi} u_\xi\|_{L_\xi^2} \quad (4.20)$$

which implies (4.16). Since $\gamma \in \Gamma_{\leq q}$, $\|\gamma\|_{\mathfrak{S}_{1,1} \cap Y} \leq q^+$. Thus (4.19) and (4.20) together give (4.17). This concludes the proof. \square

As a consequence of (4.20), we deduce that the spectrum of D_γ (and of any $D_{\gamma,\xi}$) is included in $\mathbb{R} \setminus [-1 + \kappa; 1 - \kappa]$. In order to allow for as many electrons as possible per cell, we need a more accurate estimate on the bottom of $|\sigma(D_\gamma)|$.

Lemma 4.10 (Further properties of the bottom of the spectrum of D_γ). *Let $\gamma \in \Gamma_{\leq q}$. Then*

$$\inf |\sigma(D_\gamma)| \geq \lambda_0 \geq 1 - \kappa,$$

with $\lambda_0 := 1 - \alpha \max\{C_H z + C''_{EE} q^+, \frac{C_0}{\ell} z + C_{EE} q^+\}$.

Proof. Let $\psi_\xi^+ = \Lambda_\xi^+ \psi_\xi$ and $\psi_\xi^- = \Lambda_\xi^- \psi_\xi$. Notice that $D_{\gamma,\xi} = D_\xi - \alpha z G_\ell + \alpha V_{\gamma,\xi}$ and $V_{\gamma,\xi}$ satisfies (4.13) and (4.14). Now, combining with (A.1) we have

$$\left(\psi_\xi^+, D_{\gamma,\xi} \psi_\xi^+ \right)_{H_\xi^{1/2} \times H_\xi^{-1/2}} \geq \left(1 - \alpha (C_H z + C''_{EE} \|\gamma\|_{\mathfrak{S}_{1,1} \cap Y}) \right) \|\psi_\xi^+\|_{H_\xi^{1/2}}^2$$

and

$$- \left(\psi_\xi^-, D_{\gamma,\xi} \psi_\xi^- \right)_{H_\xi^{1/2} \times H_\xi^{-1/2}} \geq \left(1 - \alpha \left(\frac{C_0}{\ell} z + C_{EE} \|\gamma\|_{\mathfrak{S}_{1,1} \cap Y} \right) \right) \|\psi_\xi^-\|_{H_\xi^{1/2}}^2.$$

We get

$$\begin{aligned} \|\psi_\xi\|_{H_\xi^{1/2}} \|D_{\gamma,\xi} \psi\|_{H_\xi^{-1/2}} &\geq \Re \left(\psi_\xi^+ - \psi_\xi^-, D_{\gamma,\xi} \psi_\xi \right)_{H_\xi^{1/2} \times H_\xi^{-1/2}} \\ &= \left(\psi_\xi^+, D_{\gamma,\xi} \psi_\xi^+ \right)_{H_\xi^{1/2} \times H_\xi^{-1/2}} - \left(\psi_\xi^-, D_{\gamma,\xi} \psi_\xi^- \right)_{H_\xi^{1/2} \times H_\xi^{-1/2}} \geq \lambda_0 \|\psi_\xi\|_{H_\xi^{1/2}}^2. \end{aligned}$$

□

Further spectral properties of the self-consistent operator D_γ are collected in the following.

Lemma 4.11 (Properties of positive eigenvalues of $D_{\gamma,\xi}$). *Assume that $\kappa < 1$ and let $\gamma \in \Gamma_{\leq q}$. We denote by $\lambda_k(\xi)$, for $k \geq 1$, the k -th positive eigenvalue (counted with multiplicity) of the mean-field operator $D_{\gamma,\xi}$. Then, there exist positive constants $c^*(k)$ and $c_*(k)$ independent of ξ , with $1 \leq c_*(k) \leq c^*(k)$ and $c_*(k) \rightarrow +\infty$ when $k \rightarrow +\infty$, such that $\lambda_k(\xi)$ is situated in the interval $[c_*(k)(1-\kappa), c^*(k)(1-\kappa)^{-1}]$. This interval is independent of γ . Moreover, there are constants $e > c^*(q+1)(1-\kappa)^{-1}$ and $M > 0$, such that each operator $D_{\gamma,\xi}$ admits at most $q + M$ eigenvalues in $[0, e]$.*

In addition, every eigenfunction $u_{k,\xi}(x)$ associated to $\lambda_k(\xi)$ lies in H_ξ^1 and satisfies

$$\|D_\xi |u_{k,\xi}\|_{L_\xi^2} \leq (1 - \kappa)^{-1} \lambda_k(\xi) \|u_{k,\xi}\|_{L_\xi^2} \leq c^*(k) (1 - \kappa)^{-2} \|u_{k,\xi}\|_{L_\xi^2}. \quad (4.21)$$

Proof. We rely on a variational characterization of eigenvalues of Dirac operators (see [10] and references therein). The proof of the condition (i)-(iii) in [10] is postponed to the end of the proof. Let

$$\Lambda_\xi^+ := 1_{\mathbb{R}^+}(D_\xi) = \frac{1}{2} + \frac{D_\xi}{2|D_\xi|}$$

and

$$\Lambda_\xi^- := 1_{\mathbb{R}^-}(D_\xi) = \frac{1}{2} - \frac{D_\xi}{2|D_\xi|}.$$

From [10, Equation (1)], the k -th positive eigenvalue $\lambda_k(\xi)$ of $D_{\gamma,\xi}$ is obtained through the formula

$$\lambda_k(\xi) := \inf_{\substack{V \text{ subspace of } \Lambda_\xi^+ H_\xi^{1/2} \\ \dim V = k}} \sup_{u_\xi \in (V \oplus \Lambda_\xi^- H_\xi^{1/2}) \setminus \{0\}} \frac{(D_{\gamma,\xi} u_\xi, u_\xi)}{\|u_\xi\|_{L_\xi^2}^2}. \quad (4.22)$$

Let $u_\xi \in (V \oplus \Lambda_\xi^- H_\xi^{1/2}) \setminus \{0\}$. We write $u_\xi = u_\xi^+ + u_\xi^-$ with

$$u_\xi^+ = \Lambda_\xi^+ u_\xi \in V, \quad u_\xi^- = \Lambda_\xi^- u_\xi \in \Lambda_\xi^- H_\xi^{1/2}.$$

By definition of Λ_ξ^\pm ,

$$(D_\xi u_\xi^+, u_\xi^+) = (|D_\xi| u_\xi^+, u_\xi^+), \quad (D_\xi u_\xi^-, u_\xi^-) = -(|D_\xi| u_\xi^-, u_\xi^-) \text{ and } (D_\xi u_\xi^+, u_\xi^-) = 0.$$

Therefore,

$$\begin{aligned}
(D_{\gamma,\xi}u_\xi, u_\xi) &= (D_\xi u_\xi, u_\xi) + ((D_{\gamma,\xi} - D_\xi)u_\xi, u_\xi) \\
&= \left(|D_\xi|u_\xi^+, u_\xi^+\right) - \left(|D_\xi|u_\xi^-, u_\xi^-\right) + \left((D_{\gamma,\xi} - D_\xi)u_\xi^+, u_\xi^+\right) + \left((D_{\gamma,\xi} - D_\xi)u_\xi^-, u_\xi^-\right) \\
&\quad + 2\Re\left((D_{\gamma,\xi} - D_\xi)u_\xi^+, u_\xi^-\right). \tag{4.23}
\end{aligned}$$

To get the lower bound, we observe that

$$\lambda_k(\xi) \geq \inf_{\substack{V \text{ subspace of } \Lambda_\xi^+ H_\xi^{1/2} \\ \dim V=k}} \sup_{u_\xi \in V \setminus \{0\}} \frac{(D_{\gamma,\xi}u_\xi, u_\xi)}{\|u_\xi\|_{L_\xi^2}^2}.$$

By (4.23) and (4.18), for any $u_\xi \in \Lambda_\xi^+ H_\xi^{1/2}$,

$$(D_{\gamma,\xi}u_\xi, u_\xi) = (|D_\xi|u_\xi, u_\xi) + ((-\alpha z G_\ell + \alpha V_\gamma)u_\xi, u_\xi) \geq (1 - \kappa)(|D_\xi|u_\xi, u_\xi).$$

Thus,

$$(1 - \kappa)^{-1}\lambda_k(\xi) \geq \inf_{\substack{V \text{ subspace of } \Lambda_\xi^+ H_\xi^{1/2} \\ \dim V=k}} \sup_{u_\xi \in V \setminus \{0\}} \frac{(|D_\xi|u_\xi, u_\xi)}{\|u_\xi\|_{L_\xi^2}^2}.$$

We define

$$c_*(k) := \inf_{\xi \in Q_\ell^*} d_k^+(\xi) = \inf_{\xi \in Q_\ell^*} \inf_{\substack{V \text{ subspace of } \Lambda_\xi^+ H_\xi^{1/2} \\ \dim V=k}} \sup_{u_\xi \in V \setminus \{0\}} \frac{(|D_\xi|u_\xi, u_\xi)}{\|u_\xi\|_{L_\xi^2}^2}.$$

Obviously, $c_*(k) \geq 1$ and $c_*(k)$ goes to infinity together with k . Also,

$$\lambda_k(\xi) \geq (1 - \kappa)c_*(k), \text{ for every } \xi \in Q_\ell^*.$$

For the upper bound, we proceed as follows. (4.18) and (4.23) yield

$$\begin{aligned}
(D_{\gamma,\xi}u_\xi, u_\xi) &= \left(|D_\xi|u_\xi^+, u_\xi^+\right) + \left((-\alpha z G_\ell + \alpha V_\gamma)u_\xi^+, u_\xi^+\right) + 2\Re\left((-\alpha z G_\ell + \alpha V_\gamma)u_\xi^+, u_\xi^-\right) \\
&\quad + \left((D_{\gamma,\xi} - D_\xi)u_\xi^-, u_\xi^-\right) - \left(|D_\xi|u_\xi^-, u_\xi^-\right) \\
&\leq (1 + \kappa)\left(|D_\xi|u_\xi^+, u_\xi^+\right) - (1 - \kappa)\left(|D_\xi|u_\xi^-, u_\xi^-\right) + 2\kappa\| |D_\xi|^{1/2}u_\xi^+ \|_{L_\xi^2} \| |D_\xi|^{1/2}u_\xi^- \|_{L_\xi^2} \\
&= (1 + \kappa)\| |D_\xi|^{1/2}u_\xi^+ \|_{L_\xi^2}^2 + 2\kappa\| |D_\xi|^{1/2}u_\xi^+ \|_{L_\xi^2} \| |D_\xi|^{1/2}u_\xi^- \|_{L_\xi^2} - (1 - \kappa)\| |D_\xi|^{1/2}u_\xi^- \|_{L_\xi^2}^2 \\
&\leq (1 - \kappa)^{-1}\| |D_\xi|^{1/2}u_\xi^+ \|_{L_\xi^2}^2,
\end{aligned}$$

by Young's inequality. Let now

$$c^*(k) := \sup_{\xi \in Q_\ell^*} d_k^+(\xi) = \sup_{\xi \in Q_\ell^*} \inf_{\substack{V \text{ subspace of } \Lambda_\xi^+ H_\xi^{1/2} \\ \dim V=k}} \sup_{u_\xi^+ \in V \setminus \{0\}} \frac{(|D_\xi|u_\xi^+, u_\xi^+)}{\|u_\xi^+\|_{L_\xi^2}^2}.$$

As $\|u_\xi^+\|_{L_\xi^2} \leq \|u_\xi\|_{L_\xi^2}$, we obtain

$$\lambda_k(\xi) \leq (1 - \kappa)^{-1}c^*(k). \tag{4.24}$$

By construction, $c_*(k) \leq c^*(k)$ and $c_*(k)$ and $c^*(k)$ are non-decreasing with respect to k . Finally, by definition of $c^*(k)$ and $c_*(k)$, for any $e > c^*(q+1)(1 - \kappa)^{-1}$, there is an integer $M \geq 2$ such that $c_*(q+M-1) \leq e < c_*(q+M)$. Therefore, $D_{\gamma,\xi}$ admits at most $q+M$ eigenvalues in $[0, e]$ for every $\xi \in Q_\ell^*$.

Using (4.20) in Lemma 4.9, we obtain

$$\lambda_k(\xi) \|u_{k,\xi}\|_{L_\xi^2} = \|D_{\gamma,\xi}u_\xi\|_{L_\xi^2} \geq (1 - \kappa)\|D_\xi u_\xi\|_{L_\xi^2}.$$

Hence (4.21).

To end the proof, it suffices to check the condition $\sup_{\xi \in Q_\ell^*} \sup_{u_\xi \in \Lambda_\xi^- H_\xi^{1/2} \setminus \{0\}} \frac{(D_{\gamma,\xi}u_\xi, u_\xi)}{\|u_\xi\|_{L_\xi^2}^2} \leq 0 < \inf_{\xi \in Q_\ell^*} \lambda_1(\xi)$ in [10]. It follows from the decomposition (4.23) of $D_{\gamma,\xi}$; namely $(D_{\gamma,\xi}\phi_\xi, \phi_\xi) \leq 0$ for every $\phi_\xi \in \Lambda_\xi^- H_\xi^{1/2}$ whenever $\kappa < 1$. \square

4.3 Properties of the minimizers of a linear problem

Recall that $B_R := \{\gamma \in X \cap Y \mid \|\gamma\|_{\mathfrak{S}_{1,\infty}} < R\}$ and $R_0 := q + M$ where M is a constant defined in Lemma 4.11. The following lemma will be used in the next sections.

Lemma 4.12. *Let $g \in \Gamma_{\leq q}$ be given, and assume $\kappa < 1$. Then for each $\epsilon_P > 0$, the minimization problem*

$$\inf_{\substack{\gamma \in \Gamma_{\leq q}, \\ \gamma = P_g^+ \gamma P_g^+}} \int_{Q_\ell^*} \text{Tr}_{L_\xi^2}[(D_{g,\xi} - \epsilon_P)\gamma_\xi] d\xi$$

admits a minimizer. Every minimizer γ_* is of the form $\gamma_* = \int_{Q_\ell^*}^\oplus 1_{[0,\nu]}(D_{g,\xi}) d\xi + \delta$, with $0 \leq \delta \leq \int_{Q_\ell^*}^\oplus 1_{\{\nu\}}(D_{g,\xi}) d\xi$ for some $\nu \in (0, \epsilon_P]$ independent of $\xi \in Q_\ell^*$.

Furthermore, for every ϵ_P , we have $\nu \leq (1-\kappa)^{-1}c^*(q+1)$ and $\gamma_* \in \overline{B}_{R_0}$. If $\epsilon_P > (1-\kappa)^{-1}c^*(q+1)$, any minimizer γ_* is independent of ϵ_P , and $\widetilde{\text{Tr}}_{L^2}(\gamma_*) = q$.

Proof. For any $\xi \in Q_\ell^*$ we can choose an orthonormal eigenbasis $\{\psi_k(\xi, \cdot)\}_{k \geq 1}$ of $D_{g,\xi} P_{g,\xi}^+$, such that

$$D_{g,\xi} P_{g,\xi}^+ = \sum_{k \geq 1} \lambda_k(\xi) |\psi_k(\xi)\rangle \langle \psi_k(\xi)|.$$

According to Lemma 4.11, each positive $\lambda_k(\xi)$ is bounded independently of ξ . Let us introduce as in [2, 14] the function

$$C : s \mapsto \frac{\ell^3}{(2\pi)^3} \sum_{k \geq 1} |\{\xi \in Q_\ell^* \mid 0 \leq \lambda_k(\xi) \leq s\}|.$$

It is non-decreasing on \mathbb{R} . In addition, by Lemma 4.11, $C(0) = 0$ and $C(+\infty) = +\infty$. Thus, there exists $\nu_1 \in [0, +\infty)$ such that

$$\lim_{s \rightarrow \nu_1^-} C(s) \leq q \leq \lim_{s \rightarrow \nu_1^+} C(s). \quad (4.25)$$

We are going to prove that every minimizer $\gamma_* \in \Gamma_{\leq q}$ is of the form

$$\gamma_* = \int_{Q_\ell^*}^\oplus 1_{[0,\nu]}(D_{g,\xi}) d\xi + \delta$$

with $0 \leq \delta \leq \int_{Q_\ell^*}^\oplus 1_{\{\nu\}}(D_{g,\xi}) d\xi$ and $\nu := \min\{\nu_1, \epsilon_P\}$. The proof is inspired by [2].

We first consider the case $\nu_1 < \epsilon_P$. According to (4.25), there is a density matrix $\tilde{\gamma} = 1_{[0,\nu_1]}(D_g) + \delta$ where $0 \leq \delta \leq 1_{\{\nu_1\}}(D_g)$ is chosen such that

$$\widetilde{\text{Tr}}_{L^2}(\tilde{\gamma}) = q.$$

For any $\gamma \in \Gamma_{\leq q}$, we write

$$\begin{aligned} & \int_{Q_\ell^*} \text{Tr}_{L_\xi^2}[(D_{g,\xi} - \epsilon_P)(\gamma_\xi - \tilde{\gamma}_\xi)] d\xi \\ &= \int_{Q_\ell^*} \text{Tr}_{L_\xi^2}[(D_{g,\xi} - \nu_1)(\gamma_\xi - \tilde{\gamma}_\xi)] d\xi + \int_{Q_\ell^*} \text{Tr}_{L_\xi^2}[(\nu_1 - \epsilon_P)(\gamma_\xi - \tilde{\gamma}_\xi)] d\xi \\ &= \int_{Q_\ell^*} \text{Tr}_{L_\xi^2}[(D_{g,\xi} - \nu_1)(\gamma_\xi - \tilde{\gamma}_\xi)] d\xi + |\nu_1 - \epsilon_P| \left| \int_{Q_\ell^*} \text{Tr}_{L_\xi^2}[\gamma_\xi - \tilde{\gamma}_\xi] d\xi \right| \\ &\geq \int_{Q_\ell^*} \text{Tr}_{L_\xi^2}[(D_{g,\xi} - \nu_1)(\gamma_\xi - \tilde{\gamma}_\xi)] d\xi. \end{aligned} \quad (4.26)$$

Since $0 \leq \gamma_\xi \leq 1_{L_\xi^2}$, we have $\langle \gamma_\xi \psi_k(\xi), \psi_k(\xi) \rangle \in [0, 1]$, for almost every $\xi \in Q_\ell^*$. Hence,

$$\begin{aligned} & \int_{Q_\ell^*} \text{Tr}_{L_\xi^2}[(D_{g,\xi} - \nu_1)(\gamma_\xi - \tilde{\gamma}_\xi)] d\xi \\ &= \int_{Q_\ell^*} \text{Tr}_{L_\xi^2}[(D_{g,\xi} - \nu_1)(\gamma_\xi - 1_{[0,\nu_1]}(D_{g,\xi}))] d\xi \end{aligned}$$

$$\begin{aligned}
&= \int_{Q_\ell^*} \sum_{\lambda_k(\xi) < \nu_1} |\lambda_k(\xi) - \nu_1| |\langle \gamma_\xi \psi_k(\xi), \psi_k(\xi) \rangle - 1| d\xi \\
&\quad + \int_{Q_\ell^*} \sum_{\lambda_k(\xi) > \nu_1} [|\lambda_k(\xi) - \nu_1| \langle \gamma_\xi \psi_k(\xi), \psi_k(\xi) \rangle] d\xi \geq 0. \tag{4.27}
\end{aligned}$$

Thus $\tilde{\gamma}$ is a minimizer. According to (4.26) and (4.27), if γ_* is a minimizer, then γ must be of the form $\gamma = f_{Q_\ell^*}^\oplus 1_{[0, \nu)}(D_g) d\xi + \delta$ with $\nu = \nu_1 = \min\{\nu_1, \epsilon_P\}$ and $\widetilde{\text{Tr}}_{L^2}(\gamma) = q$. In particular, in this case, γ_* is independent of ϵ_P .

For the case $\epsilon_P \leq \nu_1$, we prove that every minimizer γ_* satisfies $\gamma_* = f_{Q_\ell^*}^\oplus 1_{[0, \epsilon_P)}(D_{g, \xi}) d\xi + \delta$, with $0 \leq \delta \leq f_{Q_\ell^*}^\oplus 1_{\{\epsilon_P\}}(D_{g, \xi}) d\xi$ being chosen such that $\widetilde{\text{Tr}}_{L^2}(\gamma_*) \leq q$. If not, using (4.27) again (by replacing ν_1 by ϵ_P), we get

$$\int_{Q_\ell^*} \text{Tr}_{L_\xi^2}[(D_{g, \xi} - \epsilon_P)(\gamma'_\xi - 1_{[0, \epsilon_P)}(D_{g, \xi})] d\xi > 0,$$

which contradicts the fact that γ' is a minimizer. Thus any minimizer satisfies

$$\gamma_* = f_{Q_\ell^*}^\oplus 1_{[0, \nu)}(D_{g, \xi}) d\xi + \delta,$$

with $\nu = \epsilon_P = \min\{\nu_1, \epsilon_P\}$ and $0 \leq \delta \leq f_{Q_\ell^*}^\oplus 1_{\{\nu\}}(D_{g, \xi}) d\xi$ being chosen such that $\widetilde{\text{Tr}}_{L^2}(\gamma_*) \leq q$.

We turn to prove $\nu \leq (1 - \kappa)^{-1} c^*(q + 1)$, and this leads to $\gamma_* \in \overline{B}_{R_0}$. More precisely, we prove that $(1 - \kappa) c_*(q - 1) \leq \nu_1 \leq (1 - \kappa)^{-1} c^*(q + 1)$. If not, we first assume that $\nu_1 > (1 - \kappa)^{-1} c^*(q + 1)$. Then by Lemma 4.11 and (4.25),

$$q \geq \lim_{s \rightarrow \nu_1^-} C(s) \geq C((1 - \kappa)^{-1} c^*(q + 1)) \geq q + 1,$$

which contradicts (4.25). Analogously, if $\nu_1 < (1 - \kappa) c_*(q - 1)$, then

$$q \leq \lim_{s \rightarrow \nu_1^+} C(s) \leq C((1 - \kappa) c_*(q - 1)) \leq q - 1.$$

Thus, $(1 - \kappa) c_*(q - 1) \leq \nu_1 \leq (1 - \kappa)^{-1} c^*(q + 1)$, then $\nu = \min\{\nu_1, \epsilon_P\} \leq (1 - \kappa)^{-1} c^*(q + 1)$. Moreover, by Lemma 4.11, we have

$$0 \leq \gamma_{*, \xi} \leq 1_{(0, e]}(D_{g, \xi}), \quad \text{and} \quad \|\gamma_*\|_{\mathfrak{S}_{1, \infty}} \leq q + M.$$

Thus, $\gamma_* \in \overline{B}_{R_0}$. If $\epsilon_P > (1 - \kappa)^{-1} c^*(q + 1)$, then $\nu = \nu_1 < \epsilon_P$, thus any minimizer is independent of ϵ_P and satisfies $\text{Tr}_{L_\xi^2}(\gamma_*) = q$. \square

Remark 4.13. *Actually, in the proof, we show that $\sup_{\xi \in Q_\ell^*} \text{Rank}(\gamma_{*, \xi}) \leq q + M$.*

For the minimum problem given in Lemma 4.12, the following proposition gives the estimates on the minimizers in $X \cap Y$, which will be used in the proof of Proposition 5.1.

Proposition 4.14. *Assume that $\kappa < 1$. Let $\gamma, \gamma' \in \Gamma_{\leq q}$ such that*

$$0 \leq \gamma'_\xi \leq 1_{[0, (1 - \kappa)^{-1} c^*(q + 1)]}(D_{\gamma, \xi}).$$

Then,

$$\|\gamma'\|_{X \cap Y} \leq \max\{(1 - \kappa)^{-2} q c^*(q + 1), 1\}.$$

Proof. By Lemma 4.9, we have

$$\int_{Q_\ell^*} \text{Tr}_{L_\xi^2}[D_{\gamma, \xi} \gamma'_\xi] d\xi = \int_{Q_\ell^*} \text{Tr}_{L_\xi^2}[|D_{\gamma, \xi}| \gamma'_\xi] d\xi \geq (1 - \kappa) \|\gamma'\|_X.$$

Since $\gamma' \in \Gamma_{\leq q}$, we have

$$\int_{Q_\ell^*} \text{Tr}_{L_\xi^2}[D_{\gamma, \xi} \gamma'_\xi] d\xi \leq (1 - \kappa)^{-1} c^*(q + 1) \int_{Q_\ell^*} \text{Tr}_{L_\xi^2}(\gamma'_\xi) d\xi \leq q(1 - \kappa)^{-1} c^*(q + 1).$$

Then $\|\gamma'\|_X \leq (1 - \kappa)^{-2} q c^*(q + 1)$. Consequently, from the fact that $\|\gamma\|_Y \leq 1$, we deduce

$$\|\gamma'\|_{X \cap Y} \leq \max\{(1 - \kappa)^{-2} q c^*(q + 1), 1\}.$$

\square

4.4 First properties of minimizing sequences in $\Gamma_{\leq q}^+$

We prove the following.

Lemma 4.15 (Boundedness of minimizing sequences). *Assume that $\kappa < 1$. Then, there is a minimizing sequence $(\gamma_n)_{n \geq 1}$ of $I_{\leq q, R}$ in $\Gamma_{\leq q}^+$, such that for any $n \in \mathbb{N}$,*

$$\mathcal{E}^{DF}(\gamma_n) - \epsilon_P \widetilde{\text{Tr}}_{L^2}(\gamma_n) \leq 0.$$

Moreover, if $\kappa < 1 - \frac{\alpha}{2} C_{EE} q^+$, then, for every $n \geq 1$,

$$\|\gamma_n\|_{X \cap Y} \leq \max \left\{ (1 - \kappa - \frac{\alpha}{2} C_{EE} q^+)^{-1} \epsilon_P q, 1 \right\} \quad (4.28)$$

and

$$\max \left\{ \|\gamma_n |D^0|^{1/2}\|_{\mathfrak{S}_{1,1}}, \|\gamma_n\|_Y \right\} \leq \sqrt{\max \left\{ (1 - \kappa - \frac{\alpha}{2} C_{EE} q^+)^{-1} \epsilon_P q, 1 \right\}} q^+.$$

Proof. Note that the operator 0 belongs to $\Gamma_{\leq q}^+$ and satisfies $\mathcal{E}^{DF}(0) - \epsilon_P \widetilde{\text{Tr}}_{L^2}(0) = 0$. Thus, $I_{\leq q, R} = \inf_{\gamma \in \Gamma_{\leq q}^+ \cap B_R} \left[\mathcal{E}^{DF}(\gamma) - \epsilon_P \widetilde{\text{Tr}}_{L^2}(\gamma) \right] \leq 0$. In particular, there exists a minimizing sequence, such that $\mathcal{E}^{DF}(\gamma_n) - \epsilon_P \widetilde{\text{Tr}}_{L^2}(\gamma_n) \leq 0$.

For simplicity, we skip the n index in the following. As $D_{\gamma, \xi} \gamma_\xi = |D_{\gamma, \xi}| \gamma_\xi$ for any $\gamma \in \Gamma_{\leq q}^+$, by (4.13) and (4.17) we get

$$\begin{aligned} \mathcal{E}^{DF}(\gamma) - \epsilon_P \widetilde{\text{Tr}}_{L^2}(\gamma) &= \int_{Q_\ell^*} \text{Tr}_{L_\xi^2} \left[(D_{\gamma, \xi} - \epsilon_P - \frac{\alpha}{2} V_{\gamma, \xi}) \gamma_\xi \right] d\xi \\ &= \int_{Q_\ell^*} \text{Tr}_{L_\xi^2} \left[(|D_{\gamma, \xi}| - \epsilon_P - \frac{\alpha}{2} V_{\gamma, \xi}) \gamma_\xi \right] d\xi \\ &\geq \int_{Q_\ell^*} \text{Tr}_{L_\xi^2} \left[((1 - \kappa) |D_\xi| - \epsilon_P - \frac{\alpha}{2} V_{\gamma, \xi}) \gamma_\xi \right] d\xi \\ &\geq (1 - \kappa) \|\gamma\|_X - \frac{\alpha}{2} C_{EE} \|\gamma\|_{\mathfrak{S}_{1,1} \cap Y} \|\gamma\|_X - \epsilon_P \|\gamma\|_{\mathfrak{S}_{1,1}} \\ &\geq (1 - \kappa - \frac{\alpha}{2} C_{EE} q^+) \|\gamma\|_X - \epsilon_P q. \end{aligned}$$

Hence,

$$(1 - \kappa - \frac{\alpha}{2} C_{EE} q^+) \|\gamma\|_X - \epsilon_P q \leq 0.$$

Whenever $1 - \kappa - \frac{\alpha}{2} C_{EE} q^+ > 0$, (4.28) holds since $\|\gamma\|_Y \leq 1$.

The last inequality follows from Hölder's inequality and the fact that $\gamma \geq 0$; namely

$$\|\gamma |D^0|^{1/2}\|_{\mathfrak{S}_{1,1}} \leq \|\gamma^{1/2}\|_{\mathfrak{S}_{2,2}} \| |D^0|^{1/2} \|_{\mathfrak{S}_{2,2}} \leq \|\gamma\|_{\mathfrak{S}_{1,1}}^{1/2} \|\gamma\|_X^{1/2}.$$

□

From now on, we define the set

$$\mathcal{V}_0 := \left\{ \gamma \in \Gamma_{\leq q}^+ \mid \mathcal{E}^{DF}(\gamma) - \epsilon_P \widetilde{\text{Tr}}_{L^2}(\gamma) \leq 0 \right\} \quad (4.29)$$

to which the minimizing sequences belong under Assumption 3.1.

5 Approximation by a linearized problem

The aim of this section is to show the link between a minimizing sequence $(\gamma_n)_{n \geq 1}$ in \mathcal{V}_0 and the linear Dirac–Fock problem introduced in Lemma 4.12.

Proposition 5.1 (Link with the linearized problem). *Let $R > R_0 = q + M$. Under Assumption 3.1, let $(\gamma_n) \in \Gamma_{\leq q}^+ \cap B_R$ be a minimizing sequence of (3.5). Then, as n goes to infinity,*

$$\int_{Q_\ell^*} \text{Tr}_{L_\xi^2} \left[(D_{\gamma_n, \xi} - \epsilon_P) \gamma_{n, \xi} \right] d\xi - \inf_{\substack{\gamma \in \Gamma_{\leq q}^+ \\ \gamma = P_{\gamma_n}^+ \gamma P_{\gamma_n}^+}} \int_{Q_\ell^*} \text{Tr}_{L_\xi^2} \left[(D_{\gamma, \xi} - \epsilon_P) \gamma_\xi \right] d\xi \rightarrow 0. \quad (5.1)$$

This property is used in Lemma 6.2 below to build a new minimizing sequence with further regularity, and it is also used at the end of Section 6 to show some properties of the minimizers of $I_{\leq q}$.

As mentioned at the end of Section 3, the main difficulty is to deal with the nonlinear constraint $\Gamma_{\leq q}^+$. To do so, we introduce a retraction technique first used in [29]. We are going to construct a regular map θ from a locally convex set \mathcal{V} in $\Gamma_{\leq q}$ into a neighborhood of \mathcal{V}_0 in $\Gamma_{\leq q}^+$. More precisely, we will have $\mathcal{V}_0 \subset \theta(\mathcal{V}) \subset \Gamma_{\leq q}^+$. Consequently,

$$I_{\leq q} = \inf_{\gamma \in \mathcal{V}_0} (\mathcal{E}^{DF}(\gamma) - \epsilon_P \widetilde{\text{Tr}}_{L^2}(\gamma)) = \inf_{\gamma \in \mathcal{V}} (\mathcal{E}^{DF}(\theta(\gamma)) - \epsilon_P \widetilde{\text{Tr}}_{L^2}[\theta(\gamma)]). \quad (5.2)$$

The locally convex set \mathcal{V} is defined by

$$\mathcal{V} := (\mathcal{V}_0 + B_{X \cap Y}(\rho)) \cap \Gamma_{\leq q} \quad (5.3)$$

for some $\rho > 0$ small enough. The map θ is defined by

$$\theta(\gamma) = \lim_{n \rightarrow +\infty} T^n(\gamma)$$

for any $\gamma \in \mathcal{V}$ where the map T onto \mathcal{V} is given by

$$T : \gamma \mapsto P_{\gamma}^+ \gamma P_{\gamma}^+.$$

We also denote by $\text{Fix}(T)$ the set of fixed points of the map T (i.e., for any $\gamma \in \text{Fix}(T)$, $T(\gamma) = \gamma$). Obviously, $T(\gamma)$ is self-adjoint and $0 \leq T(\gamma) \leq 1$. In particular, $\Gamma_{\leq q}^+ = \Gamma_{\leq q} \cap \text{Fix}(T)$. Unfortunately, given γ in $\Gamma_{\leq q}$, $T(\gamma)$ may not stay in $\Gamma_{\leq q}^+ : P_{T(\gamma)}^+ T(\gamma) P_{T(\gamma)}^+$ may be different from $T(\gamma)$.

Now the constraint $\gamma \in \mathcal{V}$ in (5.2) is locally convex. To prove Proposition 5.1, we will study the differentiability of the new functional in (5.2).

We first introduce an admissible set \mathcal{U} for the retraction such that T maps \mathcal{U} to \mathcal{U} .

Definition 5.2 (Admissible set for the retraction). *Assume that $\kappa = \alpha(C_{Gz} + C'_{EE}q^+) < 1$ and let $\frac{\alpha}{2}C_{EE}(1 - \kappa)^{-1/2}\lambda_0^{-1/2} < A < \frac{1}{2}$. Given $1 < \tau < \frac{1}{2A}$, let $M := \max\left(\frac{2+Ag^+}{2}, \frac{1}{1-2A\tau}\right)$, then we define*

$$\mathcal{U} := \left\{ \gamma \in \Gamma_{\leq q} \mid \max\{\|\gamma\|D^0\|^{1/2}\|_{\mathfrak{S}_{1,1}}, \|\gamma\|_Y\} + M\|T(\gamma) - \gamma\|_{X \cap Y} < \tau \right\}.$$

Remark 5.3. *We must impose $\tau > 1$ in Proposition 5.4: Otherwise, any minimizer γ_* of $I_{\leq q,R}$ is not in \mathcal{U} if $q \geq 1$ since $\|\gamma_*\|_Y = 1$.*

For any differentiable function $F : \mathcal{U} \rightarrow X \cap Y$ and $a \in \mathcal{U}$, we define $dF(a)$ by

$$\lim_{x \rightarrow a, x \in \mathcal{U}} \frac{\|F(x) - F(a) - dF(a)(x - a)\|_{X \cap Y}}{\|x - a\|_{X \cap Y}} = 0.$$

Then we have the following.

Proposition 5.4 (Existence and differentiability of the retraction). *Let $\kappa, A, \tau, \mathcal{U}$ as in Definition 5.2. Then the sequence of iterated maps $(T^p)_p$ converges uniformly on $\overline{\mathcal{U}}$ to a limit θ with $\theta(\overline{\mathcal{U}}) \subset \Gamma_{\leq q}^+ \cap \overline{\mathcal{U}}$ and $\text{Fix}(T) = \Gamma_{\leq q}^+ \cap \overline{\mathcal{U}}$. We have the estimate*

$$\forall \gamma \in \overline{\mathcal{U}}, \|\theta(\gamma) - T^p(\gamma)\|_{X \cap Y} \leq \frac{k^p}{1 - k} \|T(\gamma) - \gamma\|_{X \cap Y}.$$

Moreover $\theta \in C^{1,\text{unif}}(\mathcal{U}, X \cap Y)$ and $d\theta(T^p)$ converges uniformly to $d\theta$ on \mathcal{U} .

In this way we obtain a continuous retraction θ of $\overline{\mathcal{U}}$ onto $\Gamma_{\leq q}^+ \cap \overline{\mathcal{U}}$ whose restriction to \mathcal{U} is of class $C^{1,\text{unif}}$. This map and its differential are bounded and uniformly continuous on \mathcal{U} .

For any $\gamma \in \text{Fix}(T) \cap \mathcal{U}$ and any $h \in X \cap Y$, the linear operator $h \mapsto d\theta_{\xi}(\gamma)h$ satisfies

$$P_{\gamma,\xi}^+ d\theta_{\xi}(\gamma)h P_{\gamma,\xi}^+ = P_{\gamma,\xi}^+ h_{\xi} P_{\gamma,\xi}^+ \quad \text{and} \quad P_{\gamma,\xi}^- d\theta_{\xi}(\gamma)h P_{\gamma,\xi}^- = 0,$$

where $\theta(\gamma) = \int_{Q_{\xi}^*}^{\oplus} \theta_{\xi}(\gamma) d\xi$, according to the Floquet-Bloch decomposition. 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

$$d\theta_{\xi}(\gamma)h = \begin{pmatrix} P_{\gamma,\xi}^+ h_{\xi} P_{\gamma,\xi}^+ & b_{\gamma,\xi}(h)^* \\ b_{\gamma,\xi}(h) & 0 \end{pmatrix} \quad (5.4)$$

The proof is Proposition 5.4 is postponed to the end of this section.

To apply Proposition 5.4 to the proof of Proposition 5.1, we need to verify that $\mathcal{V} \subset \mathcal{U}$ for some τ given in Definition 5.2. From Lemma 4.15, we can observe that any $\gamma \in \mathcal{V}_0$ is indeed in \mathcal{U} if

$$\tau > \sqrt{\max\{(1 - \kappa - \frac{\alpha}{2}C_{EE}q^+)^{-1}\epsilon_P q, 1\}q^+}.$$

Thus, according to the continuity of T in $X \cap Y$ (will be shown in (5.13)), we have

Corollary 5.5. *Assume that $\kappa < 1 - \frac{\alpha}{2}C_{EE}q^+$, and let A be as above. Assume in addition that*

$$2A\sqrt{\max\{(1 - \kappa - \frac{\alpha}{2}C_{EE}q^+)^{-1}\epsilon_P q, 1\}q^+} < 1.$$

Then there exist τ as in Definition 5.2 and $\rho > 0$ such that $\mathcal{V} \subset \mathcal{U}$.

We are now in the position to prove the main result of this section.

Proof of Proposition 5.1. We argue by contradiction. Otherwise, there would be an $\epsilon_0 > 0$ such that, for n large enough,

$$\int_{Q_\ell^*} \text{Tr}_{L_\xi^2}[(D_{\gamma_n, \xi} - \epsilon_P)\gamma_{n, \xi}] d\xi \geq \inf_{\substack{\gamma \in \Gamma_{\leq q} \\ \gamma = P_{\gamma_n}^+ \gamma}} \int_{Q_\ell^*} \text{Tr}_{L_\xi^2}[(D_{\gamma_n, \xi} - \epsilon_P)\gamma_\xi] d\xi + \epsilon_0.$$

By Lemma 4.12, there exists an operator $\gamma'_n \in \Gamma_{\leq q}$ such that $\gamma'_n \in \Gamma_{\leq q} \cap B_{R_0}$ (where B_{R_0} is given in (3.3) and Proposition 3.4) and γ'_n minimizes the following problem

$$\int_{Q_\ell^*} \text{Tr}_{L_\xi^2}[(D_{\gamma_n, \xi} - \epsilon_P)\gamma'_{n, \xi}] d\xi := \inf_{\substack{\gamma \in \Gamma_{\leq q} \\ \gamma = P_{\gamma_n}^+ \gamma}} \int_{Q_\ell^*} \text{Tr}_{L_\xi^2}[(D_{\gamma_n, \xi} - \epsilon_P)\gamma_\xi] d\xi.$$

From Lemma 4.12 and Proposition 4.14, $\gamma'_n \in B_R$ and $\|\gamma'_n\|_{X \cap Y}$ is uniformly bounded. So according to Corollary 5.5, there is $\sigma > 0$ such that for any n large enough and any $s \in [0, \sigma]$, $(1 - s)\gamma_n + s\gamma'_n \in \Gamma_{\leq q} \cap B_X \cap Y(\gamma_n, \rho) \cap B_R \subset \mathcal{V} \cap B_R$. Then from Proposition 5.4, the function $f_n : s \in [0, \sigma] \rightarrow (\mathcal{E}^{DF} - \epsilon_P \widetilde{\text{Tr}}_{L^2})(\theta[(1 - s)\gamma_n + s\gamma'_n])$ is of class C^1 and the sequence of derivatives (f'_n) is equicontinuous on $[0, \sigma]$. From (5.4), we infer

$$f'_n(0) = \widetilde{\text{Tr}}_{L^2}[(D_{\gamma_n} - \epsilon_P)(\gamma'_n - \gamma_n)] \leq -\frac{\epsilon_0}{2}.$$

So there is $0 < s_0 < \sigma$ independent of n such that for any $s \in [0, s_0]$ we have $f'_n(s) \leq -\frac{\epsilon_0}{4}$. Hence, for any $s \in [0, s_0]$,

$$(\mathcal{E}^{DF} - \epsilon_P \widetilde{\text{Tr}}_{L^2})(\theta[(1 - s)\gamma_n + s\gamma'_n]) = f_n(s) \leq f_n(0) - \frac{\epsilon_0 s_0}{4} = (\mathcal{E}^{DF} - \widetilde{\text{Tr}}_{L^2})(\gamma_n) - \frac{\epsilon_0 s_0}{4}.$$

But $\theta[(1 - s)\gamma_n + s\gamma'_n] \in \Gamma_{\leq q}^+ \cap B_R$ and $\mathcal{E}^{DF}(\gamma_n) - \epsilon_P \widetilde{\text{Tr}}_{L^2}(\gamma_n) \rightarrow I_{\leq q, R}$. This is a contradiction. Hence the proposition. \square

We are now in the position to prove Proposition 5.4, as in [29] for atoms. As in [29], we introduce the following set:

$$\Gamma_{\leq q, r} := \{\gamma \in X \cap Y; \text{dist}_{\sigma_{1,1} \cap Y}(\gamma, \Gamma_{\leq q}) < r\}.$$

Then analogously to Lemma 4.9 and Lemma 4.10, we have for any $\gamma \in \Gamma_{\leq q, r}$,

$$(1 - \kappa_r)|D^0| \leq |D_\gamma| \leq (1 + \kappa_r)|D^0| \quad (5.5)$$

and

$$\inf |\sigma(D_\gamma)| \geq \lambda_{0, r} \geq 1 - \kappa_r, \quad (5.6)$$

where $\kappa_r := \alpha(C_{Gz} + C'_{EE}(q^+ + 2r))$ and

$$\lambda_{0, r} := 1 - \alpha \max\{C_{Hz} + C_{EE}r + C''_{EE}(q^+ + r), \frac{C_0}{\ell}z + C_{EE}(q^+ + r)\}.$$

Recall now that $P_0^+ = 1_{\mathbb{R}^+}(D^0 - \alpha z G_\ell)$ and $\frac{\alpha}{2}C_{EE}(1 - \kappa)^{-1/2}\lambda_0^{-1/2} < A < \frac{1}{2}$ with λ_0 given in Lemma 4.10.

Lemma 5.6. *Assume that $\kappa < 1$. We introduce the map*

$$Q: \gamma \mapsto P_\gamma^+ - P_0^+$$

in such a way that $Q(\gamma) := \int_{Q_\xi^}^\oplus Q_\xi(\gamma) d\xi$ with $Q_\xi(\gamma) := P_{\gamma, \xi}^+ - P_{0, \xi}^+$.*

Then for $r > 0$ small enough, the map Q is in $C^{1, \text{lip}}(\Gamma_{\leq q, r}, \mathcal{B}(L^2(\mathbb{R}^3, \mathbb{C}^4), H^{1/2}(\mathbb{R}^3), \mathbb{C}^4))$ and we have the estimates

$$\forall \gamma \in \Gamma_{\leq q, r}, \quad \forall h \in X \cap Y: \quad \| |D^0|^{1/2} dQ(\gamma) h \|_Y < (A - r) \|h\|_{X \cap Y} \quad (5.7)$$

and

$$\forall \gamma, \gamma' \in \Gamma_{\leq q, r}, \quad \| |D^0|^{1/2} [dQ(\gamma) h - dQ(\gamma') h] \|_Y \leq K \|\gamma - \gamma'\|_{X \cap Y} \|h\|_{X \cap Y}, \quad (5.8)$$

where K is a positive constant depending only on κ which remains bounded when κ stays away from 1.

Proof. As $\kappa < 1$, by our definition of κ_r and since $\lambda_0 \geq 1 - \kappa > 0$, it is easy to see that $\kappa_r < 1$ and $\lambda_{0, r} > 0$ for r small enough.

By Lemma 4.9, $D_{\gamma, \xi}$ is a self-adjoint operator for all $\gamma \in \Gamma_{\leq q, r}$ and 0 is in its resolvent set. Then by Taylor's formula [20, Chapter VI.5, Lemma 5.6] or [16], we have

$$P_{\gamma, \xi}^\pm = \frac{1}{2} \pm \frac{1}{2\pi} \int_{-\infty}^{+\infty} (D_{\gamma, \xi} - iz)^{-1} dz \quad (5.9)$$

and, by the second resolvent identity,

$$Q_\xi(\gamma) = -\frac{\alpha}{2\pi} \int_{-\infty}^{+\infty} (D_{\gamma, \xi} - iz)^{-1} V_{\gamma, \xi} (D_{0, \xi} - iz)^{-1} dz.$$

Hence, for every $h \in X \cap Y$, we deduce from (5.9) and the second resolvent formula again, that

$$dQ_\xi(\gamma) h = dP_{\gamma, \xi}^+ h = -\frac{\alpha}{2\pi} \int_{-\infty}^{+\infty} (D_{\gamma, \xi} - iz)^{-1} V_{h, \xi} (D_{\gamma, \xi} - iz)^{-1} dz. \quad (5.10)$$

Besides, for any $u_\xi \in L_\xi^2(Q_\ell)$, we have

$$\int_{-\infty}^{+\infty} \left(u_\xi, (|D_{\gamma, \xi}|^2 + |z|^2)^{-1/2} |D_{\gamma, \xi}| (|D_{\gamma, \xi}|^2 + |z|^2)^{-1/2} u_\xi \right)_{L_\xi^2} dz = \pi \|u_\xi\|_{L_\xi^2}^2.$$

We infer from (5.6) that

$$\| |D_\gamma|^{-1} \|_Y \leq \lambda_{0, r}^{-1}.$$

Thus gathering with Lemma 4.7, for any $\phi_\xi, \psi_\xi \in L_\xi^2$ we have

$$\begin{aligned} & \left| (\psi_\xi, |D_\xi|^{1/2} dQ_\xi(\gamma) h \phi_\xi)_{L_\xi^2} \right| \\ &= \frac{\alpha}{2\pi} \left| \int_{-\infty}^{+\infty} \left(\psi_\xi, |D_\xi|^{1/2} (D_{\gamma, \xi} - iz)^{-1} V_{h, \xi} (D_{\gamma, \xi} - iz)^{-1} \phi_\xi \right)_{L_\xi^2} dz \right| \\ &\leq \frac{\alpha}{2\pi} \|V_{h, \xi}\|_{\mathcal{B}(L_\xi^2)} \left(\int_{-\infty}^{+\infty} \left\| (D_{\gamma, \xi} - iz)^{-1} |D_\xi|^{1/2} \psi_\xi \right\|_{L_\xi^2}^2 dz \right)^{1/2} \left(\int_{-\infty}^{+\infty} \left\| (D_{\gamma, \xi} - iz)^{-1} \phi_\xi \right\|_{L_\xi^2}^2 dz \right)^{1/2} \\ &\leq \frac{\alpha}{2\pi} \|V_{h, \xi}\|_{\mathcal{B}(L_\xi^2)} \| |D_\xi|^{1/2} |D_{\gamma, \xi}|^{-1/2} \phi \|_{\mathcal{B}(L_\xi^2)} \| |D_{\gamma, \xi}|^{-1/2} \| \psi_\xi \|_{L_\xi^2} \| \phi_\xi \|_{L_\xi^2} \\ &\leq \frac{\alpha}{2} C_{EE} (1 - \kappa_r)^{-1/2} \lambda_{0, r}^{-1/2} \|h\|_{X \cap Y} \| \psi_\xi \|_{L_\xi^2} \| \phi_\xi \|_{L_\xi^2}. \end{aligned} \quad (5.11)$$

Hence we obtain (5.7), i.e.,

$$\| |D^0|^{1/2} dQ(\gamma) h \|_Y \leq \frac{\alpha}{2} C_{EE} (1 - \kappa_r)^{-1/2} \lambda_{0, r}^{-1/2} \|h\|_{X \cap Y}.$$

As $A > \frac{\alpha}{2} C_{EE} (1 - \kappa)^{-1/2} \lambda_0^{-1/2}$, we know that there exists r small enough such that

$$\frac{\alpha}{2} C_{EE} (1 - \kappa_r)^{-1/2} \lambda_{0,r}^{-1/2} < A - r.$$

This proves the first inequality.

For the second inequality, we have

$$\begin{aligned} dQ_\xi(\gamma)h - dQ_\xi(\gamma')h &= -\frac{\alpha^2}{2\pi} \int_{-\infty}^{+\infty} (D_{\gamma,\xi} - iz)^{-1} V_{\gamma'-\gamma,\xi} (D_{\gamma',\xi} - iz)^{-1} V_{h,\xi} (D_{\gamma,\xi} - iz)^{-1} dz \\ &\quad - \frac{\alpha^2}{2\pi} \int_{-\infty}^{+\infty} (D_{\gamma',\xi} - iz)^{-1} V_{h,\xi} (D_{\gamma,\xi} - iz)^{-1} V_{\gamma'-\gamma,\xi} (D_{\gamma',\xi} - iz)^{-1} dz. \end{aligned}$$

Proceeding as above, we get (5.8). The fact that $Q \in C^{1,\text{lip}}(\Gamma_{\leq q,r}; \mathcal{B}(L^2, H^{1/2}))$ follows from (5.7) and (5.8). \square

Lemma 5.7. *Assume that $\kappa < 1$ and let $A > \frac{\alpha}{2} C_{EE} (1 - \kappa)^{-1/2} \lambda_0^{-1/2}$. Then, for $r > 0$ small enough, the map $T : \gamma \rightarrow P_\gamma^+ \gamma P_\gamma^+$ is well-defined and of class $\mathcal{C}^{1,1}$ on $\Gamma_{\leq q,r}$ with values in $X \cap Y$. Moreover, for any $\gamma \in \Gamma_{\leq q,r}$,*

$$\begin{aligned} \|T^2(\gamma) - T(\gamma)\|_{X \cap Y} &\leq 2A \left(\max\{\|T(\gamma)\|_{D^0}^{1/2} \|_{\mathfrak{S}_{1,1}}, \|T(\gamma)\|_Y\} \right. \\ &\quad \left. + \frac{Aq^+}{2} \|\gamma - T(\gamma)\|_{X \cap Y} \right) \|T(\gamma) - \gamma\|_{X \cap Y}. \end{aligned} \quad (5.12)$$

Moreover, there are two positive constants C_κ, L_κ such that

$$\forall \gamma \in \Gamma_{\leq q,r}, \quad \|dT(\gamma)\|_{\mathcal{B}(X \cap Y)} \leq C_\kappa (1 + \max\{\|\gamma\|_{D^0}^{1/2} \|_{\mathfrak{S}_{1,1}}, \|\gamma\|_Y\}), \quad (5.13)$$

and

$$\forall \gamma, \gamma' \in \Gamma_{\leq q,r}, \quad \|dT(\gamma') - dT(\gamma)\|_{\mathcal{B}(X \cap Y)} \leq L_\kappa (1 + \max\{\|\gamma\|_{D^0}^{1/2} \|_{\mathfrak{S}_{1,1}}, \|\gamma\|_Y\}) \|\gamma' - \gamma\|_{X \cap Y}. \quad (5.14)$$

Proof. Let $\gamma, \gamma' \in \Gamma_{\leq q,r}$. Then $P_\gamma^+ - P_{\gamma'}^+$ can be written as

$$P_\gamma^+ - P_{\gamma'}^+ = \int_0^1 dQ(\gamma' + t(\gamma - \gamma'))(\gamma - \gamma') dt.$$

From (5.7),

$$\|D^0\|^{1/2} (P_\gamma^+ - P_{\gamma'}^+) \|_Y \leq (A - r) \|\gamma - \gamma'\|_{X \cap Y}.$$

For the estimate (5.12), we have

$$\begin{aligned} T^2(\gamma) - T(\gamma) &= (P_{T(\gamma)}^+ - P_\gamma^+) T(\gamma) \left(P_{T(\gamma)}^+ - P_\gamma^+ + P_\gamma^+ \right) + P_\gamma^+ T(\gamma) (P_{T(\gamma)}^+ - P_\gamma^+) \\ &= (P_{T(\gamma)}^+ - P_\gamma^+) T(\gamma) + T(\gamma) (P_{T(\gamma)}^+ - P_\gamma^+) + (P_{T(\gamma)}^+ - P_\gamma^+) T(\gamma) (P_{T(\gamma)}^+ - P_\gamma^+). \end{aligned}$$

Then

$$\begin{aligned} \|T^2(\gamma) - T(\gamma)\|_{X \cap Y} &\leq \|(P_{T(\gamma)}^+ - P_\gamma^+) T(\gamma)\|_{X \cap Y} \\ &\quad + \|T(\gamma) (P_{T(\gamma)}^+ - P_\gamma^+)\|_{X \cap Y} + \|(P_{T(\gamma)}^+ - P_\gamma^+) T(\gamma) (P_{T(\gamma)}^+ - P_\gamma^+)\|_{X \cap Y}. \end{aligned}$$

We have

$$\|T(\gamma) (P_{T(\gamma)}^+ - P_\gamma^+)\|_{X \cap Y} \leq \|D^0\|^{1/2} (P_{T(\gamma)}^+ - P_\gamma^+) \|_Y \max\{\|T(\gamma)\|_{D^0}^{1/2} \|_{\mathfrak{S}_{1,1}}, \|T(\gamma)\|_Y\},$$

and

$$\|(P_{T(\gamma)}^+ - P_\gamma^+) T(\gamma) (P_{T(\gamma)}^+ - P_\gamma^+)\|_{X \cap Y} \leq \|D^0\|^{1/2} (P_{T(\gamma)}^+ - P_\gamma^+) \|_Y^2 \|T(\gamma)\|_{\mathfrak{S}_{1,1} \cap Y}.$$

Notice that $\|T(\gamma)\|_{\mathfrak{S}_{1,1} \cap Y} \leq \|\gamma\|_{\mathfrak{S}_{1,1} \cap Y} \leq q^+ + 2r$. Gathering together these estimates with $(A - r)(q^+ + 2r) \leq Aq^+$ for r small enough, we obtain (5.12).

We turn now to the proof of (5.13) and (5.14). From Lemma 5.6, T is in $C^1(\Gamma_{\leq q,r})$ with

$$dT(\gamma)h = (dQ_\gamma h)\gamma P_\gamma + P_\gamma \gamma (dQ_\gamma h) + P_\gamma h P_\gamma.$$

Notice that for any $\gamma \in \Gamma_{\leq q,r}$ and r small enough,

$$\| |D^0|^{1/2} P_\gamma^+ |D^0|^{-1/2} \|_Y \leq (1 - \kappa_r)^{-1/2} \| |D_\gamma|^{1/2} P_\gamma^+ |D^0|^{-1/2} \|_Y \leq \frac{(1 + \kappa_r)^{1/2}}{(1 - \kappa_r)^{1/2}} \leq 2 \frac{(1 + \kappa)^{1/2}}{(1 - \kappa)^{1/2}}. \quad (5.15)$$

Then, for r small enough,

$$\begin{aligned} \|dT(\gamma)\|_{\mathcal{B}(X \cap Y)} &\leq C(1 + \| |D^0|^{1/2} P_\gamma^+ |D^0|^{-1/2} \|_Y^2)(1 + \max\{\|\gamma\|_{\mathfrak{S}_{1,1}}, \|\gamma\|_Y\})(\|dQ_\gamma h\|_Y + \|h\|_{X \cap Y}) \\ &\leq C_\kappa(1 + \max\{\|\gamma\|_{\mathfrak{S}_{1,1}}, \|\gamma\|_Y\}). \end{aligned}$$

Finally, for the term $dT(\gamma') - dT(\gamma)$, we have

$$\begin{aligned} dT_\xi(\gamma')h - dT_\xi(\gamma)h &= (dQ_{\gamma,\xi}h)\gamma_\xi P_{\gamma,\xi} + P_{\gamma,\xi}\gamma_\xi(dQ_{\gamma,\xi}h) + P_{\gamma,\xi}h_\xi P_{\gamma,\xi} \\ &\quad - (dQ_{\gamma',\xi}h)\gamma'_\xi P_{\gamma',\xi} - P_{\gamma',\xi}\gamma'_\xi(dQ_{\gamma',\xi}h) - P_{\gamma',\xi}h_\xi P_{\gamma',\xi}. \end{aligned}$$

Proceeding in the same way as for (5.13), we can get (5.14). \square

We now show that T satisfies all the assumptions in [29, Proposition 2.2]. Before going further, we also define

$$\mathcal{U}_r := \left\{ \gamma \in \Gamma_{\leq q,r} \mid \max\{\|\gamma\|_{\mathfrak{S}_{1,1}}, \|\gamma\|_Y\} + M\|T(\gamma) - \gamma\|_{X \cap Y} < \tau \right\}.$$

Proposition 5.8. *Let κ, A, τ be as in Definition 5.2. Then for r small enough, T is in $C^0(\overline{\mathcal{U}_r}) \cap C^{1, \text{lip}}(\mathcal{U}_r, X \cap Y)$ be such that $T(\mathcal{U}_r) \subset \mathcal{U}_r$ satisfies the following estimates*

$$\sup_{\gamma \in \mathcal{U}_r} \|dT(\gamma)\|_{X \cap Y} < \infty, \quad \sup_{\gamma \in \mathcal{U}_r} \|T(\gamma) - \gamma\|_{X \cap Y} < \infty$$

and

$$\forall \gamma \in \mathcal{U}_r, \quad \|T^2(x) - T(x)\|_{X \cap Y} \leq k\|T(x) - x\|_{X \cap Y}$$

with $k := 2A\tau < 1$.

Proof. For any $\gamma \in \mathcal{U}_r$, we have

$$\|T(\gamma)\|_{\mathfrak{S}_{1,1}} \leq \|\gamma\|_{\mathfrak{S}_{1,1}} + \|(\gamma - T(\gamma))\|_{\mathfrak{S}_{1,1}} \leq \|\gamma\|_{\mathfrak{S}_{1,1}} + \|\gamma - T(\gamma)\|_X$$

and

$$\|T(\gamma)\|_Y \leq \|\gamma\|_Y \leq \|\gamma\|_Y + \|\gamma - T(\gamma)\|_Y.$$

As a result, as $M \geq \frac{2+q^+A}{2}$, (5.12) implies that

$$\|T^2(\gamma) - T(\gamma)\|_{X \cap Y} \leq k\|T(\gamma) - \gamma\|_X$$

with $k = 2a\tau < 1$. Moreover, using the inequality $M \geq \frac{1}{1-2A\tau}$,

$$\begin{aligned} \max\{\|T(\gamma)\|_{\mathfrak{S}_{1,1}}, \|T(\gamma)\|_Y\} + M\|T^2(\gamma) - T(\gamma)\|_{X \cap Y} \\ \leq \max\{\|\gamma\|_{\mathfrak{S}_{1,1}}, \|\gamma\|_Y\} + (1 + Mk)\|T(\gamma) - \gamma\|_{X \cap Y} < \tau. \end{aligned}$$

So $T(\gamma) \in \mathcal{U}_r$.

The fact that $\sup_{\gamma \in \mathcal{U}_r} \|dT(\gamma)\|_{X \cap Y} < \infty$ and dT is Lipschitz continuous on \mathcal{U}_r follows from (5.13) and (5.14). Besides, using (5.15) and $\gamma \in \mathcal{U}$, we have

$$\|T(\gamma) - \gamma\|_{X \cap Y} \leq \|T(\gamma)\|_{X \cap Y} + \|\gamma\|_{X \cap Y} \leq \frac{2}{1 - \kappa} \|\gamma\|_{X \cap Y}.$$

This ends the proof. \square

Notice that \mathcal{U}_r is an open subset of $\Gamma_{\leq q}$. Notice that $\Gamma_{\leq q} \subset \Gamma_{\leq q,r}$ and $\mathcal{U} \subset \mathcal{U}_r$ for $r > 0$. Then Proposition 5.4 follows from Proposition 5.8 and [29, Proposition 2.1 and Proposition 2.2] by choosing $U = \mathcal{U}_r$, $\Gamma = \Gamma_{\leq q,r}$ and $\mathcal{X} := \text{span}\{\gamma - \gamma' \mid \gamma, \gamma' \in \Gamma_{\leq q,r}\} = X \cap Y$. Here the notation \mathcal{X} , U and Γ is given in [29, Proposition 2.2]. The proof of (5.4) is exactly the same as in [29, Theorem 2.10]. This ends the proof of Proposition 5.4.

6 Existence of minimizers in the set B_R

In this section, we are going to prove the existence of minimizers of $I_{\leq q, R}$ (i.e., Proposition 3.4).

According to Lemma 4.15, there is a minimizing sequence $(\gamma_n)_{n \geq 1}$ in $B_R \cap \Gamma_q^+$ that is uniformly bounded in $X \cap Y$. We split $(\gamma_n)_{n \geq 1}$ into two parts: $(\tilde{\gamma}_n)_{n \geq 1}$ and $(\gamma_n - \tilde{\gamma}_n)_{n \geq 1}$ where, for each n ,

$$\tilde{\gamma}_n := p_n \gamma_n p_n \quad \text{with} \quad p_n := 1_{[0, e]}(D_{\gamma_n}) \quad (6.1)$$

with $e > c^*(q+1)(1-\kappa)^{-1}$ defined in Lemma 4.11. An important fact in this lemma is that for almost every $\xi \in Q_\ell^*$, the rank of $p_{n, \xi}$, and therefore of $\tilde{\gamma}_{n, \xi}$, is at most $q+M$. We prove in Lemma 6.1 that, for each $n \geq 1$, $\tilde{\gamma}_n \in X_\infty^2$ whereas $\gamma_n \in X$; roughly speaking, we reach a $L^\infty(Q_\ell^*; H_\xi^1(Q_\ell))$ regularity instead of a $L^2(Q_\ell^*; H_\xi^{1/2}(Q_\ell))$ regularity for the associated eigenfunctions (Lemma 6.1). Hence $(\tilde{\gamma}_n)_{n \geq 1}$ is an approximate minimizing sequence with higher regularity than $(\gamma_n)_{n \geq 1}$.

The structure of the proof of Proposition 3.4 is as follows. In Subsection 6.1, we will show $\|\gamma_n - \tilde{\gamma}_n\|_X \rightarrow 0$ when n goes to infinity. In Subsection 6.2, we study the convergence of the kernel of $(W_{\tilde{\gamma}_n, \xi})_{n \geq 1}$. Then thanks to the constraint $\gamma_n \in B_R$, we deduce the strong convergence of $(V_{\gamma_n, \xi})_{n \geq 1}$. As a result, $\|P_{\gamma_n}^+ - P_{\tilde{\gamma}_n}^+\|_Y \rightarrow 0$. Hence in Subsection 6.3, we can pass to the limit in the energy and in the constraints.

6.1 Decomposition of minimizing sequences

We start with some regularity and bound results on $\tilde{\gamma}_n$.

Lemma 6.1. *Let $\kappa < 1$. Then the sequence $(\tilde{\gamma}_n)_{n \geq 1}$ and the sequence of kernels $(\tilde{\gamma}_{n, \xi}(\cdot, \cdot))_{n \geq 1}$ are uniformly bounded in X_∞^2 and $L^\infty(Q_\ell^*; H^1(Q_\ell \times Q_\ell))$, respectively.*

Proof. We first prove that $\|p_n\|_{X_\infty^2}$ is bounded. Let $(u_{n, k}(\xi))_{k \geq 1}$ be the normalized eigenfunctions of the operator $D_{\gamma_n, \xi}$ with the corresponding eigenvalues $\lambda_{n, k}(\xi)$ counted with multiplicity. Hence,

$$p_{n, \xi} = \sum_{k=1}^{+\infty} \delta_{n, k}(\xi) |u_{n, k}(\xi)\rangle \langle u_{n, k}(\xi)|$$

with $\delta_{n, k} = 1$ if $0 \leq \lambda_{n, k}(\xi) \leq e$ and $\delta_{n, k} = 0$ otherwise.

By Lemma 4.11, we know $|\{k \in \mathbb{N}^* \mid \delta_{n, k}(\xi) = 1\}| \leq q+M$. By (4.21), for any eigenfunction $u_{n, k}(\xi)$, we have $\|\delta_{n, k}(\xi) u_{n, k}(\xi)\|_{L^\infty(Q_\ell^*; H_\xi^1(Q_\ell))} \leq (1-\kappa)^{-1}e$. Now,

$$\|p_{n, \xi}\|_{X^2(\xi)} = \sum_{k=1}^{q+M} \delta_{n, k}(\xi) \|u_{n, k}(\xi)\|_{H_\xi^1}^2 \leq (q+M) \sup_{k \geq 1} \|\delta_{n, k}(\xi) u_{n, k}(\xi)\|_{H_\xi^1}^2.$$

Hence,

$$\|p_n\|_{X_\infty^2} \leq (q+M)(1-\kappa)^{-2}e^2.$$

Since $p_n = p_n^2$, $\tilde{\gamma}_n = p_n \tilde{\gamma}_n p_n$ and $0 \leq \tilde{\gamma}_n \leq 1_{L^2(\mathbb{R}^3)}$, we have

$$\begin{aligned} \|\tilde{\gamma}_n\|_{X_\infty^2} &= \| |D^0| \tilde{\gamma}_n |D^0| \|_{\mathfrak{S}_{1, \infty}} = \| |D^0| p_n \tilde{\gamma}_n p_n |D^0| \|_{\mathfrak{S}_{1, \infty}} \\ &\leq \|\tilde{\gamma}_n\|_Y \| |D^0| p_n \|_{\mathfrak{S}_{2, \infty}}^2 \leq \|p_n\|_{X_\infty^2} \leq (q+M)(1-\kappa)^{-2}e^2. \end{aligned}$$

In terms of kernels, it writes

$$\| |D_{\xi, x}| \tilde{\gamma}_{n, \xi}(\cdot, \cdot) \|_{L^2(Q_\ell \times Q_\ell)} = \| |D_\xi| \tilde{\gamma}_{n, \xi} \|_{\mathfrak{S}_2(\xi)} \leq \|\tilde{\gamma}_{n, \xi}\|_{X^2(\xi)} \leq (q+M)(1-\kappa)^{-2}e^2,$$

the same holding for $|D_{\xi, y}| \tilde{\gamma}_{n, \xi}(\cdot, \cdot)$. Thus, $\tilde{\gamma}_{n, \xi}(x, y) \in L^\infty(Q_\ell^*; H^1(Q_\ell \times Q_\ell))$, and

$$\|\tilde{\gamma}_{n, \xi}(\cdot, \cdot)\|_{L^\infty(Q_\ell^*; H^1(Q_\ell \times Q_\ell))} \leq 2(q+M)(1-\kappa)^{-2}e^2. \quad (6.2)$$

□

We begin the proof by showing the following result as in the case of molecules [29, Lemma 3.4].

Lemma 6.2. *Let $R > R_0 = q + M$. Under Assumption 3.1, whenever $\epsilon_P > (1 - \kappa)^{-1}c^*(q + 1)$, for any minimizing sequence $(\gamma_n)_{n \geq 1}$ of (3.5) in $\Gamma_{\leq q}^+ \cap B_R$ we have*

$$\widetilde{\text{Tr}}_{L^2}(\gamma_n) \rightarrow q, \quad \|\gamma_n - \tilde{\gamma}_n\|_X \rightarrow 0.$$

Proof. According to Proposition 5.1, any minimizing sequence $(\gamma_n)_{n \geq 1}$ in $\Gamma_{\leq q}^+ \cap B_R$ satisfies (5.1). By Lemma 4.12, the minimizers of the problem

$$\inf_{\gamma \in \Gamma_{\leq q}, \gamma = P_{\gamma_n}^+ \gamma P_{\gamma_n}^+} \int_{Q_\ell^*} \text{Tr}_{L_\xi^2}[(D_{\gamma_n, \xi} - \epsilon_P)\gamma_\xi] d\xi$$

are of the form $\gamma'_n := \int_{Q_\ell^*}^\oplus 1_{[0, \nu_n]}(D_{\gamma_n, \xi}) d\xi + \delta$ with some $0 \leq \delta \leq \int_{Q_\ell^*}^\oplus 1_{\nu_n}(D_{\gamma_n, \xi}) d\xi$ such that $\widetilde{\text{Tr}}_{L^2}(\gamma'_n) = q$ and for some $\nu_n \in [0, (1 - \kappa)^{-1}c^*(q + 1)]$. We denote

$$\pi_n := \int_{Q_\ell^*}^\oplus 1_{(e, \infty)}(D_{\gamma_n, \xi}) d\xi, \quad \pi'_n := \int_{Q_\ell^*}^\oplus 1_{(\nu_n, e]}(D_{\gamma_n, \xi}) d\xi, \quad \pi''_n := \int_{Q_\ell^*}^\oplus 1_{[0, \nu_n]}(D_{\gamma_n, \xi}) d\xi.$$

We can write $p_n = \pi'_n + \pi''_n$ and $\gamma'_n = \pi''_n \gamma'_n \pi''_n$. Proceeding as for (4.26) and (4.27), we have

$$\begin{aligned} & \int_{Q_\ell^*} \text{Tr}_{L_\xi^2}[(D_{\gamma_n, \xi} - \epsilon_P)\gamma_{n, \xi}] d\xi - \int_{Q_\ell^*} \text{Tr}_{L_\xi^2}[(D_{\gamma_n, \xi} - \epsilon_P)\gamma'_{n, \xi}] d\xi \\ &= \int_{Q_\ell^*} \text{Tr}_{L_\xi^2}[(D_{\gamma_n, \xi} - \nu_n)\pi_{n, \xi} \gamma_{n, \xi} \pi_{n, \xi}] d\xi + \int_{Q_\ell^*} \text{Tr}_{L_\xi^2}[(D_{\gamma_n, \xi} - \nu_n)\pi'_{n, \xi} \gamma_{n, \xi} \pi'_{n, \xi}] d\xi \\ & \quad + \int_{Q_\ell^*} \text{Tr}_{L_\xi^2}[(D_{\gamma_n, \xi} - \nu_n)(\pi''_{n, \xi} \gamma_{n, \xi} \pi''_{n, \xi} - 1_{[0, \nu_n]}(D_{\gamma_n, \xi}))] d\xi + (\epsilon_P - \nu_n) \left(q - \widetilde{\text{Tr}}_{L^2}(\gamma_n) \right). \end{aligned}$$

We observe that the four terms in the right-hand side of the above equation are non-negative whereas, from Proposition 5.1, their sum goes to 0 as n goes to infinity. Therefore,

$$\int_{Q_\ell^*} \text{Tr}_{L_\xi^2}(\gamma_{n, \xi}) d\xi \rightarrow q \quad \text{and} \quad \int_{Q_\ell^*} \text{Tr}_{L_\xi^2}[(D_{\gamma_n, \xi} - \nu_n)\pi_{n, \xi} \gamma_{n, \xi} \pi_{n, \xi}] d\xi \rightarrow 0.$$

But $\pi_{n, \xi}(D_{\gamma_n, \xi} - \nu_n)\pi_{n, \xi} \geq (e - \nu_n)\pi_{n, \xi}$ and $\pi_{n, \xi}(D_{\gamma_n, \xi} - \nu_n)\pi_{n, \xi} = \pi_{n, \xi}(|D_{\gamma_n, \xi}| - \nu_n)\pi_{n, \xi}$. So taking a convex combination of these two estimates leads to

$$\frac{e}{e - c^*(q + 1)(1 - \kappa)^{-1}} \pi_{n, \xi}(D_{\gamma_n, \xi} - \nu_n)\pi_{n, \xi} \geq \frac{e}{e - \nu_n} (D_{\gamma_n, \xi} - \nu_n)\pi_{n, \xi} \geq \pi_{n, \xi} |D_{\gamma_n, \xi}| \pi_{n, \xi}.$$

Hence

$$\|\pi_n \gamma_n \pi_n\|_X = \int_{Q_\ell^*} \text{Tr}_{L_\xi^2}[\pi_{n, \xi} |D_\xi| \pi_{n, \xi} \gamma_{n, \xi}] d\xi \leq (1 - \kappa)^{-1} \int_{Q_\ell^*} \text{Tr}_{L_\xi^2}[\pi_{n, \xi} |D_{\gamma_n, \xi}| \pi_{n, \xi} \gamma_{n, \xi}] d\xi \rightarrow 0.$$

It remains to study the limit of $h_n := \pi_n \gamma_n p_n$ as n goes to infinity. Since $(\gamma_n)^2 \leq \gamma_n$, we have

$$(\pi_n \gamma_n \pi_n)^2 + h_n h_n^* = \pi_n (\gamma_n)^2 \pi_n \leq \pi_n \gamma_n \pi_n.$$

Hence

$$\int_{Q_\ell^*} \text{Tr}_{L_\xi^2}(|D_{\gamma_n, \xi}|^{1/2} h_{n, \xi} h_{n, \xi}^* |D_{\gamma_n, \xi}|^{1/2}) d\xi \rightarrow 0.$$

Taking any operator A in Y , by the Cauchy-Schwarz inequality,

$$\begin{aligned} & \left| \int_{Q_\ell^*} \text{Tr}_{L_\xi^2}[A_\xi |D_{\gamma_n, \xi}|^{1/2} u_{n, \xi}^* |D_{\gamma_n, \xi}|^{1/2}] d\xi \right| \\ & \leq \frac{\ell^3}{(2\pi)^3} \left\| \text{Tr}_{L_\xi^2}[|D_{\gamma_n, \xi}|^{1/2} p_{n, \xi} A_\xi^* A_\xi p_{n, \xi} |D_{\gamma_n, \xi}|^{1/2}] \right\|_{L^\infty}^{1/2} \\ & \quad \times \left(\int_{Q_\ell^*} \text{Tr}_{L_\xi^2}[|D_{\gamma_n, \xi}|^{1/2} h_{n, \xi} h_{n, \xi}^* |D_{\gamma_n, \xi}|^{1/2}] d\xi \right)^{1/2}. \end{aligned}$$

By Lemma 4.11, there is $M > 0$ 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

$$\left\| |D_{\gamma_n}|^{1/2} h_n |D_{\gamma_n}|^{1/2} \right\|_{\mathfrak{S}_{1,1}} \rightarrow 0.$$

Hence, $\|u_n\|_X \rightarrow 0$. Finally, $\|\gamma_n - \tilde{\gamma}_n\|_X \leq \|\pi_n \gamma_n \pi_n\|_X + 2\|h_n\|_X \rightarrow 0$. \square

By Lemma 6.1, up to the extraction of a subsequence, there is γ_* in $X_\infty^2 \cap Y$, such that

$$\tilde{\gamma}_n \xrightarrow{*} \gamma_* \quad \text{for the weak } * \text{-convergence in } X_\infty^2 \cap Y, \quad (6.3)$$

since X_∞^2 is a subspace of $\mathfrak{S}_{1,\infty}$ which is the dual space of $\mathfrak{S}_{\infty,1}$ and Y is the dual space of $\mathfrak{S}_{1,1}$. We immediately get the following.

Lemma 6.3 (Strong convergence of the density). *The sequence $\rho_{\tilde{\gamma}_n}^{1/2}$ converges strongly to $\rho_{\gamma_*}^{1/2}$ in $H^s(Q_\ell)$ with $0 \leq s < 1$, thus in $L^p(Q_\ell)$ for every $1 \leq p < 6$. In particular, whenever $\epsilon_P > (1 - \kappa)^{-1} c^*(q + 1)$, we have $\int_{Q_\ell} \rho_{\gamma_*} dx = q$.*

Proof. The proof is the same as in [5, p. 730] and relies on $\tilde{\gamma}_n \in X_\infty^2$. The fact that the limit of $\rho_{\tilde{\gamma}_n}^{1/2}$ is exactly $\rho_{\gamma_*}^{1/2}$ follows from [5, Eqn. (4.51) and Eqn. (4.55)] since it implies $\rho_{\tilde{\gamma}_n} \rightarrow \rho_{\gamma_*}$ in $L^1(Q_\ell)$. \square

6.2 Convergence of $(V_{\gamma_n,\xi})_{n \geq 1}$

Before going further, we introduce the following functional spaces: For $p \in [1, +\infty]$, $s \in (0, +\infty]$, let $L^p H_\xi^s := L^p(Q_\ell^*; H_\xi^s(Q_\ell \times Q_\ell; \mathcal{M}_4(\mathbb{C})))$ defined by

$$L^p H_\xi^s := \left\{ f(\cdot, x, y) \in L_{-\xi,x}^2(Q_\ell; \mathbb{C}^4) \otimes L_{\xi,y}^2(Q_\ell; \mathbb{C}^4) \mid \|f\|_{L^p(Q_\ell^*; H^s(Q_\ell \times Q_\ell))} < \infty \right\}$$

endowed with the norm $\|f\|_{L^p H_\xi^s} := \|f\|_{L^p(Q_\ell^*; H^s(Q_\ell \times Q_\ell))}$; then we also define the function space $W^{1,p} H_\xi^s := W^{1,p}(Q_\ell^*; H_\xi^s(Q_\ell \times Q_\ell)) \subset L^p H_\xi^s$ endowed with the norm

$$\|f\|_{W^{1,p} H_\xi^s} := \|f\|_{L^p H_\xi^s} + \|\nabla_\xi f(\xi, \cdot, \cdot)\|_{L^p H_\xi^s}$$

and the Hölder continuity function space $C^{0,\mu} H_\xi^s := C^{0,\mu}(Q_\ell^*; H_\xi^s(Q_\ell \times Q_\ell))$ for $\mu \in (0, 1)$, endowed with the norm

$$\|f\|_{C^{0,\mu} H_\xi^s} := \|f\|_{L^\infty H_\xi^s} + \sup_{\xi \neq \xi' \in Q_\ell^*} \frac{\|f(\xi, \cdot, \cdot) - f(\xi', \cdot, \cdot)\|_{H^s(Q_\ell \times Q_\ell)}}{|\xi - \xi'|^\mu}.$$

For any functions $f \in L^p L_\xi^2$ and $g \in L^{p'} L_\xi^2$ with $p \in [1, \infty)$ and $1/p + 1/p' = 1$, we define the product

$$\langle f, g \rangle = \int_{Q_\ell^*} \iint_{Q_\ell \times Q_\ell} \mathrm{Tr}_4[f^* g] dx dy d\xi. \quad (6.4)$$

It is easy to see that $(L^p L_\xi^2, L^{p'} L_\xi^2, \langle \cdot, \cdot \rangle)$ forms a dual pair.

First of all, we study the convergence of the kernel of $W_{\tilde{\gamma}_n,\xi}$. Recall that

$$W_{\gamma,\xi} = W_{\geq m,\gamma,\xi} + W_{< m,\gamma,\xi}, \quad \forall m \in \mathbb{N}, m \geq 2$$

where for $\eta \in 2Q_\ell^*$ and $x \in 2Q_\ell$, the kernels of $W_{\geq m,\gamma,\xi}$ and $W_{< m,\gamma,\xi}$ are respectively

$$W_{\geq m,\gamma,\xi}(x, y) := \int_{Q_\ell^*} W_{\geq m,\ell}^\infty(\xi' - \xi, x - y) \gamma_{\xi'}(x, y) d\xi'$$

and

$$W_{< m,\gamma,\xi}(x, y) := \int_{Q_\ell^*} W_{< m,\ell}^\infty(\xi' - \xi, x - y) \gamma_{\xi'}(x, y) d\xi'.$$

Lemma 6.4 (Convergence of the kernel of $(W_{\tilde{\gamma}_n, \xi})_{n \geq 1}$). *We have the following properties:*

$$(a) \quad W_{< m, \tilde{\gamma}_n, \xi} \rightarrow W_{< m, \gamma_*, \xi} \quad \text{in } L^\infty(Q_\ell^*; L_\xi^2(Q_\ell \times Q_\ell)).$$

$$(b) \quad |D_{\xi, x}|^{-1/2} |D_{\xi, y}|^{-1/2} W_{\geq m, \tilde{\gamma}_n, \xi} \rightarrow |D_{\xi, x}|^{-1/2} |D_{\xi, y}|^{-1/2} W_{\geq m, \gamma_*, \xi} \quad \text{in } L^\infty(Q_\ell^*; L_\xi^2(Q_\ell \times Q_\ell)).$$

Proof. We will prove the boundedness of the sequences, and then deduce the strong convergence by the Rellich–Kondrachov Theorem.

Uniform boundedness of $W_{< m, \tilde{\gamma}_n, \xi}$ in $C^{0, \mu}(Q_\ell^*; H_\xi^1(Q_\ell \times Q_\ell))$. It is based on Lemma 6.1, particularly (6.2). Recall

$$W_{< m, \ell}^\infty(\xi - \xi', x - y) = \frac{4\pi}{\ell^3} \sum_{\substack{|k|_\infty < m \\ k \in \mathbb{Z}^3}} \frac{1}{\left| \frac{2\pi k}{\ell} - (\xi - \xi') \right|^2} e^{i\left(\frac{2\pi k}{\ell} - (\xi - \xi')\right) \cdot (x - y)}.$$

Thus,

$$\begin{aligned} & \|W_{< m, \tilde{\gamma}_n, \eta}^\infty - W_{< m, \tilde{\gamma}_n, \eta'}^\infty\|_{H^1(Q_\ell \times Q_\ell)} \\ & \leq \frac{4\pi}{\ell^3} \sum_{\substack{|k|_\infty \leq m-1 \\ k \in \mathbb{Z}^3}} \left\| \int_{Q_\ell^*} \frac{e^{i\left(\frac{2\pi k}{\ell} - (\eta - \xi')\right) \cdot (x - y)}}{\left| \frac{2\pi k}{\ell} - (\eta - \xi') \right|^2} \tilde{\gamma}_{n, \xi'} d\xi' - \int_{Q_\ell^*} \frac{e^{i\left(\frac{2\pi k}{\ell} - (\eta' - \xi')\right) \cdot (x - y)}}{\left| \frac{2\pi k}{\ell} - (\eta' - \xi') \right|^2} \tilde{\gamma}_{n, \xi'} d\xi' \right\|_{H^1(Q_\ell \times Q_\ell)}. \end{aligned}$$

For each term on the right-hand side, we have

$$\begin{aligned} & \left\| \int_{Q_\ell^*} \frac{e^{i\left(\frac{2\pi k}{\ell} - (\eta - \xi')\right) \cdot (x - y)}}{\left| \frac{2\pi k}{\ell} - (\eta - \xi') \right|^2} \tilde{\gamma}_{n, \xi'} d\xi' - \int_{Q_\ell^*} \frac{e^{i\left(\frac{2\pi k}{\ell} - (\eta' - \xi')\right) \cdot (x - y)}}{\left| \frac{2\pi k}{\ell} - (\eta' - \xi') \right|^2} \tilde{\gamma}_{n, \xi'} d\xi' \right\|_{H^1(Q_\ell \times Q_\ell)} \\ & \leq \int_{Q_\ell^*} \left| \frac{1}{\left| \frac{2\pi k}{\ell} - (\eta' - \xi') \right|^2} - \frac{1}{\left| \frac{2\pi k}{\ell} - (\eta - \xi') \right|^2} \right| \left\| e^{i\left(\frac{2\pi k}{\ell} - (\eta - \xi')\right) \cdot (x - y)} \tilde{\gamma}_{n, \xi'} \right\|_{H_\eta^1(Q_\ell \times Q_\ell)} d\xi' \\ & \quad + \left\| \int_{Q_\ell^*} \frac{e^{i\left(\frac{2\pi k}{\ell} - (\eta - \xi')\right) \cdot (x - y)}}{\left| \frac{2\pi k}{\ell} - (\eta' - \xi') \right|^2} \tilde{\gamma}_{n, \xi'} d\xi' - \int_{Q_\ell^*} \frac{e^{i\left(\frac{2\pi k}{\ell} - (\eta' - \xi')\right) \cdot (x - y)}}{\left| \frac{2\pi k}{\ell} - (\eta' - \xi') \right|^2} \tilde{\gamma}_{n, \xi'} d\xi' \right\|_{H^1(Q_\ell \times Q_\ell)}. \end{aligned}$$

As $\eta, \xi' \in Q_\ell^*$, according to (6.2), we get

$$\left\| e^{i\left(\frac{2\pi k}{\ell} - (\eta - \xi')\right) \cdot (x - y)} \tilde{\gamma}_{n, \xi'} \right\|_{H_\eta^1(Q_\ell \times Q_\ell)} \leq C \|\tilde{\gamma}_{n, \xi'}\|_{H_{\xi'}^1(Q_\ell \times Q_\ell)} \leq C(q + M)(1 - \kappa)^{-2} e^2.$$

By the Hölder continuity of the function $\eta \mapsto \int_{Q_\ell^*} \frac{1}{|\eta - \eta'|^2} d\eta'$, there is a $0 < \mu < 1$ such that

$$\begin{aligned} & \int_{Q_\ell^*} \left| \frac{1}{\left| \frac{2\pi k}{\ell} - (\eta' - \xi') \right|^2} - \frac{1}{\left| \frac{2\pi k}{\ell} - (\eta - \xi') \right|^2} \right| \left\| e^{i\left(\frac{2\pi k}{\ell} - (\eta - \xi')\right) \cdot (x - y)} \tilde{\gamma}_{n, \xi'} \right\|_{H_\eta^1(Q_\ell \times Q_\ell)} d\xi' \\ & \leq C(q + M)(1 - \kappa)^{-2} e^2 |\eta - \eta'|^\mu. \end{aligned}$$

For the last term, note that $|e^{-i\eta \cdot z} - e^{-i\eta' \cdot z}| \leq \|\nabla_\eta e^{i\eta \cdot z}\|_{L^\infty} |\eta - \eta'| \leq C|\eta - \eta'|$ and $|\nabla_z(e^{-i\eta \cdot z} - e^{-i\eta' \cdot z})| \leq C|\eta - \eta'|$. We get

$$\begin{aligned} & \left\| \int_{Q_\ell^*} \frac{e^{i\left(\frac{2\pi k}{\ell} - (\eta - \xi')\right) \cdot (x - y)}}{\left| \frac{2\pi k}{\ell} - (\eta' - \xi') \right|^2} \tilde{\gamma}_{n, \xi'} d\xi' - \int_{Q_\ell^*} \frac{e^{i\left(\frac{2\pi k}{\ell} - (\eta' - \xi')\right) \cdot (x - y)}}{\left| \frac{2\pi k}{\ell} - (\eta' - \xi') \right|^2} \tilde{\gamma}_{n, \xi'} d\xi' \right\|_{H^1(Q_\ell \times Q_\ell)} \\ & \leq \int_{Q_\ell^*} \frac{C|\eta - \eta'|}{\left| \frac{2\pi k}{\ell} - (\eta' - \xi') \right|^2} \|\tilde{\gamma}_{n, \xi'}\|_{H_{\xi'}^1(Q_\ell \times Q_\ell)} d\xi' \\ & \leq C(q + M)(1 - \kappa)^{-2} e^2 |\eta - \eta'|. \end{aligned}$$

We finally get that there is $\mu \in (0, 1)$ such that

$$\|W_{< m, \tilde{\gamma}_n, \xi}\|_{C^{0, \mu}(Q_\ell^*; H_\xi^1(Q_\ell \times Q_\ell))} \leq C(q + M)(1 - \kappa)^{-2} e^2.$$

Boundedness of $W_{\geq m, \tilde{\gamma}_n, \xi}$ in $W^{1, \infty}(Q_\ell^*; L^2(Q_\ell \times Q_\ell))$. For $\beta = 0$ or 1 ,

$$\|\nabla_\xi^\beta W_{\geq m, \tilde{\gamma}_n, \xi}\|_{L^\infty(Q_\ell^*; L^2(Q_\ell^* \times Q_\ell^*))} \leq \int_{Q_\ell^*} \|\nabla_\xi^\beta W_{\geq m, \ell}(\xi - \xi') \tilde{\gamma}_{n, \xi'}\|_{L^\infty(Q_\ell^*; L_\xi^2(Q_\ell^* \times Q_\ell^*))} d\xi'.$$

By Corollary B.2 and Lemma B.3, we know

$$\|\nabla_\xi W_{\geq m, \ell}(\xi - \xi', x - y) \tilde{\gamma}_{n, \xi'}\|_{L^2(Q_\ell \times Q_\ell)} \leq C \|\tilde{\gamma}_{n, \xi'}\|_{H^1(Q_\ell \times Q_\ell)},$$

and

$$\|W_{\geq m, \ell}(\xi - \xi', x - y) \tilde{\gamma}_{n, \xi'}\|_{L^2(Q_\ell \times Q_\ell)} \leq C \|\tilde{\gamma}_{n, \xi'}\|_{H^1(Q_\ell \times Q_\ell)}.$$

Thus,

$$\|W_{\geq m, \tilde{\gamma}_n, \xi}\|_{W^{1, \infty}(Q_\ell^*; L^2(Q_\ell \times Q_\ell))} \leq C(q + M)(1 - \kappa)^{-2} e^2.$$

Convergence. Thanks to Rellich–Kondrachov Theorem and the boundedness of the sequences, these two sequences converge strongly up to subsequences. Now, we are going to prove that the limits are the kernels $W_{< m, \gamma_*, \xi}$ and $W_{\geq m, \gamma_*, \xi}$ respectively.

It suffices to prove that

$$W_{< m, \tilde{\gamma}_n, \xi} \xrightarrow{*} W_{< m, \gamma_*, \xi} \quad \text{and} \quad W_{\geq m, \tilde{\gamma}_n, \xi} \xrightarrow{*} W_{\geq m, \gamma_*, \xi} \quad (6.5)$$

in $L^\infty(Q_\ell^*; L^2(Q_\ell \times Q_\ell))$.

By Young's convolution inequality,

$$\begin{aligned} \|W_{< m, g, \xi}\|_{\mathfrak{S}_{\infty, 1}} &\leq \|W_{< m, g, \xi}\|_{\mathfrak{S}_{2, 1}} = \|W_{< m, g, \xi}\|_{L^1(Q_\ell^*; L^2(Q_\ell \times Q_\ell))} \\ &\leq \|W_{< m, \ell}(\xi, x - y)\|_{L^1(Q_\ell^*; L^\infty(Q_\ell \times Q_\ell))} \|g_{\xi'}(x, y)\|_{L^1(Q_\ell^*; L^2(Q_\ell \times Q_\ell))}. \end{aligned}$$

Then by (6.3) and using (6.4), for any $g_\xi(x, y) \in L^1(Q_\ell^*; L_\xi^2(Q_\ell \times Q_\ell))$,

$$\begin{aligned} \langle g_\xi, W_{< m, \tilde{\gamma}_n, \xi} \rangle &= \int_{Q_\ell^*} \text{Tr}_{L_\xi^2} [g_\xi^* W_{< m, \tilde{\gamma}_n, \xi}] d\xi = \int_{Q_\ell^*} \text{Tr}_{L_{\xi'}^2} [W_{< m, g, \xi'}^* \tilde{\gamma}_{n, \xi'}] d\xi' \\ &\rightarrow \int_{Q_\ell^*} \text{Tr}_{L_{\xi'}^2} [W_{< m, g, \xi'}^* \gamma_{*, \xi'}] d\xi' = \langle g_\xi, W_{< m, \gamma_*, \xi} \rangle. \end{aligned}$$

By Corollary B.2,

$$\begin{aligned} \||D^0|^{-1} W_{\geq m, g} |D^0|^{-1}\|_{\mathfrak{S}_{\infty, 1}} &\leq \||D^0|^{-1} W_{\geq m, g}\|_{\mathfrak{S}_{2, 1}} \\ &\leq \int_{Q_\ell^*} d\xi \||D_\xi|^{-1} W_{\geq m, \ell}(\xi - \cdot) g \cdot\|_{L^1(Q_\ell^*; L_\xi^2(Q_\ell \times Q_\ell))} \\ &\leq C \|g_{\xi'}(x, y)\|_{L^1(Q_\ell^*; L_{\xi'}^2(Q_\ell \times Q_\ell))}. \end{aligned}$$

Hence,

$$\begin{aligned} \langle g_\xi, W_{\geq m, \tilde{\gamma}_n, \xi} \rangle &= \langle W_{\geq m, g, \xi'}^*, \tilde{\gamma}_{n, \xi'} \rangle \\ &= \int_{Q_\ell^*} \text{Tr}_{L_\xi^2} [|D_{\xi'}|^{-1} W_{\geq m, g, \xi'}^* |D_{\xi'}|^{-1} |D_{\xi'}| \tilde{\gamma}_{n, \xi'} |D_{\xi'}|] d\xi' \\ &\rightarrow \int_{Q_\ell^*} \text{Tr}_{L_\xi^2} [W_{\geq m, g, \xi'}^* \gamma_{*, \xi'}] d\xi' = \langle g_\xi, W_{\geq m, \gamma_*, \xi} \rangle. \end{aligned}$$

So we have proved (6.5), hence the lemma. \square

Lemma 6.5 (Strong convergence of the electron-electron interaction). *As n goes to infinity, we have*

$$\||D^0|^{-1/2} V_{\gamma_n - \gamma_*} |D^0|^{-1/2}\|_Y \rightarrow 0.$$

Proof. As $V_{\gamma, \xi} = G_\ell * \rho_\gamma - W_{\gamma, \xi}$, we have

$$\begin{aligned} &\||D^0|^{-1/2} V_{\gamma_n - \gamma_*} |D^0|^{-1/2}\|_Y \\ &\leq \||D^0|^{-1/2} G_\ell * (\rho_{\gamma_n} - \rho_{\gamma_*}) |D^0|^{-1/2}\|_Y + \||D^0|^{-1/2} (W_{\gamma_n, \xi} - W_{\gamma_*, \xi}) |D^0|^{-1/2}\|_Y. \end{aligned}$$

For the first term in the right hand side, notice that

$$\|G_\ell * (\rho_{\gamma_n} - \rho_{\gamma_*})\|_Y \leq \|G_\ell * (\rho_{\gamma_n} - \rho_{\tilde{\gamma}_n})\|_Y + \|G_\ell * (\rho_{\tilde{\gamma}_n} - \rho_{\gamma_*})\|_Y.$$

By (4.4), we get

$$\|G_\ell * (\rho_{\gamma_n} - \rho_{\tilde{\gamma}_n})\|_Y \leq C_H \|\gamma_n - \tilde{\gamma}_n\|_X \rightarrow 0.$$

Notice that, from Lemma 6.3, we infer $\rho_{\tilde{\gamma}_n} \rightarrow \rho_{\gamma_*}$ in $L^2(Q_\ell)$. This and the fact that $G_\ell \in L^2(Q_\ell)$ yield

$$\|G_\ell * (\rho_{\tilde{\gamma}_n} - \rho_{\gamma_*})\|_{L^\infty(Q_\ell)} \rightarrow 0.$$

Thus using $|D^0|^{-1} \leq 1$, we infer

$$\||D^0|^{-1/2} G_\ell * (\rho_{\gamma_n} - \rho_{\gamma_*})|D^0|^{-1/2}\|_Y \rightarrow 0. \quad (6.6)$$

Similarly, we split the second term into two parts :

$$\||D^0|^{-1/2} (W_{\gamma_n} - W_{\gamma_*})|D^0|^{-1/2}\|_Y \leq \|W_{\gamma_n} - W_{\tilde{\gamma}_n}\|_Y + \||D^0|^{-1/2} (W_{\tilde{\gamma}_n} - W_{\gamma_*})|D^0|^{-1/2}\|_Y. \quad (6.7)$$

Since γ_n and $\tilde{\gamma}_n$ lie in B_R and since $\|\gamma_n - \tilde{\gamma}_n\|_X \rightarrow 0$, we obtain from Eqn. (4.9)

$$\|W_{\gamma_n} - W_{\tilde{\gamma}_n}\|_Y \rightarrow 0. \quad (6.8)$$

We split the second term in (6.7) into two parts. Thus by the duality of the operator $|D_{\xi,y}|^{-1/2}$, for the term associated with $W_{\geq m,\ell}^\infty$,

$$\begin{aligned} & \left\| |D_{\xi,x}|^{-1/2} \int_{Q_\ell} W_{\geq m,\tilde{\gamma}_n-\gamma_*,\xi}(x,y) [|D_{\xi,y}|^{-1/2} \psi_\xi(y)] dy \right\|_{L_\xi^2(Q_\ell)} \\ &= \left\| \int_{Q_\ell} [|D_{\xi,x}|^{-1/2} |D_{\xi,y}|^{-1/2} W_{\geq m,\tilde{\gamma}_n-\gamma_*,\xi}(x,y)] \psi_\xi(y) dy \right\|_{L_\xi^2(Q_\ell)} \\ &\leq \int_{Q_\ell} \| |D_{\xi,x}|^{-1/2} |D_{\xi,y}|^{-1/2} W_{\geq m,\tilde{\gamma}_n-\gamma_*,\xi}(\cdot,y) \|_{L_\xi^2(Q_\ell)} |\psi_\xi(y)| dy \\ &\leq \| |D_{\xi,x}|^{-1/2} |D_{\xi,y}|^{-1/2} W_{\geq m,\tilde{\gamma}_n-\gamma_*,\xi}(\cdot,\cdot) \|_{L^\infty(Q_\ell^*; L_\xi^2(Q_\ell \times Q_\ell))} \|\psi_\xi\|_{L^2(Q_\ell)}. \end{aligned}$$

For the other term, analogously we have

$$\begin{aligned} & \left\| |D_{\xi,x}|^{-1/2} \int_{Q_\ell} W_{< m,\tilde{\gamma}_n-\gamma_*,\xi}(x,y) |D_{\xi,y}|^{-1/2} \psi_\xi(y) dy \right\|_{L_\xi^2(Q_\ell)} \\ &\leq \int_{Q_\ell} \| W_{< m,\tilde{\gamma}_n-\gamma_*,\xi}(\cdot,y) \|_{L_\xi^2(Q_\ell)} |D_{\xi,y}|^{-1/2} |\psi_\xi(y)| dy \\ &\leq \| W_{< m,\tilde{\gamma}_n-\gamma_*,\xi}(\cdot,\cdot) \|_{L^\infty(Q_\ell^*; L_\xi^2(Q_\ell \times Q_\ell))} \|\psi_\xi\|_{L^2(Q_\ell)} \end{aligned}$$

Gathering these estimates with Lemma 6.4 we infer

$$\||D^0|^{-1/2} W_{\tilde{\gamma}_n-\gamma_*} |D^0|^{-1/2}\|_Y \rightarrow 0. \quad (6.9)$$

Then this lemma follows from (6.6), (6.8) and (6.9). \square

As a result, we have the following.

Corollary 6.6 (Strong convergence of the spectral projectors). *As n goes to infinity, we have*

$$\|P_{\gamma_*}^+ - P_{\gamma_n}^+\|_Y \rightarrow 0.$$

Proof. By (5.9) and the second resolvent identity, we obtain

$$\begin{aligned} \|P_{\gamma_*,\xi}^+ - P_{\gamma_n,\xi}^+\|_{\mathcal{B}(L_\xi^2)} &\leq \frac{1}{2\pi} \int_{-\infty}^{+\infty} \|(D_{\gamma_*,\xi} - iz)^{-1} V_{\gamma_n-\gamma_*,\xi} (D_{\gamma_n,\xi} - iz)^{-1}\|_{\mathcal{B}(L_\xi^2)} dz \\ &\leq \frac{1}{2\pi} \||D^0|^{-1/2} (V_{\gamma_n-\gamma_*}) |D^0|^{-1/2}\|_Y \\ &\quad \times \int_{-\infty}^{+\infty} \|(D_{\gamma_*,\xi} - iz)^{-1} |D_\xi|^{1/2}\|_{\mathcal{B}(L_\xi^2)} \| |D_\xi|^{1/2} (D_{\gamma_n,\xi} - iz)^{-1} \|_{\mathcal{B}(L_\xi^2)} dz \\ &\leq \frac{1}{4} (1 - \kappa)^{-1} \||D^0|^{-1/2} V_{\gamma_n-\gamma_*} |D^0|^{-1/2}\|_Y. \end{aligned}$$

The right-hand side goes to 0 by Lemma 6.5. \square

6.3 Existence and properties of minimizer of $I_{\leq q, R}$

The existence of minimizers of $I_{\leq q, R}$ now follows by passing to the limit in the constraint and in the energy. The proof is separated into the following two lemmas.

Lemma 6.7. *The limit γ_* lies in $\Gamma_{\leq q}^+ \cap B_R$.*

Proof. As

$$\tilde{\gamma}_n \xrightarrow{*} \gamma_* \quad \text{in} \quad X_\infty^2 \cap Y,$$

we get

$$\|\gamma_*\|_{\mathfrak{S}_{1,\infty}} \leq \liminf_{n \rightarrow \infty} \|\tilde{\gamma}_n\|_{\mathfrak{S}_{1,\infty}} \leq R, \quad \|\gamma_*\|_Y \leq \liminf_{n \rightarrow \infty} \|\tilde{\gamma}_n\|_Y \leq 1$$

and

$$\|\gamma_*\|_{X_\infty^2} \leq \liminf_{n \rightarrow \infty} \|\tilde{\gamma}_n\|_{X_\infty^2} \leq (q + M)(1 - \kappa)^{-2} e^2.$$

Thus, $\gamma_* \in \mathcal{T}$ and $\gamma_* \in X \cap Y \cap B_R$. Besides, as $\|\gamma_n - \tilde{\gamma}_n\|_X \rightarrow 0$ and $\|\rho_{\tilde{\gamma}_n}^{1/2} - \rho_{\gamma_*}^{1/2}\|_{L^2} \rightarrow 0$, we know that

$$\int_{Q_\ell^*} \text{Tr}_{L_\xi^2} \gamma_{n,\xi} d\xi \rightarrow \int_{Q_\ell^*} \text{Tr}_{L_\xi^2} \gamma_{*,\xi} d\xi \leq q.$$

Then $\gamma_* \in \Gamma_{\leq q} \cap B_R$.

To end the proof, it remains to show that $P_{\gamma_{*,\xi}}^+ \gamma_{*,\xi} = \gamma_{*,\xi}$, in the sense that for every $g \in \mathfrak{S}_{\infty,1}$,

$$\int_{Q_\ell^*} \text{Tr}_{L_\xi^2} [(P_{\gamma_{*,\xi}}^+ \gamma_{*,\xi} - \gamma_{*,\xi}) g_\xi] d\xi = 0.$$

Notice that

$$\begin{aligned} \left| \int_{Q_\ell^*} \text{Tr}_{L_\xi^2} [(P_{\gamma_{*,\xi}}^+ \gamma_{*,\xi} - \gamma_{*,\xi}) g_\xi] d\xi \right| &\leq \left| \int_{Q_\ell^*} \text{Tr}_{L_\xi^2} [(P_{\gamma_{*,\xi}}^+ - P_{\tilde{\gamma}_n,\xi}^+) \tilde{\gamma}_n g_\xi] d\xi \right| \\ &+ \left| \int_{Q_\ell^*} \text{Tr}_{L_\xi^2} [P_{\gamma_{*,\xi}}^+ (\gamma_{*,\xi} - \tilde{\gamma}_n) g_\xi] d\xi \right| + \left| \int_{Q_\ell^*} \text{Tr}_{L_\xi^2} [(\tilde{\gamma}_n - \gamma_{*,\xi}) g_\xi] d\xi \right|. \end{aligned} \quad (6.10)$$

As $g P_{\gamma_*}^+ \in \mathfrak{S}_{\infty,1}$, we know that

$$\int_{Q_\ell^*} \text{Tr}_{L_\xi^2} [P_{\gamma_{*,\xi}}^+ (\gamma_{*,\xi} - \tilde{\gamma}_n) g_\xi] d\xi \rightarrow 0 \quad \text{and} \quad \int_{Q_\ell^*} \text{Tr}_{L_\xi^2} [(\tilde{\gamma}_n - \gamma_{*,\xi}) g_\xi] d\xi \rightarrow 0.$$

For the first term in the right-hand side of (6.10), using Corollary 6.6, we have

$$\left| \int_{Q_\ell^*} \text{Tr}_{L_\xi^2} [(P_{\gamma_{*,\xi}}^+ - P_{\tilde{\gamma}_n,\xi}^+) \tilde{\gamma}_n g_\xi] d\xi \right| \leq \|P_{\gamma_*}^+ - P_{\tilde{\gamma}_n}^+\|_Y \|\tilde{\gamma}_n\|_{\mathfrak{S}_{1,1}} \|g\|_Y \rightarrow 0.$$

Consequently, letting n go to infinity,

$$\left| \int_{Q_\ell^*} \text{Tr}_{L_\xi^2} [(P_{\gamma_{*,\xi}}^+ \gamma_{*,\xi} - \gamma_{*,\xi}) g_\xi] d\xi \right| = 0.$$

Hence $\gamma_* \in \Gamma_{\leq q}^+$. This ends the proof. \square

Lemma 6.8. *The limit γ_* minimizes $I_{\leq q, R}$.*

Proof. For the kinetic energy term, we have

$$\int_{Q_\ell^*} \text{Tr}_{L_\xi^2} [D_\xi (\gamma_{n,\xi} - \gamma_{*,\xi})] d\xi = \int_{Q_\ell^*} \text{Tr}_{L_\xi^2} [D_\xi (\gamma_{n,\xi} - \tilde{\gamma}_n)] d\xi + \int_{Q_\ell^*} \text{Tr}_{L_\xi^2} [D_\xi (\tilde{\gamma}_n - \gamma_{*,\xi})] d\xi.$$

By (6.3), we know that

$$\int_{Q_\ell^*} \text{Tr}_{L_\xi^2} [D_\xi (\tilde{\gamma}_n - \gamma_{*,\xi})] d\xi = \int_{Q_\ell^*} \text{Tr}_{L_\xi^2} [|D_\xi| (\tilde{\gamma}_n - \gamma_{*,\xi}) |D_\xi| |D_\xi|^{-1} D_\xi |D_\xi|^{-1}] d\xi \rightarrow 0,$$

as $|D^0|^{-1}D^0|D^0|^{-1} \in \mathfrak{S}_{\infty,1}$. Since $\|\gamma_n - \tilde{\gamma}_n\|_X \rightarrow 0$, then $\int_{Q_\ell^*} \text{Tr}_{L_\xi^2}[D_\xi(\gamma_{n,\xi} - \tilde{\gamma}_{n,\xi})]d\xi \rightarrow 0$. Hence

$$\int_{Q_\ell^*} \text{Tr}_{L_\xi^2}[D_\xi(\gamma_{n,\xi} - \gamma_{*,\xi})]d\xi \rightarrow 0.$$

The proof for the attractive potential is similar:

$$\int_{Q_\ell^*} \text{Tr}_{L_\xi^2}(G_\ell(\gamma_{n,\xi} - \gamma_{*,\xi})) d\xi = \int_{Q_\ell^*} \text{Tr}_{L_\xi^2}(G_\ell(\gamma_{n,\xi} - \tilde{\gamma}_{n,\xi})) d\xi + \int_{Q_\ell^*} \text{Tr}_{L_\xi^2}(G_\ell(\tilde{\gamma}_{n,\xi} - \gamma_{*,\xi})) d\xi$$

and

$$\left| \int_{Q_\ell^*} \text{Tr}_{L_\xi^2}(G_\ell(\gamma_{n,\xi} - \tilde{\gamma}_{n,\xi})) d\xi \right| \leq C_H \|\gamma_n - \tilde{\gamma}\|_X \rightarrow 0.$$

As $\| |D^0|^{-1}G_\ell|D^0|^{-1} \|_{\mathfrak{S}_{\infty,1}} \leq C_G \| |D^0|^{-1} \|_{\mathfrak{S}_{\infty,1}} < +\infty$, we know that $|D^0|^{-1}G_\ell|D^0|^{-1} \in \mathfrak{S}_{\infty,1}$ and

$$\int_{Q_\ell^*} \text{Tr}_{L_\xi^2}[G_\ell(\tilde{\gamma}_{n,\xi} - \gamma_{*,\xi})]d\xi = \int_{Q_\ell^*} \text{Tr}_{L_\xi^2}[|D_\xi|(\tilde{\gamma}_{n,\xi} - \gamma_{*,\xi})|D_\xi||D_\xi|^{-1}G_\ell|D_\xi|^{-1}] d\xi \rightarrow 0.$$

For the repulsive potential, according to Lemma 6.5, we have

$$\begin{aligned} \left| \widetilde{\text{Tr}}_{L^2}(V_{\gamma_n}\gamma_n - V_{\gamma_*}\gamma_*) \right| &= \left| \widetilde{\text{Tr}}_{L^2}(V_{\gamma_n - \gamma_*}\gamma_n + V_{\gamma_n - \gamma_*}\gamma_*) \right| \\ &\leq \| |D^0|^{-1/2}V_{\gamma_n - \gamma_*}|D^0|^{-1/2} \|_Y (\|\gamma_n\|_X + \|\gamma_*\|_X) \rightarrow 0. \end{aligned}$$

The lemma follows. \square

We now know that γ_* is a minimizer of $I_{\leq q,R}$ under the condition $\gamma_* \in \Gamma_{\leq q}^+ \cap B_R$. Applying Proposition 5.1, we get

$$\int_{Q_\ell^*} \text{Tr}_{L_\xi^2}[(D_{\gamma_*,\xi} - \epsilon_P)\gamma_{*,\xi}] d\xi = \inf_{\substack{\gamma \in \Gamma_{\leq q}^+ \\ \gamma = P_{\gamma_*}^+ \gamma}} \int_{Q_\ell^*} \text{Tr}_{L_\xi^2}[(D_{\gamma_*,\xi} - \epsilon_P)\gamma_\xi] d\xi.$$

Then, with $\epsilon_P > (1 - \kappa)^{-1}c^*(q + 1)$, by Lemma 4.12, we get $\gamma_* = f_{Q_\ell^*}^\oplus 1_{[0,\nu)}(D_{\gamma_*,\xi})d\xi + \delta$ with some $0 \leq \delta \leq f_{Q_\ell^*}^\oplus 1_\nu(D_{\gamma_*,\xi})d\xi$ for $\nu \in (0, (1 - \kappa)^{-1}c^*(q + 1)]$ independently of ϵ_P . Furthermore, $\widetilde{\text{Tr}}_{L^2}(\gamma_*) = q$. Besides, if $R > R_0$, any minimizer γ_* in $\Gamma_{\leq q}^+ \cap B_R$ lies in \overline{B}_{R_0} . This proves Proposition 3.4.

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A Proof of Lemma 4.1

It suffices to prove (4.2). By interpolation, we can choose $C_H = C_G$.

To deal with (4.2), the idea is to decompose the potential G_ℓ on Q_ℓ into two parts, namely $\frac{1}{|x|}$ and $G_\ell - \frac{1}{|x|}$. The first term can be treated as the Hardy inequality on Q_ℓ , whereas the second is bounded. We begin with the second term and prove the following.

Lemma A.1. *There is a constant $C_0 > 0$ independent of ℓ such that*

$$\sup_{x \in Q_\ell} \left| G_\ell(x) - \frac{1}{|x|} \right| \leq \frac{C_0}{\ell}.$$

This implies that, for any $x \in \mathbb{R}^3$,

$$G_\ell(x) \geq -\frac{C_0}{\ell}. \quad (\text{A.1})$$

In particular, we have

$$C_0 \leq \inf_{0 < R < \frac{1}{2}} \left(\frac{3}{2R} + \frac{2\pi R^2}{5} + \frac{3}{4\pi^2 R^3} \min \left\{ \left(\frac{4\pi R^3}{3} \right)^{1/2}, \left(1 - \frac{4\pi R^3}{3} \right)^{1/2} \right\} \left(\sum_{k \in \mathbb{Z}^3 \setminus \{0\}} \frac{1}{|k|^4} \right)^{1/2} \right).$$

Proof. As $G_1(x) = \ell G_\ell(\ell x)$, it suffices to consider the case $\ell = 1$. Let $f(x) = G_1(x) - \frac{1}{|x|}$. Eqn. (2.1) yields

$$-\Delta f = 4\pi(-1 + \sum_{k \in \mathbb{Z}^3 \setminus \{0\}} \delta_k).$$

Let $B(z, R)$ be a ball of center z and radius R chosen such that $(\bigcup_{z \in Q_1} B(z, R)) \cap (\mathbb{Z}^3 \setminus \{0\}) = \emptyset$. Obviously, we can assume $0 < R < 1/2$. By the divergence theorem, for $0 \leq r \leq R$ and $z \in Q_1$ we obtain

$$\frac{d}{dr} \left(\frac{1}{4\pi r^2} \int_{\partial B(z,r)} f(s) ds \right) = \frac{1}{4\pi} \frac{d}{dr} \int_{\mathbb{S}^2} f(z + r\omega) d\omega = \frac{1}{4\pi r^2} \int_{\partial B(z,r)} \frac{\partial f(s)}{\partial n} ds = \frac{1}{4\pi r^2} \int_{B(z,r)} \Delta_x f(x) dx \quad (\text{A.2})$$

with \mathbb{S}^2 denoting the unit sphere. On the one hand, for any $z \in Q_1$,

$$\frac{1}{4\pi r^2} \left| \int_{B(z,r)} \Delta_x f dx \right| = \frac{1}{r^2} \left| \int_{B(z,r)} 1 dx \right| \leq \frac{4\pi}{3} r.$$

where the first equation holds since

$$\left(\bigcup_{z \in Q_1} B(z, r) \right) \cap \{k \in \mathbb{Z}^3 | k \neq 0\} = \emptyset, \quad \text{for } 0 \leq r \leq R.$$

Therefore, integrating (A.2) with respect to r ,

$$-\frac{8\pi^2}{3} r^2 \leq \int_{\mathbb{S}^2} f(z + r\omega) d\omega - 4\pi f(z) \leq \frac{8\pi^2}{3} r^2.$$

Since $\int_{B(z,R)} f(x) dx = \int_0^R r^2 \left(\int_{\mathbb{S}^2} f(z + r\omega) d\omega \right) dr$, integration over $[0, R]$ leads to

$$|f(z)| \leq \frac{3}{4\pi R^3} \left| \int_{B(z,R)} f(x) dx \right| + \frac{2\pi R^2}{5} \leq \frac{3}{4\pi R^3} \left| \int_{B(z,R)} G_1(x) dx \right| + \frac{3}{4\pi R^3} \left| \int_{B(z,R)} \frac{1}{|x|} dx \right| + \frac{2\pi R^2}{5}.$$

On the other hand,

$$\left| \int_{B(z,R)} G_1(x) dx \right| \leq |B(z, R)|^{1/2} \|G_1\|_{L^2(B(z,R))} \leq \left(\frac{4\pi R^3}{3} \right)^{1/2} \|G_1\|_{L^2(Q_1)} = \frac{1}{\pi} \left(\frac{4\pi R^3}{3} \sum_{k \in \mathbb{Z}^3 \setminus \{0\}} \frac{1}{|k|^4} \right)^{1/2}.$$

Using (2.2) and by the periodicity of G_1 , we also have

$$\left| \int_{B(z,R)} G_1(x) dx \right| = \left| \int_{(z+Q_1) \setminus B(z,R)} G_1(x) dx \right| \leq \frac{1}{\pi} \left(1 - \frac{4\pi R^3}{3} \right)^{1/2} \left(\sum_{k \in \mathbb{Z}^3 \setminus \{0\}} \frac{1}{|k|^4} \right)^{1/2}.$$

Thus,

$$\left| \int_{B(z,R)} G_1(x) dx \right| \leq \frac{1}{\pi} \min \left\{ \left(\frac{4\pi R^3}{3} \right)^{1/2}, \left(1 - \frac{4\pi R^3}{3} \right)^{1/2} \right\} \left(\sum_{k \in \mathbb{Z}^3 \setminus \{0\}} \frac{1}{|k|^4} \right)^{1/2}.$$

Furthermore,

$$\left| \int_{B(z,R)} \frac{1}{|x|} dx \right| \leq \int_{B(0,R)} \frac{1}{|x|} dx = 2\pi R^2.$$

Therefore, the bound holds for $\ell = 1$ and any $0 < R < \frac{1}{2}$ with

$$C_0 \leq \frac{3}{2R} + \frac{2\pi R^2}{5} + \frac{3}{4\pi^2 R^3} \min \left\{ \left(\frac{4\pi R^3}{3} \right)^{1/2}, \left(1 - \frac{4\pi R^3}{3} \right)^{1/2} \right\} \left(\sum_{k \in \mathbb{Z}^3 \setminus \{0\}} \frac{1}{|k|^4} \right)^{1/2}.$$

□

We now consider the Hardy inequality on Q_ℓ for the potential $\frac{1}{|x|}$.

Lemma A.2. *Let $u \in H^1(Q_\ell)$, then*

$$\left\| \frac{u}{|x|} \right\|_{L^2(Q_\ell)}^2 \leq \frac{4\ell + 24}{\ell} \|\nabla u\|_{L^2(Q_\ell)}^2 + \frac{48 + 24\ell}{\ell^2} \|u\|_{L^2(Q_\ell)}^2.$$

Proof. We start with the relationship:

$$0 \leq \int_{Q_\ell} \left| \nabla u + \frac{xu}{2|x|^2} \right|^2 dx.$$

Thus,

$$0 \leq \int_{Q_\ell} |\nabla u|^2 dx + \frac{1}{4} \int_{Q_\ell} \frac{|u|^2}{|x|^2} dx + \frac{1}{2} \int_{Q_\ell} \frac{\nabla |u|^2 \cdot x}{|x|^2} dx.$$

By the divergence theorem for $\int_{Q_\ell} \nabla \cdot \left(\frac{|u|^2 x}{|x|^2} \right) dx$, we obtain

$$\int_{Q_\ell} \frac{\nabla |u|^2 \cdot x}{|x|^2} dx = \int_{\partial Q_\ell} \frac{\vec{n}x |u|^2}{|x|^2} dx - \int_{Q_\ell} \frac{|u|^2}{|x|^2} dx.$$

where \vec{n} is the outward pointing unit normal at each point on the boundary ∂Q_ℓ . To end this proof, it suffices to estimate $\int_{\partial Q_\ell} \frac{\vec{n}x |u|^2}{|x|^2}$.

Let

$$A^{2,3}(x_1) = \int_{(-\frac{\ell}{2}, \frac{\ell}{2})^2} |u|^2(x_1, x_2, x_3) dx_2 dx_3.$$

As $|\vec{n} \cdot x| = \frac{\ell}{2}$ and $|x| \geq \frac{\ell}{2}$ for any $x \in \partial Q_\ell$, we have

$$\left| \int_{\partial Q_\ell} \frac{\vec{n}x |u|^2}{|x|^2} dx \right| \leq \frac{2}{\ell} \int_{\partial Q_\ell} |u|^2 dx = \frac{2}{\ell} \left(A^{2,3}(-\frac{\ell}{2}) + A^{2,3}(\frac{\ell}{2}) + A^{1,3}(-\frac{\ell}{2}) + A^{1,3}(\frac{\ell}{2}) + A^{1,2}(-\frac{\ell}{2}) + A^{1,2}(\frac{\ell}{2}) \right). \quad (\text{A.3})$$

Let $x_1^{(0)} \in (-\frac{\ell}{2}, \frac{\ell}{2}]$ such that

$$A^{2,3}(x_1^{(0)}) \leq \int_{(-\frac{\ell}{2}, \frac{\ell}{2})} A^{2,3}(x_1) dx_1 = \frac{1}{\ell} \int_{(-\frac{\ell}{2}, \frac{\ell}{2})} A^{2,3}(x_1) dx_1 = \frac{1}{\ell} \int_{Q_\ell} |u|^2 dx.$$

Then we have

$$A^{2,3}(-\frac{\ell}{2}) + A^{2,3}(\frac{\ell}{2}) = \left[\int_{x_1^{(0)}}^{\frac{\ell}{2}} - \int_{-\frac{\ell}{2}}^{x_1^{(0)}} \right] \frac{d}{dx_1} A^{2,3} dx_1 + 2A^{2,3}(x_1^{(0)}) \leq 2A^{2,3}(x_1^{(0)}) + \int_{(-\frac{\ell}{2}, \frac{\ell}{2})} \left| \frac{d}{dx_1} A^{2,3} \right| dx_1.$$

As

$$\int_{(-\frac{\ell}{2}, \frac{\ell}{2}] \left| \frac{d}{dx_1} A^{2,3}(x_1) \right| dx_1 \leq 2 \int_{Q_\ell} |u| \left| \frac{\partial}{\partial x_1} u \right| \leq 2 \|u\|_{L^2(Q_\ell)} \|\nabla u\|_{L^2(Q_\ell)},$$

we get

$$A^{2,3}\left(-\frac{\ell}{2}\right) + A^{2,3}\left(\frac{\ell}{2}\right) \leq \frac{2}{\ell} \|u\|_{L^2(Q_\ell)}^2 + 2 \|u\|_{L^2(Q_\ell)} \|\nabla u\|_{L^2(Q_\ell)}.$$

Inserting this into (A.3), we can conclude

$$0 \leq \|\nabla u\|_{L^2(Q_\ell)}^2 - \frac{1}{4} \left\| \frac{u}{|x|} \right\|_{L^2(Q_\ell)}^2 + \frac{6}{\ell^2} \|u\|_{L^2(Q_\ell)}^2 + \frac{6}{\ell} \|u\|_{L^2(Q_\ell)} \|\nabla u\|_{L^2(Q_\ell)}.$$

As a result, by the Cauchy-Schwarz inequality

$$\left\| \frac{u}{|x|} \right\|_{L^2(Q_\ell)}^2 \leq \frac{4\ell + 12}{\ell} \|\nabla u\|_{L^2(Q_\ell)}^2 + \frac{24 + 12\ell}{\ell^2} \|u\|_{L^2(Q_\ell)}^2.$$

□

Combining Lemma A.1 and A.2, we obtain

$$C_G := 2 \left(1 + \frac{C_0}{\ell} \right) \max \left\{ \sqrt{1 + \frac{3}{\ell}}, \sqrt{\frac{3}{\ell} + \frac{6}{\ell^2}} \right\}. \quad (\text{A.4})$$

We now turn to the estimates on $W_{\gamma, \xi}$.

B Proof of Lemma 4.5

We first study the property of W_ℓ^∞ , then we prove Lemma 4.5.

Properties of W_ℓ^∞

Recall that $W_\ell^\infty(\eta, x) = W_{\geq m, \ell}(\eta, x) + W_{< m, \ell}(\eta, x)$ is given by (4.7). We are going to prove the Hardy type inequalities for $W_{\geq m, \ell}$. A natural idea is to compare it with the potential G_ℓ .

Proposition B.1 (Singularities for the potential $W_{\geq m, \ell}$). *For every $m \geq 2$, there exists a positive constant $C_{\geq m}$ such that, for any $\ell > 0$, we have*

$$\sup_{\substack{\eta \in 2Q_\ell^* \\ x \in Q_\ell}} |W_{\geq m, \ell}(\eta, x) - G_\ell(x)| \leq \frac{C_{\geq m}}{\ell} \quad (\text{B.1})$$

with

$$C_{\geq m} \leq \inf_{0 < R < 1/2} \left\{ \frac{\sqrt{3}}{2(\pi R)^{3/2}} \frac{m^2 + 2}{(m-1)^2} \left(\sum_{|k|_\infty \geq m} \frac{1}{|k|^4} \right)^{1/2} + \frac{2\pi[(2m-1)^3 + 1]R^2}{5} \right. \\ \left. + \frac{3}{4\pi^2 R^3} \min \left\{ \left(\frac{4\pi R^3}{3} \right)^{1/2}, \left(1 - \frac{4\pi R^3}{3} \right)^{1/2} \right\} \left(\sum_{k \in \mathbb{Z}^3 \setminus \{0\}} \frac{1}{|k|^4} \right)^{1/2} \right\}.$$

Proof. The proof is similar to Lemma A.1. Notice that

$$W_\ell^\infty(\eta, x) = \lambda W_{\lambda \ell}^\infty\left(\frac{\eta}{\lambda}, \lambda x\right), \quad \eta \in \mathbb{R}^3, x \in \mathbb{R}^3.$$

We therefore take $\ell = 1$. Observe, from (2.17), that

$$-\Delta_z W_1^\infty(\eta, x) = 4\pi \sum_{k \in \mathbb{Z}^3} e^{-i\eta \cdot k} \delta_k(x).$$

Let $f(\eta, x) = W_{\geq m, 1}(\eta, x) - G_1(x)$. Then

$$-\Delta_x f(\eta, x) = 4\pi \sum_{\substack{k \neq 0 \\ k \in \mathbb{Z}^3}} (e^{-i\eta \cdot k} - 1) \delta_k(x) + 4\pi - 4\pi \sum_{\substack{|k|_\infty < m \\ k \in \mathbb{Z}^3}} e^{i(2\pi k - \eta) \cdot x}.$$

Let $B(z, R)$ be a ball of center z and radius R chosen such that $(\bigcup_{z \in Q_1} B(z, R)) \cap \{k \in \mathbb{Z}^3 | k \neq 0\} = \emptyset$. Obviously, we can assume $0 < R < 1/2$. Analogous to (A.2), for $0 \leq r \leq R$ and $z \in Q_1$ we obtain

$$\frac{d}{dr} \left(\frac{1}{4\pi r^2} \int_{\partial B(z, r)} f(\eta, s) ds \right) = \frac{1}{4\pi r^2} \int_{B(z, r)} \Delta_x f(\eta, x) dx. \quad (\text{B.2})$$

On the one hand, for any $z \in Q_1$,

$$\frac{1}{4\pi r^2} \left| \int_{B(z, r)} \Delta_x f dx \right| = \frac{1}{r^2} \left| \int_{B(z, r)} \left(1 - \sum_{\substack{k \in \mathbb{Z}^3 \\ |k|_\infty \leq m-1}} e^{i(2\pi k - \eta) \cdot x} \right) dx \right| \leq \frac{4\pi[(2m-1)^3 + 1]}{3} r,$$

where the first equality holds since

$$\left(\bigcup_{z \in Q_1} B(z, r) \right) \cap \{k \in \mathbb{Z}^3 | k \neq 0\} = \emptyset, \quad \text{for } 0 \leq r \leq R.$$

Therefore, integrating (B.2) with respect to r ,

$$-\frac{8\pi^2[(2m-1)^3 + 1]}{3} r^2 \leq \int_{\mathbb{S}^2} f(\eta, z + r\omega) d\omega - 4\pi f(\eta, z) \leq \frac{8\pi^2[(2m-1)^3 + 1]}{3} r^2.$$

Then integration over $[0, R]$ leads to

$$|f(\eta, z)| \leq \frac{3}{4\pi R^3} \left| \int_{B(z, R)} f(\eta, x) dx \right| + \frac{2\pi[(2m-1)^3 + 1]R^2}{5}.$$

On the other hand,

$$\left| \int_{B(z, R)} G_1(x) dx \right| \leq \frac{1}{\pi} \min \left\{ \left(\frac{4\pi R^3}{3} \right)^{1/2}, \left(1 - \frac{4\pi R^3}{3} \right)^{1/2} \right\} \left(\sum_{k \in \mathbb{Z}^3 \setminus \{0\}} \frac{1}{|k|^4} \right)^{1/2}.$$

Furthermore, according to the quasi-periodicity of $W_{\geq m, 1}$ with respect to $z \in \mathbb{R}^3$, for any $\eta \in 2Q_1^*$,

$$\begin{aligned} \left| \int_{B(z, R)} W_{\geq m, 1}(\eta, x) dx \right| &\leq |B(z, R)|^{1/2} \|W_{\geq m, 1}\|_{L^2(B(z, R))} \leq \left(\frac{4\pi R^3}{3} \right)^{1/2} \|W_{\geq m, 1}\|_{L^2(Q_1)} \\ &\leq 4\pi \left(\frac{4\pi R^3}{3} \right)^{1/2} \left(\sum_{|k|_\infty \geq m} \frac{1}{|2\pi k - \eta|^4} \right)^{1/2} \\ &\leq 4\pi \left(\frac{4\pi R^3}{3} \right)^{1/2} \sup_{\substack{|k|_\infty \geq m \\ \eta \in 2Q_1^*}} \frac{|2\pi k|^2}{|2\pi k - \eta|^2} \left(\sum_{|k|_\infty \geq m} \frac{1}{|2\pi k|^4} \right)^{1/2} \\ &= \left(\frac{4\pi R^3}{3} \right)^{1/2} \frac{m^2 + 2}{\pi(m-1)^2} \left(\sum_{|k|_\infty \geq m} \frac{1}{|k|^4} \right)^{1/2}. \end{aligned}$$

Therefore, the bound (B.1) holds for $\ell = 1$ with

$$C_{\geq m} \leq \frac{\sqrt{3}}{2(\pi R)^{3/2}} \frac{m^2 + 2}{(m-1)^2} \left(\sum_{|k|_\infty \geq m} \frac{1}{|k|^4} \right)^{1/2} + \frac{2\pi[(2m-1)^3 + 1]R^2}{5}$$

$$+ \frac{3}{4\pi^2 R^3} \min \left\{ \left(\frac{4\pi R^3}{3} \right)^{1/2}, \left(1 - \frac{4\pi R^3}{3} \right)^{1/2} \right\} \left(\sum_{k \in \mathbb{Z}^3 \setminus \{0\}} \frac{1}{|k|^4} \right)^{1/2},$$

for any $0 < R < \frac{1}{2}$. The corresponding result for any $\ell > 0$ follows immediately by a scaling argument. \square

We can immediately conclude from Lemma 4.1 and Proposition B.1 the following.

Corollary B.2 (Hardy-type inequalities for the potential $W_{\geq m, \ell}$). *For $m \geq 2$, we have*

$$\| |W_{\geq m, \ell}|^{1/2} |D_\xi|^{-1/2} \|_{L^\infty(2Q_\ell^*; \mathcal{B}(L_\xi^2))} \leq \left(C_H + \frac{C_{\geq m}}{\ell} \right) \quad (\text{B.3})$$

and

$$\| |W_{\geq m, \ell}| |D_\xi|^{-1} \|_{L^\infty(2Q_\ell^*; \mathcal{B}(L_\xi^2))} \leq \left(C_G + \frac{C_{\geq m}}{\ell} \right). \quad (\text{B.4})$$

We also have the following estimate on W_ℓ^∞ .

Lemma B.3. *Let $m \geq 2$. There is a constant $C = C(\ell, m)$ such that*

$$\sup_{\eta \in 2Q_\ell^*} \|\nabla_\eta W_{\geq m, \ell}(\eta, \cdot)\|_{L^\infty(Q_\ell)} \leq C. \quad (\text{B.5})$$

Proof. Take $\ell = 1$ for simplicity. Notice that

$$-\Delta_x \nabla_\eta W_{\geq m, 1}(\eta, x) = -4\pi \sum_{k \in \mathbb{Z}^3 \setminus \{0\}} i k e^{-i\eta \cdot k} \delta_k(x) + 4\pi \sum_{\substack{|k|_\infty < m \\ k \in \mathbb{Z}^3}} i x e^{i(2\pi k - \eta) \cdot x},$$

from which we obtain

$$|\Delta_x \nabla_\eta W_{\geq m, 1}(\eta, x)| \leq C$$

for any $\eta \in 2Q_\ell^*$ and $x \in Q_\ell$. Following the proof of Lemma B.1, we know

$$|\nabla_\eta W_{\geq m, 1}(\eta, x)| \leq C.$$

The corresponding result for any $\ell > 0$ follows immediately by a scaling argument as for Lemma B.1. \square

Estimates for the exchange term

We consider now the exchange term. Let $\psi_\xi \in H_\xi^{1/2}$. As

$$\|W_{\gamma, \xi} \psi_\xi\|_{L_\xi^2} = \sup_{\phi_\xi \in L_\xi^2, \|\phi_\xi\|_{L_\xi^2} = 1} |(\phi_\xi, W_{\gamma, \xi} \psi_\xi)|, \quad (\text{B.6})$$

we only need to study the inner product $(W_{\gamma, \xi} \psi_\xi, \phi_\xi)$. For $m \geq 2$, $\xi, \xi' \in Q_\ell^*$ and $x, y \in Q_\ell$,

$$W_\ell^\infty(\xi - \xi', x - y) = W_{\geq m, \ell}(\xi - \xi', x - y) + W_{< m, \ell}(\xi - \xi', x - y). \quad (\text{B.7})$$

For the term that carries all singularities in the x variable (i.e., $W_{\geq m, \ell}$), we use the decomposition (2.10) and Corollary B.2. As $\gamma \in X \cap Y$, for any $\xi \in Q_\ell^*$ we have

$$|D_\xi|^{1/2} \gamma_\xi |D_\xi|^{1/2} = \sum_{n \geq 1} \lambda_n(\xi) |v_n(\xi, \cdot)\rangle \langle v_n(\xi, \cdot)| \quad (\text{B.8})$$

with $(v_n(\xi, \cdot), v_m(\xi, \cdot))_{L_\xi^2} = \delta_{m, n}$ and $\|\gamma\|_X = \int_{Q_\ell^*} \sum_{n \geq 1} |\lambda_n(\xi)| d\xi$. Hence

$$\gamma_\xi = \sum_{n \geq 1} \lambda_n(\xi) |u_n(\xi, \cdot)\rangle \langle u_n(\xi, \cdot)|$$

with $u_n(\xi, \cdot) = |D_\xi|^{-1/2} v_n(\xi, \cdot)$. Now, we have

$$\begin{aligned}
& \left| \int_{Q_\ell^*} d\xi' \int_{Q_\ell \times Q_\ell} W_{\geq m, \ell}(\xi - \xi', x - y) \phi_\xi^*(x) \gamma_{\xi'}(x, y) \psi_\xi(y) dx dy \right| \\
& \leq \int_{Q_\ell^*} d\xi' \sum_{n \geq 1} |\lambda_n(\xi)| \int_{Q_\ell \times Q_\ell} |W_{\geq m, \ell}(\xi - \xi', x - y)| |u_n(\xi', x)| |u_n(\xi', y)| |\psi_\xi(y)| |\phi_\xi^*(x)| dx dy \\
& \leq \int_{Q_\ell^*} d\xi' \sum_{n \geq 1} |\lambda_n(\xi)| \left(\int_{Q_\ell} |\psi_\xi(y)|^2 dy \int_{Q_\ell} |W_{\geq m, \ell}(\xi - \xi', x - y)| |u_n(\xi', x)|^2 dx \right)^{1/2} \\
& \quad \times \left(\int_{Q_\ell} |\phi_\xi^*(x)|^2 dx \int_{Q_\ell} |W_{\geq m, \ell}(\xi - \xi', x - y)| |u_n(\xi', y)|^2 dy \right)^{1/2} \\
& \leq \left(\int_{Q_\ell^*} \left(C_H + \frac{C_{\geq m}}{\ell} \right) \sum_{n \geq 1} |\lambda_n(\xi)| \| |D_\xi|^{1/2} u_n(\xi', \cdot) \|_{L^2(\xi')}^2 d\xi' \right) \|\psi_\xi\|_{L_\xi^2} \|\phi_\xi\|_{L_\xi^2} \\
& \leq \left(C_H + \frac{C_{\geq m}}{\ell} \right) \|\gamma\|_X \|\psi_\xi\|_{L_\xi^2} \|\phi_\xi\|_{L_\xi^2}. \tag{B.9}
\end{aligned}$$

Using the Cauchy-Schwarz inequality, we can also argue as follows:

$$\begin{aligned}
& \left| \int_{Q_\ell^*} d\xi' \iint_{Q_\ell \times Q_\ell} W_{\geq m, \ell}(\xi - \xi', x - y) \phi_\xi^*(x) \gamma_{\xi'}(x, y) \psi_\xi(y) dx dy \right| \\
& \leq \int_{Q_\ell^*} \left(\iint_{Q_\ell \times Q_\ell} \rho_{\gamma_{\xi'}}(y) |\phi_\xi^*(x)|^2 dx dy \right)^{1/2} \left(\iint_{Q_\ell \times Q_\ell} \rho_{\gamma_{\xi'}}(x) |W_{\geq m, \ell}(\xi - \xi', x - y)|^2 |\psi_\xi(y)|^2 dx dy \right)^{1/2} d\xi' \\
& \leq \left(C_G + \frac{C_{\geq m}}{\ell} \right) \|\gamma\|_{\mathfrak{S}_{1,1}} \| |D_\xi| \psi_\xi \|_{L_\xi^2} \|\phi_\xi\|_{L_\xi^2}. \tag{B.10}
\end{aligned}$$

We now study the contribution of the term involving $W_{< m, \ell}$, that carries the singularities in the η variable. We first observe that

$$\gamma_{\xi' + \frac{2k\pi}{\ell}}(x, y) = e^{\frac{2ik\pi}{\ell} \cdot (x-y)} \gamma_{\xi'}(x, y) \quad \text{for every } \xi' \in Q_\ell^*, k \in \mathbb{Z}^3 \text{ and } x, y \in \mathbb{R}^3.$$

In particular, $\rho_{\gamma_{\xi' + \frac{2k\pi}{\ell}}} = \rho_{\gamma_{\xi'}}$ for every $\xi' \in Q_\ell^*$ and $k \in \mathbb{Z}^3$, and the function of $\xi \mapsto \text{Tr}_{L_\xi^2}(\gamma_\xi)$ is Q_ℓ^* -periodic. Next, we write

$$\begin{aligned}
& \left| \int_{Q_\ell^*} d\xi' \iint_{Q_\ell \times Q_\ell} \frac{4\pi}{\ell^3} \sum_{\substack{k \in \mathbb{Z}^3 \\ |k|_\infty \leq m-1}} \frac{e^{-i(\xi' - \xi - \frac{2\pi k}{\ell}) \cdot (x-y)}}{|\xi' - \xi - \frac{2\pi k}{\ell}|^2} \phi_\xi^*(x) \gamma_{\xi'}(x, y) \psi_\xi(y) dx dy \right| \\
& \leq \frac{4\pi}{\ell^3} \sum_{\substack{k \in \mathbb{Z}^3 \\ |k|_\infty \leq m-1}} \int_{Q_\ell^* + \frac{2k\pi}{\ell}} \frac{d\xi'}{|\xi' - \xi|^2} \iint_{Q_\ell \times Q_\ell} \rho_{|\gamma_{\xi'}|}^{1/2}(x) \rho_{|\gamma_{\xi'}|}^{1/2}(y) |\psi_\xi(y)| |\phi_\xi^*(x)| dx dy \\
& = \frac{1}{2\pi^2} \int_{(2m-1)Q_\ell^*} \frac{d\xi'}{|\xi' - \xi|^2} \iint_{Q_\ell \times Q_\ell} \rho_{|\gamma_{\xi'}|}^{1/2}(x) \rho_{|\gamma_{\xi'}|}^{1/2}(y) |\psi_\xi(y)| |\phi_\xi^*(x)| dx dy \\
& \leq \frac{1}{2\pi^2} \int_{(2m-1)Q_\ell^*} \frac{\|\gamma_{\xi'}\|_{\mathfrak{S}_1(\xi')}}{|\xi' - \xi|^2} d\xi' \|\psi_\xi\|_{L_\xi^2} \|\phi_\xi\|_{L_\xi^2}, \tag{B.11}
\end{aligned}$$

where the last estimate follows from the Cauchy-Schwarz inequality. Here and below we use the fact that

$$\sum_{\substack{k \in \mathbb{Z}^3 \\ |k|_\infty \leq m-1}} \int_{Q_\ell^*} f(\xi' - \frac{2\pi k}{\ell}) d\xi' = \sum_{\substack{k \in \mathbb{Z}^3 \\ |k|_\infty \leq m-1}} \int_{\frac{2\pi k}{\ell} + Q_\ell^*} f(\xi') d\xi' = \frac{\ell^3}{(2\pi)^3} \int_{(2m-1)Q_\ell^*} f(\xi') d\xi',$$

since $(Q_\ell^* + 2\pi k/\ell) \cap (Q_\ell^* + 2\pi k'/\ell) = \emptyset$ whenever $k, k' \in \mathbb{Z}^3$ with $k \neq k'$. We focus on the quantity inside the brackets in the last inequality. By Hölder's inequality, for $\gamma \in \mathfrak{S}_{1,\infty}$ and some constant $C'_{\leq m,\ell}$, we obtain

$$\begin{aligned} \int_{(2m-1)Q_\ell^*} \frac{\|\gamma_{\xi'}\|_{\mathfrak{S}_1(\xi')}}{|\xi' - \xi|^2} d\xi' &\leq \left(\int_{(2m-1)Q_\ell^*} \frac{d\xi'}{|\xi' - \xi|^{8/3}} \right)^{3/4} \left(\int_{(2m-1)Q_\ell^*} \|\gamma_{\xi'}\|_{\mathfrak{S}_1(\xi')}^4 d\xi' \right)^{1/4} \\ &\leq C'_{\leq m,\ell} \|\gamma\|_{\mathfrak{S}_{1,\infty}}^{3/4} \|\gamma\|_{\mathfrak{S}_{1,1}}^{1/4}. \end{aligned} \quad (\text{B.12})$$

Alternatively, by using the fact that the γ_ξ 's are bounded operators on L_ξ^2 uniformly on $\xi \in Q_\ell^*$,

$$\begin{aligned} &\left| \int_{Q_\ell^*} \iint_{Q_\ell \times Q_\ell} \frac{4\pi}{\ell^3} \sum_{\substack{k \in \mathbb{Z}^3 \\ |k|_\infty \leq m-1}} \frac{e^{-i(\xi' - \xi - \frac{2\pi k}{\ell}) \cdot (x-y)}}{|\xi' - \xi - \frac{2\pi k}{\ell}|^2} \phi_\xi^*(x) \gamma_{\xi'}(x, y) \psi_\xi(y) dx dy d\xi' \right| \\ &\leq \frac{4\pi}{\ell^3} \left| \sum_{\substack{k \in \mathbb{Z}^3 \\ |k|_\infty \leq m-1}} \int_{Q_\ell^* + \frac{2k\pi}{\ell}} \iint_{Q_\ell \times Q_\ell} \frac{e^{-i(\xi' - \xi) \cdot (x-y)}}{|\xi' - \xi|^2} \phi_\xi^*(x) \gamma_{\xi'}(x, y) \psi_\xi(y) dx dy d\xi' \right| \\ &\leq \frac{4\pi}{\ell^3} \sum_{\substack{k \in \mathbb{Z}^3 \\ |k|_\infty \leq m-1}} \int_{Q_\ell^* + \frac{2k\pi}{\ell}} \frac{d\xi'}{|\xi' - \xi|^2} \left| \left(e^{i(\xi' - \xi) \cdot (\cdot)} \phi_\xi(\cdot), \gamma_{\xi'} e^{i(\xi' - \xi) \cdot (\cdot)} \psi_\xi(\cdot) \right)_{L^2} \right| \\ &\leq C_{\leq m,\ell} \operatorname{ess\,sup}_{\xi' \in Q_\ell^*} \|\gamma_{\xi'}\|_{\mathcal{B}(L_\xi^2)} \|\psi_\xi\|_{L_\xi^2} \|\phi_\xi\|_{L_\xi^2} \\ &= C_{\leq m,\ell} \|\gamma\|_Y \|\psi_\xi\|_{L_\xi^2} \|\phi_\xi\|_{L_\xi^2} \end{aligned} \quad (\text{B.13})$$

with

$$C_{\leq m,\ell} = \frac{4\pi}{\ell^3} \sup_{\xi \in Q_\ell^*} \sum_{\substack{k \in \mathbb{Z}^3 \\ |k|_\infty \leq (m-1)}} \int_{Q_\ell^* + \frac{2k\pi}{\ell}} \frac{d\xi'}{|\xi' - \xi|^2} = \frac{(2m-1)}{2\pi\ell} \int_{[-1,1]^3} \frac{d\xi'}{|\xi'|^2}. \quad (\text{B.14})$$

Since $\|\gamma\|_{\mathfrak{S}_{1,1}} \leq \|\gamma\|_X$ and $|D^0|^{-1/2} \leq 1$, the statement of the lemma follows: from (B.9) and (B.13), we obtain (4.8); from (B.9) and (B.12), we obtain (4.9); from (B.10) and (B.13), we obtain (4.10). More precisely,

$$C_W = C_H + C_\ell, \quad C'_W = C_G + C_\ell, \quad C''_W = C_H + C'_\ell, \quad (\text{B.15})$$

with

$$C_\ell := \inf_{\substack{m \in \mathbb{N} \\ m \geq 2}} \left(\frac{C_{\geq m}}{\ell} + C_{\leq m,\ell} \right), \quad C'_\ell := \inf_{\substack{m \in \mathbb{N} \\ m \geq 2}} \left(\frac{C_{\geq m}}{\ell} + C'_{\leq m,\ell} \right). \quad (\text{B.16})$$

C Proof of Lemma 4.7

Analogous to (B.6), we have

$$\|V_{\gamma,\xi} \psi_\xi\|_{L_\xi^2} = \sup_{\phi_\xi \in L_\xi^2, \|\phi_\xi\|_{L_\xi^2} = 1} |(\phi_\xi, V_{\gamma,\xi} \psi_\xi)|. \quad (\text{C.1})$$

We can rewrite as $W_\ell^\infty = W_{< m,\ell}^\infty + G_\ell + (W_{\geq m,\ell}^\infty - G_\ell)$. According to Proposition B.1 and (B.13), the terms associated to $W_{< m,\ell}^\infty$ and $(W_{\geq m,\ell}^\infty - G_\ell)$ are easily bounded. So the aim of this section is to get a better estimate on the following term :

$$\iint_{Q_\ell \times Q_\ell} G_\ell(x-y) \rho_\gamma(y) \phi_\xi^*(x) \psi_\xi(x) dx dy - \int_{Q_\ell^*} d\xi' \iint_{Q_\ell \times Q_\ell} G_\ell(x-y) \phi_\xi^*(x) \gamma_{\xi'}(x, y) \psi_\xi(y) dx dy.$$

From now on, for any function $f \in L^2(Q_\ell, \mathbb{C}^4)$, we denote $f := (f^\alpha)_{1 \leq \alpha \leq 4}$. We use the decomposition (2.10) for $\gamma \in \mathfrak{S}_{1,1} \cap Y$. Then as $G(x) = G(-x)$, for almost every $\xi \in Q_\ell^*$,

$$\begin{aligned}
& \iint_{Q_\ell \times Q_\ell} G_\ell(x-y) \left[\rho_{\gamma_{\xi'}}(y) \phi_\xi^*(x) \psi_\xi(x) - \phi_\xi^*(x) \gamma_{\xi'}(x, y) \psi_\xi(y) \right] dx dy \\
&= \sum_{n \geq 1} \lambda_n(\xi') \iint_{Q_\ell \times Q_\ell} G_\ell(x-y) \left(|u_n(\xi', y)|^2 \phi_\xi^*(x) \psi_\xi(x) - \phi_\xi^*(x) u_n(\xi', x) u_n^*(\xi', y) \psi_\xi(y) \right) dx dy \\
&= \frac{1}{2} \sum_{n \geq 1} \sum_{1 \leq \alpha, \beta \leq 4} \lambda_n(\xi') \iint_{Q_\ell \times Q_\ell} G_\ell(x-y) \left(u_n^\alpha(\xi', y) \phi_\xi^\beta(x) - \phi_\xi^\alpha(y) u_n^\beta(\xi', x) \right)^* \\
&\quad \times \left(u_n^\alpha(\xi', y) \psi_\xi^\beta(x) - \psi_\xi^\alpha(y) u_n^\beta(\xi', x) \right) dx dy. \tag{C.2}
\end{aligned}$$

Estimate for (4.12). By Lemma A.1, we have

$$\begin{aligned}
& \left| \sum_{1 \leq \alpha, \beta \leq 4} \iint_{Q_\ell \times Q_\ell} G_\ell(x-y) \left(u_n^\alpha(\xi', y) \phi_\xi^\beta(x) - \phi_\xi^\alpha(y) u_n^\beta(\xi', x) \right)^* \left(u_n^\alpha(\xi', y) \psi_\xi^\beta(x) - \psi_\xi^\alpha(y) u_n^\beta(\xi', x) \right) dx dy \right| \\
&\leq \left(\sum_{1 \leq \alpha, \beta \leq 4} \iint_{Q_\ell \times Q_\ell} |G_\ell(x-y)|^2 \left| u_n^\alpha(\xi', y) \psi_\xi^\beta(x) - u_n^\beta(\xi', x) \psi_\xi^\alpha(y) \right|^2 dx dy \right)^{1/2} \\
&\quad \times \left(\sum_{1 \leq \alpha, \beta \leq 4} \iint_{Q_\ell \times Q_\ell} \left| u_n^\alpha(\xi', y) \phi_\xi^\beta(x) - u_n^\beta(\xi', x) \phi_\xi^\alpha(y) \right|^2 dx dy \right)^{1/2}. \tag{C.3}
\end{aligned}$$

Thus according to the Cauchy-Schwarz inequality, we have

$$\begin{aligned}
& \sum_{1 \leq \alpha, \beta \leq 4} \left| \iint_{Q_\ell \times Q_\ell} G_\ell(x-y) \left(u_n^\alpha(\xi', y) \phi_\xi^\beta(x) - \phi_\xi^\alpha(y) u_n^\beta(\xi', x) \right)^* \left(u_n^\alpha(\xi', y) \psi_\xi^\beta(x) - \psi_\xi^\alpha(y) u_n^\beta(\xi', x) \right) dx dy \right| \\
&\leq 2 \left(\sum_{1 \leq \alpha, \beta \leq 4} \iint_{Q_\ell \times Q_\ell} |G_\ell(x-y)|^2 |u_n(\xi', y)|^2 |\psi_\xi(x)|^2 dx dy \right)^{1/2} \left(\iint_{Q_\ell \times Q_\ell} |u_n^*(\xi', y)|^2 |\phi_\xi^*(x)|^2 dx dy \right)^{1/2} \\
&\leq 2C_G \|\phi_\xi\|_{L_\xi^2} \|D_\xi |\psi_\xi|\|_{L_\xi^2}.
\end{aligned}$$

Substituting this inequality into (C.2) and using the decomposition (2.11), we get

$$\begin{aligned}
& \left| \iint_{Q_\ell \times Q_\ell} G_\ell(x-y) \left(\rho_{\gamma_{\xi'}}(y) \phi_\xi^*(x) \psi_\xi(x) - \phi_\xi^*(x) \gamma_{\xi'}(x, y) \psi_\xi(y) \right) dx dy \right| \\
&\leq C_G \sum_{n \geq 1} |\lambda_n(\xi')| \|\phi_\xi\|_{L_\xi^2} \|D_\xi |\psi_\xi|\|_{L_\xi^2} = C_G \|\gamma_{\xi'}\|_{\mathfrak{S}_1(\xi')} \|\phi_\xi\|_{L_\xi^2} \|D_\xi |\psi_\xi|\|_{L_\xi^2},
\end{aligned}$$

from which we get

$$\begin{aligned}
& \left| \iint_{Q_\ell \times Q_\ell} G_\ell(x-y) \rho_\gamma(y) \phi_\xi^*(x) \psi_\xi(x) dx dy - \int_{Q_\ell^*} d\xi' \iint_{Q_\ell \times Q_\ell} G_\ell(x-y) \phi_\xi^*(x) \gamma_{\xi'}(x, y) \psi_\xi(y) dx dy \right| \\
&\leq C_G \|\gamma\|_{\mathfrak{S}_{1,1}} \|\phi_\xi\|_{L_\xi^2} \|D_\xi |\psi_\xi|\|_{L_\xi^2}. \tag{C.4}
\end{aligned}$$

Combining (C.4) with Proposition B.1 and (B.13), we get for any $\phi_\xi \in L_\xi^2$ and $\psi_\xi \in H_\xi^1$,

$$|(\phi_\xi, V_{\gamma, \xi} \psi_\xi)| \leq (C_G + C_\ell) \|\gamma\|_{\mathfrak{S}_{1,1} \cap Y} \|\phi_\xi\|_{L_\xi^2} \|D_\xi |\psi_\xi|\|_{L_\xi^2},$$

hence (4.12) with

$$C'_{EE} := C_G + C_\ell \tag{C.5}$$

with C_ℓ given in (B.16).

Estimate for (4.11). As $\gamma \in X \cap Y$, we use the decomposition (B.8) for γ_ξ . Analogous to (C.3), we also have

$$\left| \sum_{1 \leq \alpha, \beta \leq 4} \iint_{Q_\ell \times Q_\ell} G_\ell(x-y) \left(u_n^\alpha(\xi', y) \phi_\xi^\beta(x) - \phi_\xi^\alpha(y) u_n^\beta(\xi', x) \right)^* \left(u_n^\alpha(\xi', y) \psi_\xi^\beta(x) - \psi_\xi^\alpha(y) u_n^\beta(\xi', x) \right) dx dy \right| \\ \leq 2 \left(\iint_{Q_\ell \times Q_\ell} |G_\ell(x-y)| |u_n(\xi', y)|^2 |\psi_\xi(x)|^2 dx dy \right)^{1/2} \left(\iint_{Q_\ell \times Q_\ell} |G_\ell(x-y)| |u_n^*(\xi', y)|^2 |\phi_\xi^*(x)|^2 dx dy \right)^{1/2}$$

from which by the decomposition (B.8) we get

$$\left| \iint_{Q_\ell \times Q_\ell} G_\ell(x-y) \rho_\gamma(y) \phi_\xi^*(x) \psi_\xi(x) dx dy - \int_{Q_\ell^*} d\xi' \iint_{Q_\ell \times Q_\ell} G_\ell(x-y) \phi_\xi^*(x) \gamma_{\xi'}(x, y) \psi_\xi(y) dx dy \right| \\ \leq \left(\int_{Q_{\xi'}} d\xi' \sum_{n \geq 1} |\lambda_n(\xi')| \iint_{Q_\ell \times Q_\ell} |G_\ell(x-y)| |u_n(\xi', y)|^2 |\psi_\xi(x)|^2 dx dy \right)^{1/2} \\ \times \left(\int_{Q_{\xi'}} d\xi' \sum_{n \geq 1} |\lambda_n(\xi')| \iint_{Q_\ell \times Q_\ell} |G_\ell(x-y)| |u_n(\xi', y)|^2 |\phi_\xi^*(x)|^2 dx dy \right)^{1/2} \\ \leq C_H \|\gamma\|_X \|\phi_\xi\|_{L_\xi^2} \|\psi_\xi\|_{L_\xi^2} \quad (C.6)$$

where the last inequality holds by using Lemma 4.1.

Combining (C.6) with Proposition B.1 and estimate (B.13), we get for any $\phi_\xi \in L_\xi^2$ and $\psi_\xi \in H_\xi^1$,

$$|(\phi_\xi, V_{\gamma, \xi} \psi_\xi)| \leq (C_H + C_\ell) \|\gamma\|_{X \cap Y} \|\phi_\xi\|_{L_\xi^2} \|D_\xi |\psi_\xi|\|_{L_\xi^2},$$

hence (4.12) and

$$C_{EE} := C_H + C_\ell. \quad (C.7)$$

Estimate for (4.13). Combining with Proposition B.1 and estimate (B.13), analogous to (C.6) it can be derived directly from:

$$\left| \iint_{Q_\ell \times Q_\ell} G_\ell(x-y) \rho_\gamma(y) \psi_\xi^*(x) \psi_\xi(x) dx dy - \int_{Q_\ell^*} d\xi' \iint_{Q_\ell \times Q_\ell} G_\ell(x-y) \psi_\xi^*(x) \gamma_{\xi'}(x, y) \psi_\xi(y) dx dy \right| \\ \leq \left(\int_{Q_{\xi'}} d\xi' \sum_{n \geq 1} |\lambda_n(\xi')| \iint_{Q_\ell \times Q_\ell} |G_\ell(x-y)| |u_n(\xi', y)|^2 |\psi_\xi(x)|^2 dx dy \right) \\ \leq C_H \|\gamma\|_{\mathfrak{S}_{1,1}} \|D_\xi |^{1/2} \psi_\xi\|_{L_\xi^2}^2$$

using the decomposition (2.10) for γ_ξ . Hence (4.13) and C_{EE} .

Estimate for (4.14). Notice that $|\gamma_{\xi'}(x, y)| \leq \rho_{\gamma_{\xi'}}(x)^{1/2} \rho_{\gamma_{\xi'}}(y)^{1/2}$ since $\gamma \geq 0$. Thus, according to Lemma A.1 and the Cauchy-Schwarz inequality,

$$\int_{Q_\ell^*} d\xi' \iint_{Q_\ell \times Q_\ell} G_\ell(x-y) \psi_\xi^*(x) \gamma_{\xi'}(x, y) \psi_\xi(y) dx dy - \iint_{Q_\ell \times Q_\ell} G_\ell(x-y) \rho_\gamma(x) |\psi_\xi(y)|^2 dx dy \\ \leq \iint_{Q_\ell \times Q_\ell} (|G_\ell(x-y)| - G_\ell(x-y)) \rho_\gamma(y) |\psi_\xi(x)|^2 dx dy \leq \frac{2C_0}{\ell} \|\gamma\|_{\mathfrak{S}_{1,1}} \|\psi\|_{L_\xi^2}^2.$$

Combining with Proposition B.1 and (B.13), we get

$$(\psi_\xi, V_{\gamma, \xi} \psi_\xi) \geq -\left(\frac{C_0}{\ell} + C_\ell\right) \|\gamma\|_{\mathfrak{S}_{1,1} \cap Y} \|\psi_\xi\|_{L_\xi^2}^2,$$

hence (4.13) and

$$C_{EE}'' = \frac{2C_0}{\ell} + C_\ell. \quad (C.8)$$

D Numerical results about constants

In this section, we will show the numerical results about the constants used in Remark 2.8 under the condition $\ell = 1000$. Next, we show that Assumption 2.6 is satisfied for $q \leq 17$ for the neutral systems.

We compute numerically the value of the bound of the potential $G_\ell - \frac{1}{|x|}$. First of all, we calculate

$$\sum_{k \in \mathbb{Z}^3 \setminus \{0\}} \frac{1}{|k|^4} \approx 16.512.$$

Thus, $C_0 \approx 5.019$ and we can choose $C_H = C_G \approx 2.011$. Concerning the estimates involving the potential W_ℓ , we set $m = 2$. When $R \approx \frac{1}{2}$,

$$|C_{\geq 2}| \leq 20.912, \quad C_{\leq 2, 1000} \approx 0.010.$$

Thus, we get $C_W \approx 2.042$, and $C'_W \approx 2.042$. Then, $C_{EE} \approx 2.052$, $C'_{EE} \approx 2.052$ and $C''_{EE} \approx 0.041$.

Finally, we estimate $c^*(q)$ which is given by (2.24). Let $u_{p,\xi}(x) = e^{(2i\pi p/\ell + i\xi) \cdot x}$ with $p \in \mathbb{Z}^3$. Then $(u_{p,\xi})_{p \in \mathbb{Z}^3}$ is an orthogonal basis on $L^2_\xi(Q_\ell)$. Obviously, $(\Lambda^+ u_{p,\xi})_p$ is equally an orthogonal basis on $L^2_\xi(Q_\ell)$. Let

$$V_q = \text{Span}\{\Lambda^+ u_{p,\xi}(x) \mid p = (j, 0, 0), j \in \{1, \dots, q\}\}.$$

Then

$$c^*(q) \leq \sup_{\xi \in Q_\ell^*} \sup_{u_\xi^+ \in V_q} \frac{\| |D_\xi|^{1/2} u_\xi^+ \|_{L^2_\xi}^2}{\|u_\xi^+\|_{L^2_\xi}^2} \leq \sqrt{1 + \frac{4\pi^2(q+1)^2}{\ell^2}}.$$

Now we can check Assumption 2.6 for $z = q = 17$. The calculation leads to $A_0 \approx 0.012$ and $c^*(17) \leq 1.006$. Hence

- $\kappa + \frac{\alpha}{2} C_{EE} q^+ \approx 0.630 < 1$,
- $2A_0 \sqrt{\max\{(1 - \kappa - \frac{\alpha}{2} C_{EE} q^+)^{-1} (1 - \kappa)^{-1} c^*(q+1)q, 1\}} q^+ \approx 0.973 < 1$.

Consequently, Assumption 2.6 is satisfied for $q \leq 17$ whenever $\ell = 1000$.

Bibliography

- [1] V. Bach. “Error bound for the Hartree-Fock energy of atoms and molecules”. In: *Comm. Math. Phys.* 147.3 (1992), pp. 527–548.
- [2] E. Cancès, A. Deleurence, and M. Lewin. “A new approach to the modeling of local defects in crystals: the reduced Hartree-Fock case”. In: *Comm. Math. Phys.* 281.1 (2008), pp. 129–177.
- [3] I. Catto, C. Le Bris, and P. L. Lions. *The mathematical theory of thermodynamic limits: Thomas-Fermi type models*. Oxford Mathematical Monographs. The Clarendon Press, Oxford University Press, New York, 1998, pp. xiv+277. ISBN: 0-19-850161-7.
- [4] I. Catto, C. Le Bris, and P. L. Lions. “Recent mathematical results on the quantum modeling of crystals”. In: *Mathematical models and methods for ab initio quantum chemistry*. Vol. 74. Lecture Notes in Chem. Springer, Berlin, 2000, pp. 95–119.
- [5] I. Catto, C. Le Bris, and P. L. Lions. “On the thermodynamic limit for Hartree-Fock type models”. In: *Ann. Inst. H. Poincaré C Anal. Non Linéaire* 18.6 (2001), pp. 687–760.
- [6] I. Catto, C. Le Bris, and P. L. Lions. “On some periodic Hartree-type models for crystals”. In: *Ann. Inst. H. Poincaré C Anal. Non Linéaire* 19.2 (2002), pp. 143–190.
- [7] N. E. Christensen. “Relativistic band structure calculations”. In: *International Journal of Quantum Chemistry* 25.1 (1984), pp. 233–261.
- [8] N. E. Christensen and B. O. Seraphin. “Relativistic Band Calculation and the Optical Properties of Gold”. In: *Phys. Rev. B* 4 (10 Nov. 1971), pp. 3321–3344.
- [9] J. P. Desclaux. “Relativistic Dirac-Fock expectation values for atoms with $Z = 1$ to $Z = 120$ ”. In: *Atomic Data and Nuclear Data Tables* 12.4 (1973), pp. 311–406.

- [10] J. Dolbeault, M. J. Esteban, and E. Séré. “On the eigenvalues of operators with gaps. Application to Dirac operators”. In: *J. Funct. Anal.* 174.1 (2000), pp. 208–226. Corrigendum in: *J. Funct. Anal.* 284.1 (2023), 109651.
- [11] H. Eschrig, M. Richter, and I. Opahle. “Chapter 12 - Relativistic Solid State Calculations”. In: *Relativistic Electronic Structure Theory*. Ed. by Peter Schwerdtfeger. Vol. 14. Theoretical and Computational Chemistry. Elsevier, 2004, pp. 723–776.
- [12] M. J. Esteban and E. Séré. “Solutions of the Dirac-Fock equations for atoms and molecules”. In: *Comm. Math. Phys.* 203.3 (1999), pp. 499–530.
- [13] M. J. Esteban and E. Séré. “Nonrelativistic limit of the Dirac-Fock equations”. In: *Ann. Henri Poincaré* 2.5 (2001), pp. 941–961.
- [14] M. Ghimenti and M. Lewin. “Properties of periodic Hartree-Fock minimizers”. In: *Calc. Var. Partial Differential Equations* 35.1 (2009), pp. 39–56.
- [15] I. P. Grant. “Relativistic calculation of atomic structures”. In: *Advances in Physics* 19.82 (1970), pp. 747–811.
- [16] M. Griesemer, R. T. Lewis, and H. Siedentop. “A minimax principle for eigenvalues in spectral gaps: Dirac operators with Coulomb potentials”. In: *Doc. Math.* 4 (1999), pp. 275–283.
- [17] I.W. Herbst. “Spectral theory of the operator $(p^2 + m^2)^{1/2} - Ze^2/r$ ”. In: *Comm. Math. Phys.* 53.3 (1977), pp. 285–294.
- [18] M. Huber and H. Siedentop. “Solutions of the Dirac-Fock equations and the energy of the electron-positron field”. In: *Arch. Ration. Mech. Anal.* 184.1 (2007), pp. 1–22.
- [19] M. Kadec, M. Repisky, and K. Ruud. “All-electron fully relativistic Kohn-Sham theory for solids based on the Dirac-Coulomb Hamiltonian and Gaussian-type functions”. In: *Phys. Rev. B* 99 (20 2019), p. 205103.
- [20] T. Kato. *Perturbation theory for linear operators*. Classics in Mathematics. Reprint of the 1980 edition. Springer-Verlag, Berlin, 1995, pp. xxii+619. ISBN: 3-540-58661-X.
- [21] Y. K. Kim. “Relativistic self-consistent-field theory for closed-shell atoms”. In: *Phys. Rev.* 154 (1 Feb. 1967), pp. 17–39.
- [22] E. H. Lieb. “Variational principle for many-fermion systems”. In: *Phys. Rev. Lett.* 46.7 (1981), pp. 457–459.
- [23] E. H. Lieb and B. Simon. “The Thomas-Fermi theory of atoms, molecules and solids”. In: *Advances in Math.* 23.1 (1977), pp. 22–116.
- [24] P. L. Lions. “Solutions of Hartree-Fock equations for Coulomb systems”. In: *Comm. Math. Phys.* 109.1 (1987), pp. 33–97.
- [25] M. H. Mittleman. “Theory of relativistic effects on atoms: Configuration-space Hamiltonian”. In: *Phys. Rev. A* 24 (3 Sept. 1981), pp. 1167–1175.
- [26] E. Paturel. “Solutions of the Dirac-Fock equations without projector”. In: *Ann. Henri Poincaré* 1.6 (2000), pp. 1123–1157.
- [27] P. Pyykkö and J. P. Desclaux. “Relativity and the periodic system of elements”. In: *Accounts of Chemical Research* 12.8 (1979), pp. 276–281.
- [28] M. Reed and B. Simon. *Methods of modern mathematical physics. IV. Analysis of operators*. Academic Press [Harcourt Brace Jovanovich, Publishers], New York-London, 1978, pp. xv+396. ISBN: 0-12-585004-2.
- [29] E. Séré. “A new definition of the Dirac-Fock ground state”. Preprint arXiv:2211.10196, 2022.