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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 fully 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 [8, 7] 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 [23, 3, 5, 6] – 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 [21, 15, 9]. 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 DF 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, $Z \leqslant 124$). 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 introduced a density matrix formulation of the Dirac–Fock model [18]. Recently, one of us proved

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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].

Inspired by this work, 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 [22, 1], and we prove the existence of minimizers. Our result shows that these minimizers solve a self-consistent equation, as established in [14] for the periodic Hartree–Fock model. Our theory can be used to calculate the ground-state of neutral crystals with at least 17 electrons per cell.

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

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

By convention, we choose G_ℓ such that

$$\int_{Q_\ell} G_\ell \, dx = 0. \tag{2.2}$$

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

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

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 $L^2(Q_\ell^*) \bigotimes L^2(Q_\ell; \mathbb{C}^4)$, where $Q_\ell^* = [-\frac{\pi}{\ell}, \frac{\pi}{\ell})^3$ is the so-called reciprocical 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 $U : L^2(\mathbb{R}^3;\mathbb{C}^4) \to L^2(Q_\ell^*) \bigotimes L^2(Q_\ell;\mathbb{C}^4)$ is given by

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

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

$$L^2_\xi(Q_\ell;\mathbb{C}^4) = \left\{\psi \in L^2_{\mathrm{loc}}(\mathbb{R}^3;\mathbb{C}^4) \,\middle|\, e^{-i\xi\cdot x}\psi \text{ is } Q_\ell\text{-periodic}\right\},$$

which will be denoted by L^2_ξ 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

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

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

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

with coefficients

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

The Hilbert space L^2_ξ is endowed with the norm

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

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

$$H^s_\xi(Q_\ell;\mathbb{C}^4) := L^2_\xi(Q_\ell;\mathbb{C}^4) \cap H^s_{\mathrm{loc}}(\mathbb{R}^3;\mathbb{C}^4)$$

for every real number s, endowed with the norm

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

To simplify the notation, we simply write here and below H^s_ξ 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 $\mathcal{L}_\xi$ acting on L^2_ξ and defined by

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

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

$$D^0 = \fint^{\oplus}_{Q_\ell^*} D_\xi\, d\xi. \tag{2.7}$$

where the D_ξ's are self-adjoint operators on L^2_ξ with domains H^1_ξ and form-domains $H^{1/2}_\xi$. Note that $D_\xi^2 = 1 - \Delta_\xi$, where $-\Delta = \fint^{\oplus}_{Q_\ell^*} -\Delta_\xi d\xi$. For every function $\phi_\xi \in H^1_\xi$, 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,

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

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

$$d^+_n(\xi) \geqslant 1, \quad \lim_{n\to\infty} d^+_n(\xi) = +\infty.$$

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

$$\bigcup_{\xi\in Q^*_\ell} \sigma(D_\xi) = \bigcup_{\xi\in Q^*_\ell} \bigcup_{n\geqslant 1} \left\{d^-_n(\xi), d^+_n(\xi)\right\} = \sigma(D^0) = (-\infty, -1] \cup [+1, +\infty). \tag{2.9}$$

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 $\mathcal{B}(L^2_\xi)$ for $\mathcal{B}(L^2_\xi(Q_\ell);\mathbb{C}^4)$. The space of bounded operators on $⨏^\oplus_{Q^*_\ell} L^2_\xi\, d\xi = L^2(Q^*_\ell)\otimes L^2(Q_\ell;\mathbb{C}^4)$ which commute with the translations of $\ell\mathbb{Z}^3$ is denoted by Y. It is isomorphic to $L^\infty(Q^*_\ell;\mathcal{B}(L^2_\xi))$. Moreover, for every $h = ⨏^\oplus_{Q^*_\ell} h_\xi\, d\xi \in Y$,

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

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

$$\mathfrak{S}_s(\xi) := \left\{h \in \mathcal{B}(L^2_\xi) \,\middle|\, \mathrm{Tr}_{L^2_\xi}(|h|^s) < \infty\right\}$$

endowed with the norm

$$\|h\|_{\mathfrak{S}_s(\xi)} = \left(\mathrm{Tr}_{L^2_\xi}(|h|^s)\right)^{1/s}.$$

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

$$\mathfrak{S}_{s,t} := \left\{h = ⨏^\oplus_{Q^*_\ell} h_\xi\, d\xi \,\middle|\, h_\xi \in \mathfrak{S}_s(\xi) \text{ a.e. } \xi \in Q^*_\ell, \|h_\xi\|_{\mathfrak{S}_s(\xi)} \in L^t(Q^*_\ell)\right\}$$

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

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

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

$$X^\alpha(\xi) = \left\{h \in \mathcal{B}(L^2_\xi) \,\middle|\, |D_\xi|^{\alpha/2} h |D_\xi|^{\alpha/2} \in \mathfrak{S}_1(\xi)\right\}$$

endowed with the norm

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

and

$$X^\alpha_s := \left\{h = ⨏^\oplus_{Q^*_\ell} h_\xi\, d\xi \,\middle|\, h_\xi \in \mathfrak{S}_1(\xi) \text{ a.e. } \xi \in Q^*_\ell, \int_{Q^*_\ell} \||D_\xi|^{\alpha/2} h_\xi |D_\xi|^{\alpha/2}\|^s_{\mathfrak{S}_1(\xi)} d\xi < \infty\right\}$$

endowed with the norm

$$\|h\|_{X^\alpha_s} = \left(\fint_{Q^*_\ell} \| |D_\xi|^{\alpha/2} h_\xi |D_\xi|^{\alpha/2} \|^s_{\mathfrak{S}_1(\xi)} d\xi \right)^{1/s} = \| |D^0|^{\alpha/2} h |D^0|^{\alpha/2} \|_{\mathfrak{S}_{1,s}}.$$

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

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

Remark 2.2 (Projectors)**.** *According to [1, 22, 14] 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 2.3. *For $\gamma \in \mathcal{T}$ and for almost every ξ in Q^*_ℓ, the operator γ_ξ is compact on L^2_ξ and admits a complete set of eigenfunctions $(u_n(\xi,\cdot))_{n\geqslant 1}$ in L^2_ξ (actually lying in $H^{1/2}_\xi$), corresponding to a non-decreasing sequence of eigenvalues $0 \leqslant \lambda_n(\xi) \leqslant 1$ (counted with their multiplicity). This is expressed as*

$$\gamma_\xi = \sum_{n\geqslant 1} \lambda_n(\xi) \left| u_n(\xi,\cdot) \right\rangle \left\langle u_n(\xi,\cdot) \right| , \; (u_n(\xi,\cdot), u_m(\xi,\cdot))_{L^2_\xi} = \delta_{n,m} \tag{2.10}$$

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

$$\gamma_\xi(x,y) = \sum_{n\geqslant 1} \lambda_n(\xi) u_n(\xi,x) u^*_n(\xi,y). \tag{2.11}$$

*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 $\varphi \in L^2_\xi$,*

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

By definition of the trace of an operator,

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

This allows us to define

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

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

Definition 2.4 (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*

$$\gamma(x,y) = \fint_{Q^*_\ell} \gamma_\xi(x,y)\,d\xi \tag{2.12}$$

and

$$\rho_\gamma(x) = \fint_{Q^*_\ell} \mathrm{Tr}_4 \gamma_\xi(x,x)\,d\xi, \tag{2.13}$$

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*

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

and

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

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

$$|\gamma(x, y)|^2 \leqslant \rho_\gamma(x)\, \rho_\gamma(y), \qquad a.e.\ x, y \in \mathbb{R}^3. \tag{2.15}$$

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* $|h(x, y)|^2 \leqslant \rho_{|h|}(x)\rho_{|h|}(y)$ *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 :

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

and

$$\Gamma_{\leqslant q} := \left\{\gamma \in \mathcal{T} \,\middle|\, \|\gamma\|_{\mathfrak{S}_{1,1}} \leqslant q\right\}.$$

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

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

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

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 $\mathrm{Tr}_{L^2_\xi}[D_\xi \gamma_\xi]$ is not really a trace, it is just a notation for the rigorous mathematical object $\mathrm{Tr}_{L^2_\xi}[|D_\xi|^{1/2}\gamma_\xi |D_\xi|^{1/2} \mathrm{sign}(D_\xi)]$. 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

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

(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 $\gamma \in \Gamma_{\leqslant q}$, we now define the mean-field periodic Dirac operator

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

where

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

with

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

and

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

(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 $\Gamma_{\leqslant q}$ with h in $\mathcal{T}$, then the right derivative of $t \mapsto \mathcal{E}^{DF}(\gamma + th)$ at $t = 0$ is $\fint_{Q_\ell^*} \mathrm{Tr}_{L^2_\xi}(D_{\gamma,\xi} h_\xi)\,d\xi$.

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

2.3 Ground-state energy and main result

In most situations of physical and chemical interest, the negative energy states of Dirac–Fock models are irrelevant for the description of electrons.The ground- energy and state should thus be defined on the positive spectral subspaces of the corresponding Dirac–Fock operator. Let

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

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

$$\Gamma_q^+ := \left\{\gamma \in \Gamma_q \,\middle|\, \gamma = P_\gamma^+ \gamma P_\gamma^+\right\}$$

and the ground-state energy

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

Our main result is the following.

Theorem 2.5 (Existence of a minimizer)**.** *Under some conditions on α, q, z and ℓ that are detailed in Assumption 2.6 below, there exists $\gamma_* \in \Gamma_q^+$ such that*

$$\mathcal{E}^{DF}(\gamma_*) = I_q = \min_{\gamma \in \Gamma_q^+} \mathcal{E}^{DF}(\gamma). \tag{2.20}$$

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

$$\gamma = 1_{[0,\nu)}(D_\gamma) + \delta \tag{2.21}$$

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

$$c^*(k) := \sup_{\xi \in Q_\ell^*} d_k^+(\xi) \tag{2.22}$$

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

Assumption 2.6. *Let $q^+ := \max\{q, 1\}$, $\kappa := \alpha\left(C_G z + C'_{EE} q^+\right)$ 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.

Remark 2.7. *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 $q \leqslant 17$. 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 $\Gamma_{\leqslant q}^+$ defined by

$$\Gamma_{\leqslant q}^+ := \left\{\gamma \in \Gamma_{\leqslant q} \,\middle|\, \gamma = P_\gamma^+ \gamma P_\gamma^+\right\}.$$

However, a direct computation shows that 0 is a minimizer. To overcome this problem, we next subtract a penalization term $\epsilon_P \widetilde{\mathrm{Tr}}_{L^2}(\gamma)$, for some parameter $\epsilon_P > 0$ to be chosen later, and first study the minimization problem for the penalized functional with relaxed constraint :

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

We prove below that, when ϵ_P is sufficiently large, every minimizer of problem $I_{\leqslant q}$ 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 2.5 read as follows.

Assumption 3.1. *Let $q^+ = \max\{q, 1\}$, $\kappa := \alpha\,(C_G z + C'_{EE} q^+)$ 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 $\gamma_* \in \Gamma_{\leqslant q}^+$ such that*

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

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

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

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

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 (2.21).*

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 $I_{\leqslant q}$ lies in Γ_q^+. Thus,

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

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

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

□

We therefore focus on the proof of Theorem 3.2. We consider a minimizing sequence $(\gamma_n)_{n\geqslant 1}$ in $\Gamma^+_{\leqslant q}$ and first prove that it is bounded for the norm of $X \cap Y$ (Lemma 4.15). The singular behaviour of the potential $W^\infty_\ell(\xi, x)$ with respect to $\xi \in Q^*_\ell$ (of order $1/|\xi|^2$) leads to the failure of the direct convergence study. Whereas in the Hartree–Fock model, the potential W^∞_ℓ can be controlled directly by the Schrödinger operator [5], it is not the case for the Dirac operator D^0. We overcome this difficulty by first considering existence of minimizers into the following set

$$B_R := \left\{\gamma \in X \cap Y \,\middle|\, \|\gamma\|_{\mathfrak{S}_{1,\infty}} < R\right\} \tag{3.3}$$

with R large enough. For density matrices in this set, the exchange term is well-controlled. Moreover, it turns out the minimizers in this set do not saturate the constraint $\|\gamma\|_{\mathfrak{S}_{1,\infty}} < R$. 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 4.15 below. Under Assumption 3.1, if $\epsilon_P > (1-\kappa)^{-1}c^*(q+1)$ and for any $R > R_0$, there exists γ_* in $\Gamma^+_{\leqslant q} \cap B_R$ such that*

$$I_{\leqslant q,R} := \min_{\gamma\in\Gamma^+_{\leqslant q}\cap B_R} \left[\mathcal{E}^{DF}(\gamma) - \epsilon_P \widetilde{\mathrm{Tr}}_{L^2}(\gamma)\right] = \mathcal{E}^{DF}(\gamma_*) - \epsilon_P \widetilde{\mathrm{Tr}}_{L^2}(\gamma_*). \tag{3.4}$$

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

$$\gamma = \mathbb{1}_{[0,\nu)}(D_\gamma) + \delta \tag{3.5}$$

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

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 $I_{\leqslant q}$ is achieved. Any minimizer γ_* of (3.4) is a minimizer of $I_{\leqslant q}$. It satisfies $\widetilde{\mathrm{Tr}}_{L^2}(\gamma_*) = q$ and γ_* lies in $\mathfrak{S}_{1,\infty}$.*

Proof of Corollary 3.5. The proof follows immediately from the fact that any minimizer in B_R lies in $\overline{R}_{R_0}$ and by observing that $R \mapsto I_{\leqslant q,R}$ is non-increasing with $I_{\leqslant q} = \lim_{R\to+\infty} I_{\leqslant q,R}$. ☐

Next sections are devoted to the proof of Proposition 3.4.

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 first estimates on minimizing sequences.

In Section 5, we study the linearization problem associated to (3.4). We conclude that the minimizers of (3.4) 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 $\Gamma^+_{\leqslant q}$ 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 $\theta : \mathcal{V} \to \mathcal{V}$ on an open neighborhood $\mathcal{V}$ of the minimizing sequence of (3.4) in $\Gamma^+_{\leqslant q}$ such that $\theta(\gamma) = P^+_{\theta(\gamma)}\theta(\gamma)P^+_{\theta(\gamma)}$. Next, we consider an equivalent minimization problem with locally convex constraint ; namely

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

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*

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

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

Moreover, there exists a positive constant $C_G = C_G(\ell)$ with $C_G \geqslant C_H$ 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 $A \leqslant B$ is equivalent to : For almost every $\xi \in Q_\ell^*$, $A_\xi \leqslant B_\xi$ in the sense of operators on L^2_ξ.*

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,*

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

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 [20, 17].

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*

$$\|\rho_\gamma * G_\ell\|_Y \leqslant C_H\,\|\gamma\|_X \tag{4.4}$$

and

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

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

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

Indeed, the bound (4.1) in Lemma 4.1 yields

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

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

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

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 $x \in \mathbb{R}^3$.

□

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

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

with

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

and

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

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 $W_{\geqslant m,\ell}(\eta, x)$ 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*

$$\begin{aligned} \|W_\gamma\|_Y &\leqslant C_W\,\|\gamma\|_{X\cap Y} && \text{if } \gamma \in X \cap Y, && (4.8)\\ \|W_\gamma\|_Y &\leqslant C''_W\,(\|\gamma\|_X + \|\gamma\|^{3/4}_{\mathfrak{S}_{1,\infty}}\|\gamma\|^{1/4}_{\mathfrak{S}_{1,1}}) && \text{if } \gamma \in X \cap \mathfrak{S}_{1,\infty}, && (4.9)\\ \|W_\gamma\,|D^0|^{-1}\|_Y &\leqslant C'_W\,\|\gamma\|_{\mathfrak{S}_{1,1}\cap Y} && \text{if } \gamma \in \mathfrak{S}_{1,1} \cap Y. && (4.10) \end{aligned}$$

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*

$$\|V_{\gamma,\xi}\|_Y \leqslant C_{EE}\,\|\gamma\|_{X\cap Y} \tag{4.11}$$

and

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

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

$$\left|(\psi_\xi, V_{\gamma,\xi}\psi_\xi)_{L^2_\xi}\right| \leqslant C_{EE}\|\gamma\|_{\mathfrak{S}_{1,1}\cap Y}\|\psi_\xi\|^2_{H^{1/2}_\xi} \tag{4.13}$$

Furthermore, if $\gamma \geqslant 0$, for any $\psi \in L^2_\xi$,

$$-C''_{EE}\|\gamma\|_{\mathfrak{S}_{1,1}\cap Y}\|\psi_\xi\|^2_{L^2_\xi} \leqslant (\psi_\xi, V_{\gamma,\xi}\psi_\xi)_{L^2_\xi}. \tag{4.14}$$

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 $\kappa := \alpha\left(C_G z + C'_{EE} q^+\right)$. 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^2_ξ with domain H^1_ξ and form-domain $H^{1/2}_\xi$. In addition, the following holds*

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

and

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

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

$$(1-\kappa)\,|D^0| \leqslant |D_\gamma| \leqslant (1+\kappa)\,|D^0|. \tag{4.17}$$

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

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

In particular, D_γ is self-adjoint on $\fint^{\oplus}_{Q^*_\ell} H^1_\xi\, d\xi$ 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 $u_\xi \in H^1_\xi(Q_\ell)$. We have

$$\|D_{\gamma,\xi}\, u_\xi\|_{L^2_\xi} \leqslant \left(1 + \alpha\, C_G z + \alpha C'_{EE}\|\gamma\|_{\mathfrak{S}_{1,1}\cap Y}\right)\, \|D_\xi\, u_\xi\|_{L^2_\xi}, \tag{4.19}$$

which implies (4.15). On the other hand,

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

Hence,

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

which implies (4.16). Since $\gamma \in \Gamma_{\leqslant q}$, $\|\gamma\|_{\mathfrak{S}_{1,1}\cap Y} \leqslant q^+$. 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 $\mathbb{R}\backslash[-1+\kappa; 1-\kappa]$. 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 $\gamma \in \Gamma_{\leqslant q}$. Then*

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

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

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

and

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

We get

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

$\square$

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 $\gamma \in \Gamma_{\leqslant q}$. We denote by $\lambda_k(\xi)$, for $k \geqslant 1$, 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 $1 \leqslant c_*(k) \leqslant c^*(k)$ and $c_*(k) \to +\infty$ when $k \to +\infty$, 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^1_ξ and satisfies

$$\||D_\xi| u_{k,\xi}\|_{L^2_\xi} \leqslant (1-\kappa)^{-1}\, \lambda_k(\xi)\, \|u_{k,\xi}\|_{L^2_\xi} \leqslant c^*(k)\, (1-\kappa)^{-2}\, \|u_{k,\xi}\|_{L^2_\xi}. \tag{4.21}$$

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

$$\lambda_k(\xi) := \inf_{\substack{V \text{ subspace of } \Lambda^+_\xi H^{1/2}_\xi \\ \dim V = k}} \ \sup_{u_\xi \in (V \bigoplus \Lambda^-_\xi H^{1/2}_\xi)\setminus\{0\}} \frac{(D_{\gamma,\xi}\, u_\xi, u_\xi)}{\|u_\xi\|^2_{L^2_\xi}}. \tag{4.22}$$

Let $u_\xi \in (V \bigoplus \Lambda^-_\xi H^{1/2}_\xi)\setminus\{0\}$. We write $u_\xi = u^+_\xi + u^-_\xi$ with

$$u^+_\xi = \Lambda^+_\xi u_\xi \in V, \quad u^-_\xi = \Lambda^-_\xi u_\xi \in \Lambda^-_\xi H^{1/2}_\xi.$$

By definition of $\Lambda^\pm_\xi$,

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

Therefore,

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

To get the lower bound, we observe that

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

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

$$(D_{\gamma,\xi}\, u_\xi, u_\xi) = (|D_\xi|\, u_\xi, u_\xi) + ((D_{\gamma,\xi} - D_\xi)\, u_\xi, u_\xi) \geqslant (1-\kappa)\, (|D_\xi|\, u_\xi, u_\xi)\,.$$

Thus,

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

We define

$$c_*(k) := \inf_{\xi \in Q^*_\ell} d^+_k(\xi) = \inf_{\xi \in Q^*_\ell} \ \inf_{\substack{V \text{ subspace of } \Lambda^+_\xi H^{1/2}_\xi \\ \dim V = k}} \ \sup_{u_\xi \in V\setminus\{0\}} \frac{(|D_\xi| u_\xi, u_\xi)}{\|u_\xi\|^2_{L^2_\xi}}.$$

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

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

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

$$\begin{aligned}
(D_{\gamma,\xi}u_\xi, u_\xi) &= \Big(|D_\xi|\, u_\xi^+, u_\xi^+\Big) + \Big((D_{\gamma,\xi}-D_\xi)\, u_\xi^+, u_\xi^+\Big) + 2\Re\Big((D_{\gamma,\xi}-D_\xi)\, u_\xi^+, u_\xi^-\Big) \\
&\quad + \Big((D_{\gamma,\xi}-D_\xi)\, u_\xi^-, u_\xi^-\Big) - \Big(|D_\xi|\, u_\xi^-, u_\xi^-\Big) \\
&\leqslant (1+\kappa)\ \Big(|D_\xi|\, u_\xi^+, u_\xi^+\Big) - (1-\kappa)\ \Big(|D_\xi|\, u_\xi^-, u_\xi^-\Big) + 2\,\kappa\, \||D_\xi|^{1/2}u_\xi^+\|_{L^2_\xi}\, \||D_\xi|^{1/2}u_\xi^-\|_{L^2_\xi} \\
&= (1+\kappa)\||D_\xi|^{1/2}u_\xi^+\|^2_{L^2_\xi} + 2\,\kappa\, \||D_\xi|^{1/2}u_\xi^+\|_{L^2_\xi}\, \||D_\xi|^{1/2}u_\xi^-\|_{L^2_\xi} - (1-\kappa)\||D_\xi|^{1/2}u_\xi^-\|^2_{L^2_\xi} \\
&\leqslant (1-\kappa)^{-1}\||D_\xi|^{1/2}u_\xi^+\|^2_{L^2_\xi},
\end{aligned}$$

by Young's inequality. Let now

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

As $\|u_\xi^+\|_{L^2_\xi} \leqslant \|u_\xi\|_{L^2_\xi}$, we obtain

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

By construction, $c_*(k) \leqslant c^*(k)$ 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 $M \geqslant 2$ such that $c_*(q+M-1) \leqslant e < c_*(q+M)$. 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

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

Hence (4.21).

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

4.3 Properties of the minimizers of a linear problem

Recall that $B_R := \big\{\gamma \in X \cap Y \,\big|\, \|\gamma\|_{\mathfrak{S}_{1,\infty}} < R\big\}$ 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 $g \in \Gamma_{\leqslant q}$ be given, and assume $\kappa < 1$. Then for each $\epsilon_P > 0$, the minimization problem*

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

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

Furthermore, for every ϵ_P, we have $\nu \leqslant (1-\kappa)^{-1}c^*(q+1)$ 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 $\widetilde{\mathrm{Tr}}_{L^2}(\gamma_*) = q$.

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

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

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

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

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

$$\lim_{s \to \nu_1^-} C(s) \leqslant q \leqslant \lim_{s \to \nu_1^+} C(s). \tag{4.25}$$

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

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

with $0 \leqslant \delta \leqslant \fint_{Q_\ell^*}^{\oplus} 1_{\{\nu\}}(D_{g,\xi}) d\xi$ 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 $\widetilde{\gamma} = 1_{[0,\nu_1)}(D_g) + \delta$ where $0 \leqslant \delta \leqslant 1_{\{\nu_1\}}(D_g)$ is chosen such that

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

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

$$\begin{aligned}
&\fint_{Q_\ell^*} \mathrm{Tr}_{L^2_\xi}((D_{g,\xi} - \epsilon_P)(\gamma_\xi - \widetilde{\gamma}_\xi)) d\xi \\
&= \fint_{Q_\ell^*} \mathrm{Tr}_{L^2_\xi}((D_{g,\xi} - \nu_1)(\gamma_\xi - \widetilde{\gamma}_\xi)) d\xi + \fint_{Q_\ell^*} \mathrm{Tr}_{L^2_\xi}(\nu_1 - \epsilon_P)(\gamma_\xi - \widetilde{\gamma}_\xi)) d\xi \\
&= \fint_{Q_\ell^*} \mathrm{Tr}_{L^2_\xi}((D_{g,\xi} - \nu_1)(\gamma_\xi - \widetilde{\gamma}_\xi)) d\xi + |\nu_1 - \epsilon_P| \left| \fint_{Q_\ell^*} \mathrm{Tr}_{L^2_\xi}(\gamma_\xi - \widetilde{\gamma}_\xi) d\xi \right| \\
&\geqslant \fint_{Q_\ell^*} \mathrm{Tr}_{L^2_\xi}((D_{g,\xi} - \nu_1)(\gamma_\xi - \widetilde{\gamma}_\xi)) d\xi.
\end{aligned} \tag{4.26}$$

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

$$\begin{aligned}
&\fint_{Q_\ell^*} \mathrm{Tr}_{L^2_\xi}((D_{g,\xi} - \nu_1)(\gamma_\xi - \widetilde{\gamma}_\xi)) d\xi \\
&\quad = \fint_{Q_\ell^*} \mathrm{Tr}_{L^2_\xi}[(D_{g,\xi} - \nu_1)(\gamma_\xi - 1_{[0,\nu_1)}(D_{g,\xi})]\, d\xi \\
&\quad = \fint_{Q_\ell^*} \sum_{\lambda_k(\xi) < \nu_1} |\lambda_k(\xi) - \nu_1|\, |\langle \gamma_\xi \psi_k(\xi), \psi_k(\xi) \rangle - 1|\, d\xi \\
&\qquad\qquad + \fint_{Q_\ell^*} \sum_{\lambda_k(\xi) > \nu_1} [|\lambda_k(\xi) - \nu_1|\, \langle \gamma_\xi \psi_k(\xi), \psi_k(\xi) \rangle]\, d\xi \geqslant 0.
\end{aligned} \tag{4.27}$$

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

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

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

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

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

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

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

$$q \geqslant \lim_{s\to v_1^-} C(s) \geqslant C((1-\kappa)^{-1}c^*(q+1)) \geqslant q+1,$$

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

$$q \leqslant \lim_{s\to v_1^+} C(s) \leqslant C((1-\kappa)c^*(q-1)) \leqslant q-1.$$

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

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

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 $\mathrm{Tr}_{L_\xi^2}(\gamma_*) = q$. □

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

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* $\gamma, \gamma' \in \Gamma_{\leqslant q}$ *such that*

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

Then,

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

Proof. By Lemma 4.9, we have

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

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

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

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

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

□

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

We prove the following.

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

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

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

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

and

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

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

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

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

Hence,

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

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

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

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

$\square$

From now on, we define the set

$$\mathcal{V}_0 := \left\{\gamma\in\Gamma^+_{\leqslant q}\,\middle|\,\mathcal{E}^{DF}(\gamma) - \epsilon_P\widetilde{\mathrm{Tr}}_{L^2}(\gamma) \leqslant 0\right\} \tag{4.29}$$

to which the minimizing sequences belong, at least from a certain rank, under Assumption 3.1.

5 Approximation by a linearized problem

The aim of this section is to show the link between a minimizing sequence $(\gamma_n)_{n\geqslant 1}$ 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 $(\gamma_n) \in \Gamma^+_{\leqslant q} \cap B_R$ be a minimizing sequence of (3.4). Then, as n goes to infinity,*

$$\fint_{Q^*_\ell} \mathrm{Tr}_{L^2_\xi}\left[(D_{\gamma_n,\xi} - \epsilon_P)\gamma_{n,\xi}\right] d\xi - \inf_{\substack{\gamma\in\Gamma_{\leqslant q}\\ \gamma = P^+_{\gamma_n}\gamma P^+_{\gamma_n}}} \fint_{Q^*_\ell} \mathrm{Tr}_{L^2_\xi}\left[(D_{\gamma_n,\xi} - \epsilon_P)\gamma_\xi\right] d\xi \to 0. \tag{5.1}$$

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 $I_{\leqslant q}$.

As mentioned at the end of Section 3, the main difficulty is to deal with the nonlinear constraint $\Gamma^+_{\leqslant q}$. 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 $\Gamma_{\leqslant q}$ into a neighborhood of $\mathcal{V}_0$ in $\Gamma^+_{\leqslant q}$. More precisely, we will have $\mathcal{V}_0 \subset \theta(\mathcal{V}) \subset \Gamma^+_{\leqslant q}$. Consequently,

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

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

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

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

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

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 $\mathrm{Fix}(T)$ the set of fixed points of the map T (i.e., for any $\gamma \in \mathrm{Fix}(T)$, $T(\gamma) = \gamma$). Obviously, $T(\gamma)$ is self-adjoint and $0 \leqslant T(\gamma) \leqslant 1$. In particular, $\Gamma^+_{\leqslant q} = \Gamma_{\leqslant q} \cap \mathrm{Fix}(T)$. Unfortunately, given γ in $\Gamma_{\leqslant q}$, $T(\gamma)$ may not stay in $\Gamma^+_{\leqslant q}$: $P^+_{T(\gamma)}T(\gamma)P^+_{T(\gamma)}$ 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 a 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* $\kappa = \alpha\left(C_G z + C'_{EE}q^+\right) < 1$ *and let* $A := \frac{\alpha}{2}C_{EE}(1-\kappa)^{-1/2}\lambda_0^{-1/2} < \frac{1}{2}$. *Given* $1 < \tau < \frac{1}{2A}$, *let* $M := \max\left(\frac{2+Aq^+}{2}, \frac{1}{1-2A\tau}\right)$, *then we define*

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

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

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

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

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* $\theta(\overline{\mathcal{U}}) \subset \Gamma^+_{\leqslant q} \cap \overline{\mathcal{U}}$ *and* $\mathit{Fix}(T) = \Gamma^+_{\leqslant q} \cap \overline{\mathcal{U}}$. *We have the estimate*

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

Moreover $\theta \in C^{1,unif}(\mathcal{U}, X\cap Y)$ *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* $\Gamma^+_{\leqslant q} \cap \overline{\mathcal{U}}$ *whose restriction to* $\mathcal{U}$ *is of class* $C^{1,unif}$. *This map and its differential are bounded and uniformly continuous on* $\mathcal{U}$.

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

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

where $\theta(\gamma) = \fint^{\oplus}_{Q^*_\ell} \theta_\xi(\gamma)d\xi$, *according to the Floquet-Bloch decomposition. In other words, the splitting* $L^2_\xi = P^+_{\gamma,\xi}L^2_\xi \oplus P^-_{\gamma,\xi}L^2_\xi$ *gives a block decomposition of* $d\theta_\xi(\gamma)h$ *of the form*

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

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 (5.11)), 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,

$$\fint_{Q_\ell^*} \mathrm{Tr}_{L^2_\xi}((D_{\gamma_n,\xi} - \epsilon_P)\gamma_{n,\xi})d\xi \geqslant \inf_{\substack{\gamma\in\Gamma_{\leqslant q},\\ \gamma = P^+_{\gamma_n}\gamma}} \fint_{Q_\ell^*} \mathrm{Tr}_{L^2_\xi}\big[(D_{\gamma_n,\xi} - \epsilon_P)\gamma\big]d\xi + \epsilon_0.$$

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

$$\fint_{Q_\ell^*} \mathrm{Tr}_{L^2_\xi}\big[(D_{\gamma_n,\xi} - \epsilon_P)\gamma_{n,\xi}'\big]\, d\xi := \inf_{\substack{\gamma\in\Gamma_{\leqslant q},\\ \gamma = P^+_{\gamma_n}\gamma}} \fint_{Q_\ell^*} \mathrm{Tr}_{L^2_\xi}\big[(D_{\gamma_n,\xi} - \epsilon_P)\gamma_\xi\big]\, d\xi.$$

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

$$f_n'(0) = \widetilde{\mathrm{Tr}}_{L^2}\big(D_{\gamma_n} - \epsilon_P)(\gamma_n' - \gamma_m)\big) \leqslant -\frac{\epsilon_0}{2}.$$

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

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

But $\theta[(1-s)\gamma_n + s\gamma_n'] \in \Gamma^+_{\leqslant q}\bigcap B_R$ and $\mathcal{E}^{DF}(\gamma_n) - \epsilon_P\widetilde{\mathrm{Tr}}_{L^2}(\gamma_n) \to I_{\leqslant q,R}$. This is a contradiction. Hence the proposition. ◻

We are now in the position to prove Proposition 5.4. This is essentially the same as in [29]. Recall now that $P_0^+ = 1_{\mathbb{R}^+}(D^0 - \alpha z G_\ell)$ and $A = \frac{\alpha}{2}C_{EE}\,(1-\kappa)^{-1/2}\lambda_0^{-1/2}$ with λ_0 given in Lemma 4.10.

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

$$Q\colon \gamma \longmapsto P_\gamma^+ - P_0^+$$

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

Then the map Q is in $C^{1,lip}(\Gamma_{\leqslant q}, \mathcal{B}(L^2(\mathbb{R}^3,\mathbb{C}^4), H^{1/2}(\mathbb{R}^3),\mathbb{C}^4))$ and we have the estimates

$$\forall\gamma\in\Gamma_{\leqslant q},\quad \forall h\in X\cap Y:\quad \||D^0|^{1/2}dQ(\gamma)h\|_Y \leqslant A\|h\|_{X\cap Y} \tag{5.5}$$

and

$$\forall\gamma,\gamma'\in\Gamma_{\leqslant q}\quad, \||D^0|^{1/2}[dQ(\gamma)h - dQ(\gamma')h]|D^0|^{1/2}\|_Y \leqslant K\|\gamma-\gamma'\|_{X\cap Y}\|h\|_{X\cap Y}, \tag{5.6}$$

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

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

$$P^{\pm}_{\gamma,\xi} = \frac{1}{2} \pm \frac{1}{2\pi} \int_{-\infty}^{+\infty} (D_{\gamma,\xi} - iz)^{-1} dz \tag{5.7}$$

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 (5.7) and the second resolvent formula again, that

$$dQ_\xi(\gamma)h = dP^{+}_{\gamma,\xi}\, h = -\frac{\alpha}{2\pi} \int_{-\infty}^{+\infty} (D_{\gamma,\xi} - iz)^{-1} V_{h,\xi} (D_{\gamma,\xi} - iz)^{-1} dz. \tag{5.8}$$

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

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

We infer from Lemma 4.10 that

$$\||D_\gamma|^{-1}\|_Y \leqslant \lambda_0^{-1}.$$

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

$$\begin{aligned}
&\Big|(\psi_\xi, |D_\xi|^{1/2} dQ_\xi(\gamma) h \phi_\xi)_{L^2_\xi}\Big| \\
&\quad = \frac{\alpha}{2\pi} \left| \int_{-\infty}^{+\infty} \Big(\psi_\xi, |D_\xi|^{1/2} (D_{\gamma,\xi} - iz)^{-1} V_{h,\xi} (D_{\gamma,\xi} - iz)^{-1} \phi_\xi \Big)_{L^2_\xi} dz \right| \\
&\quad \leqslant \frac{\alpha}{2\pi} \|V_{h,\xi}\|_{\mathcal{B}(L^2_\xi)} \left(\int_{-\infty}^{+\infty} \Big\| (D_{\gamma,\xi} - iz)^{-1} |D_\xi|^{1/2} \psi_\xi \Big\|^2_{L^2_\xi} dz \right)^{1/2} \left(\int_{-\infty}^{+\infty} \|(D_{\gamma,\xi} - iz)^{-1} \phi_\xi\|^2_{L^2_\xi} dz \right)^{1/2} \\
&\quad \leqslant \frac{\alpha}{2\pi} \|V_{h,\xi}\|_{\mathcal{B}(L^2_\xi)} \||D_\xi|^{1/2} |D_{\gamma,\xi}|^{-1/2} \phi\|_{\mathcal{B}(L^2_\xi)} \||D_{\gamma,\xi}|^{-1/2}\|_{\mathcal{B}(L^2_\xi)} \|\psi_\xi\|_{L^2_\xi} \|\phi_\xi\|_{L^2_\xi} \\
&\quad \leqslant \frac{\alpha}{2} C_{EE} (1-\kappa)^{-1/2} \lambda_0^{-1/2} \|h\|_{X\cap Y} \|\psi_\xi\|_{L^2_\xi} \|\phi_\xi\|_{L^2_\xi}.
\end{aligned} \tag{5.9}$$

Hence we obtain (5.5), i.e.,

$$\||D^0|^{1/2} dQ(\gamma) h |D^0|^{1/2}\|_Y \leqslant \frac{\alpha}{2} C_{EE} (1-\kappa)^{-1/2} \lambda_0^{-1/2} \|h\|_{X\cap Y}.$$

For the second inequality, we have

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

Proceeding as above, we get (5.6). The fact that $Q \in C^{1,\mathrm{lip}}(\Gamma_{\leqslant q}, \mathcal{B}(L^2, H^{1/2}))$ follows from (5.5) and (5.6). $\square$

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

$$\begin{aligned}
\|T^2(\gamma) - T(\gamma)\|_{X\cap Y} \leqslant 2A \Big(&\max\{\|T(\gamma)|D^0|^{1/2}\|_{\mathfrak{S}_{1,1}}, \|T(\gamma)\|_Y\} \\
&+ \frac{Aq^+}{2} \|\gamma - T(\gamma)\|_{X\cap Y} \Big) \|T(\gamma) - \gamma\|_{X\cap Y}.
\end{aligned} \tag{5.10}$$

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

$$\forall\,\gamma\in\Gamma_{\leqslant q},\quad \|dT(\gamma)\|_{\mathcal{B}(X\cap Y)}\leqslant C_\kappa(1+\max\{\|\gamma|D^0|^{1/2}\|_{\mathfrak{S}_{1,1}},\|\gamma\|_Y\}), \tag{5.11}$$

and

$$\forall\,\gamma,\gamma'\in\Gamma_{\leqslant q},\ \|dT(\gamma')-dT(\gamma)\|_{\mathcal{B}(X\cap Y)}\leqslant L_\kappa(1+\max\{\|\gamma|D^0|^{1/2}\|_{\mathfrak{S}_{1,1}},\|\gamma\|_Y\})\|\gamma'-\gamma\|_{X\cap Y}. \tag{5.12}$$

Proof. Let $\gamma,\gamma'\in\Gamma_{\leqslant q}$. 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 (5.5),

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

For the estimate (5.10), 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

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

We have

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

and

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

Notice that $\|T(\gamma)\|_{\mathfrak{S}_{1,1}\cap Y}\leqslant\|\gamma\|_{\mathfrak{S}_{1,1}\cap Y}\leqslant q^+$. Gathering together these estimates, we obtain (5.10).

We turn now to the proof of (5.11) and (5.12). From Lemma 5.6, T is in $C^1(\Gamma_{\leqslant q})$ with

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

Notice that for any $\gamma\in\Gamma_{\leqslant q}$,

$$\||D^0|^{1/2}P^+_\gamma|D^0|^{-1/2}\|_Y\leqslant(1-\kappa)^{-1/2}\||D_\gamma|^{1/2}P^+_\gamma|D^0|^{-1/2}\|_Y\leqslant\frac{(1+\kappa)^{1/2}}{(1-\kappa)^{1/2}}. \tag{5.13}$$

Then,

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

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

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

Proceeding in the same way as for (5.11), we can get (5.12). □

We now show that T satisfies all the assumptions in [29, Proposition 2.2].

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

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

and

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

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

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

$$\|T(\gamma)|D^0|^{1/2}\|_{\mathfrak{S}_{1,1}} \leqslant \|\gamma|D^0|^{1/2}\|_{\mathfrak{S}_{1,1}} + \|(\gamma - T(\gamma))|D^0|^{1/2}\|_{\mathfrak{S}_{1,1}} \leqslant \|\gamma|D^0|^{1/2}\|_{\mathfrak{S}_{1,1}} + \|\gamma - T(\gamma)\|_X$$

and

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

As a result, as $M \geqslant \frac{2+q^+A}{2}$, (5.10) implies that

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

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

$$\begin{aligned}\max\{\|T(\gamma)|D^0|^{1/2}\|_{\mathfrak{S}_{1,1}}, \|T(\gamma)\|_Y\} + M\|T^2(\gamma) - T(\gamma)\|_{X \cap Y}\\ \leqslant \max\{\|\gamma|D^0|^{1/2}\|_{\mathfrak{S}_{1,1}}, \|\gamma\|_Y\} + (1 + Mk)\|T(\gamma) - \gamma\|_{X \cap Y} < \tau.\end{aligned}$$

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

The fact that $\sup_{\gamma \in \mathcal{U}} \|dT(\gamma)\|_{X \cap Y} < \infty$ and dT is Lipschitzian on $\mathcal{U}$ follows from (5.11) and (5.12). Besides, using (5.13) and $\gamma \in \mathcal{U}$, we have

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

This ends the proof. ☐

Notice that $\mathcal{U}$ is an open subset of $\Gamma_{\leqslant q}$. Then Proposition 5.4 follows from Proposition 5.8 and [29, Proposition 2.1 and Proposition 2.2] by choosing $U = \mathcal{U}$, $\Gamma = \Gamma_{\leqslant q}$ and $\mathcal{X} := \overline{\operatorname{span}\{\gamma - \gamma' \mid \gamma, \gamma' \in \Gamma_{\leqslant q}\}} = X \cap Y$. Here the notations $\mathcal{X}$, U and Γ are 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 $I_{\leqslant q,R}$ (i.e., Proposition 3.4).

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

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

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 $\widetilde{\gamma}_{n,\xi}$, is at most $q + M$. We prove in Lemma 6.1 that, for each $n \geqslant 1$, $\widetilde{\gamma}_n \in X_\infty^2$ 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 $(\widetilde{\gamma}_n)_{n\geqslant 1}$ is an approximate minimizing sequence with higher regularity than $(\gamma_n)_{n\geqslant 1}$.

The structure of the proof of Proposition 3.4 is as follows. In Subsection 6.1, we will show $\|\gamma_n - \widetilde{\gamma}_n\|_X \to 0$ when n goes to infinity. In Subsection 6.2, we study the convergence of the kernel of $(W_{\widetilde{\gamma}_n,\xi})_{n\geqslant 1}$. Then thanks to the constraint $\gamma_n \in B_R$, we deduce the strong convergence of $(V_{\gamma_n,\xi})_{n\geqslant 1}$. As a result, $\|P_{\gamma_*}^+ - P_{\gamma_n}^+\|_Y \to 0$. 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 $\widetilde{\gamma}_n$.

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

Proof. We first prove that $\|p_n\|_{X^2_\infty}$ is bounded. Let $(u_{n,k}(\xi))_{k\geqslant 1}$ 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 $0 \leqslant \lambda_{n,k}(\xi) \leqslant e$ and $\delta_{n,k} = 0$ otherwise.

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

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

Hence,

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

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

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

In terms of kernels, it writes

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

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

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

$\square$

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 $(\gamma_n)_{n\geqslant 1}$ of (3.4) in $\Gamma^+_{\leqslant q} \cap B_R$ we have*

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

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

$$\inf_{\gamma \in \Gamma_{\leqslant q},\, \gamma = P^+_{\gamma_n} \gamma P^+_{\gamma_n}} \fint_{Q^*_\ell} \mathrm{Tr}_{L^2_\xi}\big[(D_{\gamma_n,\xi} - \epsilon_P)\gamma_\xi\big]\, d\xi$$

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

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

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

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

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,

$$\fint_{Q_\ell^*} \mathrm{Tr}_{L^2_\xi}(\gamma_{n,\xi})\, d\xi \to q \text{ and } \fint_{Q_\ell^*} \mathrm{Tr}_{L^2_\xi}[(D_{\gamma_n,\xi}-\nu_n)\pi_{n,\xi}\gamma_{n,\xi}\pi_{n,\xi}]\, d\xi \to 0.$$

But $\pi_{n,\xi}(D_{\gamma_n,\xi}-\nu_n)\pi_{n,\xi} \geqslant (e-\nu_n)\pi_{n,\xi}$ 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

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

Hence

$$\|\pi_n\gamma_n\pi_n\|_X = \fint_{Q_\ell^*} \mathrm{Tr}_{L^2_\xi}[\pi_{n,\xi}|D_\xi|\pi_{n,\xi}\gamma_{n,\xi}]\, d\xi \leqslant (1-\kappa)^{-1}\fint_{Q_\ell^*} \mathrm{Tr}_{L^2_\xi}[\pi_{n,\xi}|D_{\gamma_n,\xi}|\pi_{n,\xi}\gamma_{n,\xi}]\, d\xi \to 0.$$

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

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

Hence

$$\fint_{Q_\ell^*} \mathrm{Tr}_{L^2_\xi}(|D_{\gamma_n,\xi}|^{1/2}h_{n,\xi}h_{n,\xi}^*|D_{\gamma_n,\xi}|^{1/2})\, d\xi \to 0.$$

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

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

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 $\big\|p_n|D_{\gamma_n}|^{1/2}\big\|_Y \leqslant e^{1/2}$. As a consequence,

$$\|\mathrm{Tr}_{L^2_\xi}(|D_{\gamma_n,\xi}|^{1/2}p_{n,\xi}A_\xi^*A_\xi p_{n,\xi}|D_{\gamma_n,\xi}|^{1/2})\|_{L^\infty} \leqslant (q+M)e\|A\|_Y^2.$$

So we have

$$\Big\||D_{\gamma_n}|^{1/2}h_n|D_{\gamma_n}|^{1/2}\Big\|_{\mathfrak{S}_{1,1}} \to 0.$$

Hence, $\|u_n\|_X \to 0$. Finally, $\|\gamma_n - \widetilde{\gamma}_n\|_X \leqslant \|\pi_n\gamma_n\pi_n\|_X + 2\|h_n\|_X \to 0$. ☐

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

$$\widetilde{\gamma}_n \overset{*}{\rightharpoonup} \gamma_* \quad \text{for the weak } *\text{-convergence in } X_\infty^2 \cap Y, \tag{6.3}$$

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 $\rho_{\widetilde{\gamma}_n}^{1/2}$ converges strongly to $\rho_{\gamma_*}^{1/2}$ in $H^s(Q_\ell)$ with $0 \leqslant s < 1$, thus in $L^p(Q_\ell)$ for every $1 \leqslant p < 6$. 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 $\widetilde{\gamma}_n \in X_\infty^2$. The fact that the limit of $\rho_{\widetilde{\gamma}_n}^{1/2}$ is exactly $\rho_{\gamma_*}^{1/2}$ follows from [5, Eqn. (4.51) and Eqn. (4.55)] since it implies $\rho_{\widetilde{\gamma}_n} \to \rho_{\gamma_*}$ in $L^1(Q_\ell)$. ☐

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

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

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

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

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

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

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

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

$$\langle f, g\rangle = \fint_{Q^*_\ell} \iint_{Q_\ell\times Q_\ell} \mathrm{Tr}_4[f^*g]\,dx\,dy\,d\xi. \tag{6.4}$$

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

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

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

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

$$W_{\geqslant m,\gamma,\xi}(x,y) := \fint_{Q^*_\ell} W^\infty_{\geqslant m,\ell}(\xi'-\xi, x-y)\,\gamma_{\xi'}(x,y)\,d\xi'$$

and

$$W_{<m,\gamma,\xi}(x,y) := \fint_{Q^*_\ell} W^\infty_{<m,\ell}(\xi'-\xi, x-y)\,\gamma_{\xi'}(x,y)d\xi'.$$

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

(a) $W_{<m,\widetilde{\gamma}_n,\xi} \to W_{<m,\gamma_*,\xi}$ *in* $L^\infty(Q^*_\ell; L^2_\xi(Q_\ell\times Q_\ell))$.

(b) $|D_{\xi,x}|^{-1/2}|D_{\xi,y}|^{-1/2}W_{\geqslant m,\widetilde{\gamma}_n,\xi} \to |D_{\xi,x}|^{-1/2}|D_{\xi,y}|^{-1/2}W_{\geqslant m,\gamma_*,\xi}$ *in* $L^\infty(Q^*_\ell; L^2_\xi(Q_\ell\times Q_\ell))$.

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

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

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

Thus,

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

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

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

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

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

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

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

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

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

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

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

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

$$
\|\nabla_\xi^\beta W_{\geqslant m,\widetilde{\gamma}_n,\xi}\|_{L^\infty(Q_\ell^*;L^2(Q_\ell^*\times Q_\ell^*))} \leqslant \fint_{Q_\ell^*} \|\nabla_\xi^\beta W_{\geqslant m,\ell}(\xi-\xi')\widetilde{\gamma}_{n,\xi'}\|_{L^\infty(Q_\ell^*;L^2_\xi(Q_\ell^*\times Q_\ell^*))} d\xi'.
$$

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

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

and

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

Thus,

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

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 $W_{\geqslant m,\gamma_*,\xi}$ respectively.

It suffices to prove that

$$
W_{<m,\widetilde{\gamma}_n,\xi} \overset{*}{\rightharpoonup} W_{<m,\gamma_*,\xi} \quad \text{and} \quad W_{\geqslant m,\widetilde{\gamma}_n,\xi} \overset{*}{\rightharpoonup} W_{\geqslant m,\gamma_*,\xi} \tag{6.5}
$$

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

By Young's convolution inequality,

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

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

$$\begin{aligned}\langle g_\xi, W_{<m,\widetilde{\gamma}_n,\xi}\rangle &= \fint_{Q_\ell^*} \mathrm{Tr}_{L^2_\xi}[g_\xi^* W_{<m,\widetilde{\gamma}_n,\xi}]\, d\xi = \fint_{Q_\ell^*} \mathrm{Tr}_{L^2_{\xi'}}[W^*_{<m,g,\xi'}\widetilde{\gamma}_{n,\xi'}]\, d\xi' \\ &\to \fint_{Q_\ell^*} \mathrm{Tr}_{L^2_{\xi'}}[W^*_{<m,g,\xi'}\gamma_{*,\xi'}] d\xi' = \langle g_\xi, W_{<m,\gamma_*,\xi}\rangle .\end{aligned}$$

By Corollary B.2,

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

Hence,

$$\begin{aligned}\langle g_\xi, W_{\geqslant m,\widetilde{\gamma}_n,\xi}\rangle &= \langle W_{\geqslant m,g,\xi'}, \widetilde{\gamma}_{n,\xi'}\rangle \\ &= \fint_{Q_\ell^*} \mathrm{Tr}_{L^2_\xi}[|D_{\xi'}|^{-1}W^*_{\geqslant m,g,\xi'}|D_{\xi'}|^{-1}|D_{\xi'}|\widetilde{\gamma}_{n,\xi'}|D_{\xi'}|]\, d\xi' \\ &\to \fint_{Q_\ell^*} \mathrm{Tr}_{L^2_\xi}[W^*_{\geqslant m,g,\xi'}\gamma_{*,\xi'}] d\xi' = \langle g_\xi, W_{\geqslant m,\gamma_*,\xi}\rangle .\end{aligned}$$

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

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

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

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

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

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

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

By (4.4), we get

$$\|G_\ell * (\rho_{\gamma_n} - \rho_{\widetilde{\gamma}_n})\|_Y \leqslant C_H\|\gamma_n - \widetilde{\gamma}_n\|_X \to 0.$$

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

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

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

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

Similarly, we split the second term into two parts :

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

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

$$\|W_{\gamma_n} - W_{\widetilde{\gamma}_n}\|_Y \to 0. \tag{6.8}$$

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 $W^{\infty}_{\geqslant m,\ell}$,

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

For the other term, analogously we have

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

Gathering these estimates with Lemma 6.4 we infer

$$\| |D^0|^{-1/2} W_{\widetilde{\gamma}_n-\gamma_*} |D^0|^{-1/2} \|_Y \to 0. \tag{6.9}$$

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

As a result, we have the following.

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

$$\|P^+_{\gamma_*} - P^+_{\gamma_n}\|_Y \to 0.$$

Proof. By (5.7) and the second resolvent identity, we obtain

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

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

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

The existence of minimizers of $I_{\leqslant q,R}$ 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 $\Gamma^+_{\leqslant q} \cap B_R$.*

Proof. As

$$\widetilde{\gamma}_n \overset{*}{\rightharpoonup} \gamma_* \quad \text{in} \quad X^2_\infty \cap Y,$$

we get

$$\|\gamma_*\|_{\mathfrak{S}_{1,\infty}} \leqslant \liminf_{n\to\infty} \|\widetilde{\gamma}_n\|_{\mathfrak{S}_{1,\infty}} \leqslant R, \quad \|\gamma_*\|_Y \leqslant \liminf_{n\to\infty} \|\widetilde{\gamma}_n\|_Y \leqslant 1$$

and

$$\|\gamma_*\|_{X^2_\infty} \leqslant \liminf_{n\to\infty} \|\widetilde{\gamma}_n\|_{X^2_\infty} \leqslant (q+M)(1-\kappa)^{-2}e^2.$$

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

$$\fint_{Q_\ell^*} \mathrm{Tr}_{L^2_\xi} \gamma_{n,\xi} d\xi \to \fint_{Q_\ell^*} \mathrm{Tr}_{L^2_\xi} \gamma_{*,\xi}\, d\xi \leqslant q.$$

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

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

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

Notice that

$$\begin{aligned} \left|\int_{Q_\ell^*} \mathrm{Tr}_{L^2_\xi}[(P^+_{\gamma_*,\xi}\gamma_{*,\xi} - \gamma_{*,\xi})g_\xi]\, d\xi\right| &\leqslant \left|\int_{Q_\ell^*} \mathrm{Tr}_{L^2_\xi}[(P^+_{\gamma_*,\xi} - P^+_{\gamma_n,\xi})\widetilde{\gamma}_{n,\xi} g_\xi]\, d\xi\right| \\ &+ \left|\int_{Q_\ell^*} \mathrm{Tr}_{L^2_\xi}[P^+_{\gamma_*,\xi}(\gamma_{*,\xi} - \widetilde{\gamma}_{n,\xi})g_\xi]\, d\xi\right| + \left|\int_{Q_\ell^*} \mathrm{Tr}_{L^2_\xi}[(\widetilde{\gamma}_{n,\xi} - \gamma_{*,\xi})g_\xi]\, d\xi\right|. \end{aligned} \tag{6.10}$$

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

$$\int_{Q_\ell^*} \mathrm{Tr}_{L^2_\xi}[P^+_{\gamma_*,\xi}(\gamma_{*,\xi} - \widetilde{\gamma}_{n,\xi})g_\xi]\, d\xi \to 0 \quad \text{and} \quad \int_{Q_\ell^*} \mathrm{Tr}_{L^2_\xi}[(\widetilde{\gamma}_{n,\xi} - \gamma_{*,\xi})g_\xi]\, d\xi \to 0.$$

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

$$\left|\int_{Q_\ell^*} \mathrm{Tr}_{L^2_\xi}[(P^+_{\gamma_*,\xi} - P^+_{\gamma_n,\xi})\widetilde{\gamma}_{n,\xi} g_\xi]\, d\xi\right| \leqslant \|P^+_{\gamma_*} - P^+_{\gamma_n}\|_Y \|\widetilde{\gamma}_n\|_{\mathfrak{S}_{1,1}} \|g\|_Y \to 0.$$

Consequently, letting n go to infinity,

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

Hence $\gamma_* \in \Gamma^+_{\leqslant q}$. This ends the proof. ☐

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

Proof. For the kinetic energy term, we have

$$\int_{Q_\ell^*} \mathrm{Tr}_{L^2_\xi}[D_\xi(\gamma_{n,\xi} - \gamma_{*,\xi})]\, d\xi = \int_{Q_\ell^*} \mathrm{Tr}_{L^2_\xi}[D_\xi(\gamma_{n,\xi} - \widetilde{\gamma}_{n,\xi})]\, d\xi + \int_{Q_\ell^*} \mathrm{Tr}_{L^2_\xi}[D_\xi(\widetilde{\gamma}_{n,\xi} - \gamma_{*,\xi})]\, d\xi.$$

By (6.3), we know that

$$\int_{Q_\ell^*} \mathrm{Tr}_{L^2_\xi}[D_\xi(\widetilde{\gamma}_{n,\xi} - \gamma_{*,\xi})]\, d\xi = \int_{Q_\ell^*} \mathrm{Tr}_{L^2_\xi}[|D_\xi|(\widetilde{\gamma}_{n,\xi} - \gamma_{*,\xi})|D_\xi||D_\xi|^{-1}D_\xi|D_\xi|^{-1}]\, d\xi \to 0,$$

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

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

The proof for the attractive potential is similar:

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

and

$$\left|\int_{Q_\ell^*} \mathrm{Tr}_{L^2_\xi}(G_\ell(\gamma_{n,\xi} - \widetilde{\gamma}_{n,\xi}))\, d\xi\right| \leqslant C_H \|\gamma_n - \widetilde{\gamma}\|_X \to 0.$$

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

$$\int_{Q_\ell^*} \mathrm{Tr}_{L^2_\xi}[G_\ell(\widetilde{\gamma}_{n,\xi} - \gamma_{*,\xi})]d\xi = \int_{Q_\ell^*} \mathrm{Tr}_{L^2_\xi}[|D_\xi|(\widetilde{\gamma}_{n,\xi} - \gamma_{*,\xi})|D_\xi||D_\xi|^{-1}G_\ell|D_\xi|^{-1}]\, d\xi \to 0.$$

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

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

The lemma follows. $\square$

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

$$\int_{Q_\ell^*} \mathrm{Tr}_{L^2_\xi}\big[(D_{\gamma_*,\xi} - \epsilon_P)\gamma_{*,\xi}\big]\, d\xi = \inf_{\substack{\gamma\in\Gamma_{\leqslant q}\\ \gamma = P^+_{\gamma_*}\gamma}} \int_{Q_\ell^*} \mathrm{Tr}_{L^2_\xi}\big[(D_{\gamma_*,\xi} - \epsilon_P)\gamma_\xi\big]\, d\xi.$$

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

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*

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

This implies

$$G_\ell(x) \geqslant -\frac{C_0}{\ell}. \tag{A.1}$$

In particular, we have

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

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 $(\cup_{z\in Q_1}B(z,R)) \cap (\mathbb{Z}^3\setminus\{0\}) = \varnothing$. Obviously, we can assume $0 < R < 1/2$. By the divergence theorem, for $0 \leqslant r \leqslant R$ and $z \in Q_1$ we obtain

$$\frac{d}{dr}\left(\frac{1}{4\pi r^2}\int_{\partial B(z,r)} f(s)\, ds\right) = \frac{1}{4\pi}\frac{d}{dr}\int_{\mathbb{S}^2} f(z + r\omega)d\omega$$

$$= \frac{1}{4\pi r^2}\int_{\partial B(z,r)} \frac{\partial f(s)}{\partial n}\,ds = \frac{1}{4\pi r^2}\int_{B(z,r)} \Delta_x f(x)\,dx \tag{A.2}$$

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

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

where the first equation holds since

$$(\cup_{z\in Q_1} B(z,r)) \cap \{k \in \mathbb{Z}^3 | k \neq 0\} = \varnothing, \quad \text{for } 0 \leqslant r \leqslant R.$$

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

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

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

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

On the other hand,

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

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

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

Thus,

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

Furthermore,

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

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

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

□

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*

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

Proof. We start with the relationship:

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

Thus,

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

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

$$A^{2,3}(x_1) = \int_{(-\frac{\ell}{2},\frac{\ell}{2}]^2} |u|^2(x_1,x_2,x_3)dx_2dx_3.$$

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

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

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

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

Then we have

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

As

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

we get

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

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

$$0 \leqslant \|\nabla u\|^2_{L^2(Q_\ell)} - \frac{1}{4}\left\|\frac{u}{|x|}\right\|^2_{L^2(Q_\ell)} + \frac{12}{\ell^2}\|u\|^2_{L^2(Q_\ell)} + \frac{12}{\ell}\|u\|_{L^2(Q_\ell)}\|\nabla u\|_{L^2(Q_\ell)}.$$

As a result, by the Cauchy-Schwarz inequality

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

□

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

$$C_G := 2\sqrt{1+\frac{C_0}{\ell}}\max\left\{\sqrt{1+\frac{6}{\ell}}, \sqrt{\frac{24+C_0}{4\ell}+\frac{12}{\ell^2}}\right\}. \tag{A.4}$$

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

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

$$\sup_{\substack{\eta\in 2Q_\ell^*\\ x\in Q_\ell}} \left| W_{\geqslant m,\ell}(\eta,x) - G_\ell(x)\right| \leqslant \frac{C_{\geqslant m}}{\ell} \tag{B.1}$$

with

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

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 $f(\eta,x) = W_{\geqslant m,1}(\eta,x) - G_1(x)$. 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 $(\cup_{z\in Q_1} B(z,R)) \cap \{k\in\mathbb{Z}^3 | k\neq 0\} = \varnothing$. Obviously, we can assume $0<R<1/2$. Analogous to (A.2), for $0\leqslant r\leqslant R$ and $z\in Q_1$ we obtain

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

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

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

where the first equality holds since

$$(\cup_{z\in Q_1} B(z,r)) \cap \{k\in\mathbb{Z}^3|k\neq 0\} = \varnothing, \quad \text{for } 0\leqslant r\leqslant R.$$

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

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

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

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

On the other hand,

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

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

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

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

$$\begin{aligned}
C_{\geqslant m} &\leqslant \frac{\sqrt{3}}{2(\pi R)^{3/2}}\frac{m^2+2}{(m-1)^2}\left(\sum_{|k|_\infty\geqslant m}\frac{1}{|k|^4}\right)^{1/2} + \frac{2\pi[(2m-1)^3+1]R^2}{5} \\
&\quad + \frac{3}{4\pi^2 R^3}\min\left\{\left(\frac{4\pi R^3}{3}\right)^{1/2}, \left(1-\frac{4\pi R^3}{3}\right)^{1/2}\right\}\left(\sum_{k\in\mathbb{Z}^3\setminus\{0\}}\frac{1}{|k|^4}\right)^{1/2},
\end{aligned}$$

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

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

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

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

and

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

We also have the following estimate on W_ℓ^∞.

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

$$\sup_{\eta\in 2Q_\ell^*}\|\nabla_\eta W_{\geqslant m,\ell}(\eta,\cdot)\|_{L^\infty(Q_\ell)} \leqslant C. \tag{B.5}$$

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

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

from which we obtain

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

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

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

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

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

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

$$W_\ell^\infty\Big(\xi - \xi', x - y\Big) = W_{\geqslant m,\ell}\Big(\xi - \xi', x - y\Big) + W_{<m,\ell}\Big(\xi - \xi', x - y\Big). \tag{B.7}$$

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

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

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

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

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

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

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

$$\begin{aligned}
&\left|\fint_{Q_\ell^*} d\xi' \iint_{Q_\ell\times Q_\ell} W_{\geqslant m,\ell}\Big(\xi-\xi', x-y\Big)\phi_\xi^*(x)\gamma_{\xi'}(x,y)\psi_\xi(y)dxdy\right| \\
&\quad\leqslant \fint_{Q_\ell^*}\left(\iint_{Q_\ell\times Q_\ell}\rho_{\gamma_{\xi'}}(y)\,|\phi_\xi^*(x)|^2\,dxdy\right)^{1/2}\left(\iint_{Q_\ell\times Q_\ell}\rho_{\gamma_{\xi'}}(x)\left|W_{\geqslant m,\ell}(\xi-\xi',x-y)\right|^2|\psi_\xi(y)|^2\,dxdy\right)^{1/2} d\xi'
\end{aligned}$$

$$\leqslant \left(C_G + \frac{C_{\geqslant m}}{\ell}\right) \|\gamma\|_{\mathfrak{S}_{1,1}} \||D_\xi|\psi_\xi\|_{L^2_\xi} \|\phi_\xi\|_{L^2_\xi}. \tag{B.10}$$

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 $\xi \mapsto \mathrm{Tr}_{L^2_\xi}(\gamma_\xi)$ is Q_ℓ^*-periodic. Next, we write

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

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

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

since $(Q_\ell^* + 2\pi k/\ell) \cap (Q_\ell^* + 2\pi k'/\ell) = \varnothing$ 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 $C'_{\leqslant m,\ell}$, we obtain

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

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

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

$$= C_{\leqslant m,\ell}\,\|\gamma\|_Y\,\|\psi_\xi\|_{L^2_\xi}\,\|\phi_\xi\|_{L^2_\xi} \tag{B.13}$$

with

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

Since $\|\gamma\|_{\mathfrak{S}_{1,1}}\leqslant\|\gamma\|_X$ and $|D^0|^{-1/2}\leqslant 1$, 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,

$$C_W = C_H + C_\ell,\quad C_W' = C_G + C_\ell,\quad C_W'' = C_H + C_\ell', \tag{B.15}$$

with

$$C_\ell := \inf_{\substack{m\in\mathbb{N}\\ m\geqslant 2}}\left(\frac{C_{\geqslant m}}{\ell} + C_{\leqslant m,\ell}\right),\quad C_\ell' := \inf_{\substack{m\in\mathbb{N}\\ m\geqslant 2}}\left(\frac{C_{\geqslant m}}{\ell} + C_{\leqslant m,\ell}'\right). \tag{B.16}$$

C Proof of Lemma 4.7

Analogous to (B.6), we have

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

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

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

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

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

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

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

Thus according to the Cauchy-Schwarz inequality, we have

$$\sum_{1\leqslant\alpha,\beta\leqslant 4}\left|\iint_{Q_\ell\times Q_\ell} G_\ell(x-y)\left(u_n^\alpha(\xi',y)\phi_\xi^\beta(x)-\phi_\xi^\alpha(y)u_n^\beta(\xi',x)\right)^*\left(u_n^\alpha(\xi',y)\psi_\xi^\beta(x)-\psi_\xi^\alpha(y)u_n^\beta(\xi',x)\right)dxdy\right|$$
$$\leqslant 2\left(\sum_{1\leqslant\alpha,\beta\leqslant 4}\iint_{Q_\ell\times Q_\ell}|G_\ell(x-y)|^2|u_n(\xi',y)|^2|\psi_\xi(x)|^2dxdy\right)^{1/2}\left(\iint_{Q_\ell\times Q_\ell}|u_n^*(\xi',y)|^2|\phi_\xi^*(x)|^2dxdy\right)^{1/2}$$
$$\leqslant 2C_G\|\phi_\xi\|_{L^2_\xi}\||D_\xi|\psi_\xi\|_{L^2_\xi}.$$

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

$$\left|\iint_{Q_\ell\times Q_\ell} G_\ell(x-y)\left(\rho_{\gamma_{\xi'}}(y)\phi_\xi^*(x)\psi_\xi(x)-\phi_\xi^*(x)\gamma_{\xi'}(x,y)\psi_\xi(y)\right)dxdy\right|$$
$$\leqslant C_G\sum_{n\geqslant 1}|\lambda_n(\xi')|\|\phi_\xi\|_{L^2_\xi}\||D_\xi|\psi_\xi\|_{L^2_\xi}=C_G\|\gamma_{\xi'}\|_{\mathfrak{S}_1(\xi')}\|\phi_\xi\|_{L^2_\xi}\||D_\xi|\psi_\xi\|_{L^2_\xi},$$

from which we get

$$\left|\iint_{Q_\ell\times Q_\ell} G_\ell(x-y)\rho_\gamma(y)\phi_\xi^*(x)\psi_\xi(x)\,dxdy-\fint_{Q_\ell^*}d\xi'\iint_{Q_\ell\times Q_\ell} G_\ell(x-y)\phi_\xi^*(x)\gamma_{\xi'}(x,y)\psi_\xi(y)\,dxdy\right|$$
$$\leqslant C_G\|\gamma\|_{\mathfrak{S}_{1,1}}\|\phi_\xi\|_{L^2_\xi}\||D_\xi|\psi_\xi\|_{L^2_\xi}. \tag{C.4}$$

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

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

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

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

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

$$\left|\iint_{Q_\ell\times Q_\ell} G_\ell(x-y)\rho_\gamma(y)\phi_\xi^*(x)\psi_\xi(x)dxdy-\fint_{Q_\ell^*}d\xi'\iint_{Q_\ell\times Q_\ell} G_\ell(x-y)\phi_\xi^*(x)\gamma_{\xi'}(x,y)\psi_\xi(y)\,dxdy\right|$$
$$\leqslant\left(\fint_{Q_{\xi'}}d\xi'\sum_{n\geqslant 1}|\lambda_n(\xi')|\iint_{Q_\ell\times Q_\ell}|G_\ell(x-y)||u_n(\xi',y)|^2|\psi_\xi(x)|^2dxdy\right)^{1/2}$$
$$\times\left(\fint_{Q_{\xi'}}d\xi'\sum_{n\geqslant 1}|\lambda_n(\xi')|\iint_{Q_\ell\times Q_\ell}|G_\ell(x-y)||u_n(\xi',y)|^2|\phi_\xi^*(x)|^2dxdy\right)^{1/2}$$
$$\leqslant C_H\|\gamma\|_X\|\phi_\xi\|_{L^2_\xi}\|\psi_\xi\|_{L^2_\xi} \tag{C.6}$$

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 $\phi_\xi\in L^2_\xi$ and $\psi_\xi\in H^1_\xi$,

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

hence (4.12) and

$$C_{EE} := C_H + C_\ell. \tag{C.7}$$

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

$$\begin{aligned}
&\left| \iint_{Q_\ell \times Q_\ell} G_\ell(x-y)\rho_\gamma(y)\psi_\xi^*(x)\psi_\xi(x)dxdy - \fint_{Q_\ell^*} d\xi' \iint_{Q_\ell\times Q_\ell} G_\ell(x-y)\psi_\xi^*(x)\gamma_{\xi'}(x,y)\psi_\xi(y)\,dxdy \right| \\
&\quad \leqslant \left(\fint_{Q_{\xi'}} d\xi' \sum_{n\geqslant 1} |\lambda_n(\xi')| \iint_{Q_\ell\times Q_\ell} |G_\ell(x-y)||u_n(\xi',y)|^2|\psi_\xi(x)|^2 dxdy \right) \\
&\quad \leqslant C_H \|\gamma\|_{\mathfrak{S}_{1,1}} \||D_\xi|^{1/2}\psi_\xi\|^2_{L^2_\xi}
\end{aligned}$$

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

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

$$\begin{aligned}
&\fint_{Q_\ell^*} d\xi' \iint_{Q_\ell\times Q_\ell} G_\ell(x-y)\psi_\xi^*(x)\gamma_{\xi'}(x,y)\psi_\xi(y)\,dxdy - \iint_{Q_\ell\times Q_\ell} G_\ell(x-y)\rho_\gamma(x)|\psi_\xi(y)|^2\,dxdy \\
&\quad \leqslant \iint_{Q_\ell\times Q_\ell} (|G_\ell(x-y)| - G_\ell(x-y))\rho_\gamma(y)|\psi_\xi(x)|^2\,dxdy \leqslant \frac{2C_0}{\ell}\|\gamma\|_{\mathfrak{S}_{1,1}}\|\psi\|^2_{L^2_\xi}.
\end{aligned}$$

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

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

hence (4.13) and

$$C''_{EE} = \frac{2C_0}{\ell} + C_\ell. \tag{C.8}$$

D Numerical results about constants

In this section, we will show the numerical results about the constants used in Remark 2.7 under the condition $\ell = 1000$. Next, we show that Assumption 2.6 is satisfied for $q \leqslant 17$ 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 $R \approx \frac{1}{2}$,

$$|C_{\geqslant 2}| \leqslant 20.912, \quad C_{\leqslant 2,1000} \approx 0.010.$$

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 (2.22). 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

$$V_q = \mathrm{Span}\{\Lambda^+ u_{p,\xi}(x) \,|\, p = (j,0,0), j \in \{1,\cdots,q\}\}.$$

Then

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

Now we can check Assumption 2.6 for $z = q = 17$. The calculation leads to $A_0 \approx 0.012$ and $c^*(17) \leqslant 1.006$. 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 $q \leqslant 17$ whenever $\ell = 1000$.

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