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Properties of periodic Dirac–Fock functional and minimizers

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Abstract

Existence of minimizers for the Dirac–Fock model for crystals was recently proved by Patrel and Séré and the authors [9]. In this paper, inspired by Ghimenti and Lewin’s result [12] for the periodic Hartree–Fock model, we prove that the Fermi level of any periodic Dirac–Fock minimizer is either empty or totally filled when $\frac{\alpha}{c} \leq C_{\text{cri}}$ and $\alpha > 0$. Here c is the speed of light, α is the fine structure constant, and C_{cri} is a constant only depending on the number of electrons and on the charge of nuclei per cell. More importantly, we provide an explicit upper bound for C_{cri} .

Our result implies that any minimizer of the periodic Dirac–Fock model is a projector when $\frac{\alpha}{c} \leq C_{\text{cri}}$ and $\alpha > 0$. In particular, the non-relativistic regime (i.e., $c \gg 1$) and the weak coupling regime (i.e., $0 < \alpha \ll 1$) are covered.

The proof is based on a delicate study of a second-order expansion of the periodic Dirac–Fock functional composed with a retraction that was introduced by Séré in [23] for atoms and molecules and later extended to the case of crystals in [9].

1 Introduction

The Hartree–Fock (HF) model is commonly used in non-relativistic chemistry and quantum physics to calculate ground- or bound state energies of atoms and molecules. In this model, the state of the electrons is represented by a so-called density matrix γ which is a self-adjoint trace-class operator $0 \leq \gamma \leq 1$ acting on the space $L^2(\mathbb{R}^3; \mathbb{C})$. Its finite trace represents the number N of electrons ($N \in \mathbb{N}^* := \mathbb{N} \setminus \{0\}$). When the nuclear charge $Z > N - 1$, existence of a ground state for the HF model expressed in terms of N -particle wave-functions goes back to Lieb and Simon [18]. This existence result has been extended later to excited states by Lions [19] (see also the recent review paper by Bach [2] and the references therein). Existence of minimizers for the HF functional involving one-particle density matrices is due to Lieb [16] (see also Bach [1]). Additionally, it is shown in [16] that any HF minimizer γ is automatically a projector of the form $\gamma = \sum_{n=1}^N |\psi_n\rangle \langle \psi_n|$ with the ψ_i ’s being the eigenfunctions corresponding to the smallest eigenvalues (counted with multiplicity) of the mean-field self-adjoint HF operator H_γ ,

$$H_\gamma \psi_n = \epsilon_n \psi_n,$$

with spectrum $\sigma(H_\gamma) = \{\epsilon_1 \leq \epsilon_2 \leq \dots \leq \epsilon_N \leq \dots\} \cup [0, +\infty)$ where $\epsilon_j < 0$ for any $j \in \mathbb{N}^*$. Furthermore, Bach, Lieb, Loss, and Solovej proved that shells are always completely filled in the HF model [3]. Mathematically, this property writes $\epsilon_N < \epsilon_{N+1}$. In particular, any minimizer of the HF functional solves the following self-consistent equation

$$\gamma = \mathbb{1}_{(-\infty, \epsilon_N]}(H_\gamma),$$

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where $\mathbb{1}_I(H)$ denotes the spectral projection of the self-adjoint operator H on the set $I \subset \mathbb{R}$. Efficient numerical methods in the HF theory rely on these properties (see e.g., [7]).

This result has been later extended by Ghimenti and Lewin in [12] to the periodic HF model for neutral crystals introduced and studied by Catto, Le Bris and Lions in [8]. They proved that any minimizer γ of the periodic HF energy is always a projector (of infinite rank), that solves the self-consistent equation

$$\gamma = \mathbb{1}_{(-\infty, \nu)}(H_\gamma) + \epsilon \mathbb{1}_{\{\nu\}}(H_\gamma) \quad (1.1)$$

with $\epsilon \in \{0, 1\}$, and $\nu \in \mathbb{R}$ may be an eigenvalue of the periodic mean-field HF operator H_γ (with infinite multiplicity due to the invariance by translations of the lattice). In [6], a similar result was proved by Cancès, Deleurence, and Lewin for the reduced HF model for crystals where the exchange term is neglected. Relying on [24], they show that the spectrum of the corresponding self-adjoint operator is purely absolutely continuous. Hence ν cannot be an eigenvalue and one can take $\epsilon = 0$ in (1.1). In particular, there are no unfilled shells in the reduced HF theory either. Unfortunately, we do not know whether the spectrum of the periodic HF operator is also purely absolutely continuous because of the non-local feature of the exchange term. Therefore, the proof of Ghimenti and Marco rely on different arguments based on a careful analysis of the exchange term.

When heavy nuclei are involved (that is, Z is large), it is expected that the electrons closest to the nucleus move at very high velocities, thus requiring a relativistic treatment. It is widely believed that Quantum Electrodynamics (QED) is an adequate framework to deal with relativistic effects. It is shown that the shells are always completely filled for the Bogoliubov–Dirac–Fock model in QED [13]. The proof relies on the fact that the corresponding functional is bounded from below and on the positive definiteness of the nonlinear term. However, this theory leads to divergence problems: it is not easy to give meaning to different physical quantities appearing in QED, such as the energy and the charge density of the vacuum.

Alternatively, the Dirac–Fock model (DF) for atoms and molecules is one of the most attractive models in relativistic computational chemistry. It is a variant of the HF model in which the Laplace operator $-\frac{1}{2}\Delta$ entering the kinetic energy term is replaced by the free Dirac operator \mathcal{D}^c where the superscript c stands for the speed of light. Unlike the QED models, the DF functional is not bounded from below. It is therefore difficult to give a rigorous definition of the ground state energy. However, results on existence of critical points – that is, solutions to the DF equations – can be found in [10, 21]. These solutions provide an infinite number of finite rank projectors as critical points of the DF functional. It is also proved in [11] that, up to subsequences, the projector with the smallest energy among these critical points converges to a minimizer of the Hartree–Fock energy in the non-relativistic limit; that is, when the speed of light goes to infinity.

Recently, in the spirit of Lieb’s variational principle (see, e.g., [1, 16]), Séré redefined the DF ground state energy for atoms and molecules by using the density matrix formalism [23]. Using a retraction technique, he proved that the DF ground state energy admits a minimizer γ on a suitable subset of density matrix, and that γ satisfies the self-consistent equation

$$\gamma = \mathbb{1}_{(0, \nu)}(\mathcal{D}_\gamma^c) + \delta, \quad \text{with } 0 \leq \delta \leq \mathbb{1}_{\{\nu\}}(\mathcal{D}_\gamma^c),$$

for some Lagrange multiplier ν associated with the charge constraint. Later on, by using Séré’s retraction technique, Meng [20] mathematically justifies Mittleman’s approach to the DF model: the DF model is an approximation of a max-min problem coming from the electron-positron field (see, e.g., [4, 5, 14]). As a byproduct, he shows that the shells in the DF theory of atoms and molecules are completely filled when the fine structure constant α is small enough or the speed of light c is large enough under some conditions on Z and N . This is an immediate consequence of a second-order expansion of a new DF functional, which is the composition of the DF functional with the retraction introduced by Séré in [23].

Finally, one can construct the periodic DF model for crystals by replacing the Schrödinger operator in the periodic HF model by the Dirac operator. Recently, together with Paturel and Séré, we have studied this new model in [9]. We have shown that the energy of the periodic DF model admits a minimizer that solves the self-consistent equation

$$\gamma = \mathbb{1}_{(0,\nu)}(\mathcal{D}_\gamma^c) + \delta, \quad \text{with } 0 \leq \delta \leq \mathbb{1}_{\{\nu\}}(\mathcal{D}_\gamma^c).$$

Here γ and \mathcal{D}_γ^c are a periodic density matrix and the periodic mean-field DF operator respectively. In the present paper, inspired by the results of one of us [20], we investigate the properties of the DF functional and minimizers in crystals. We mimic the proof of Ghimenti and Lewin for the periodic HF model [12] and obtain a similar result. More precisely, we show that when $\alpha > 0$ and $\frac{\alpha}{c} \leq C_{\text{cri}}$ (with C_{cri} given in Lemma 4.6), any minimizer γ of the periodic DF ground state energy is always a projector that solves a self-consistent equation of the form

$$\gamma = \mathbb{1}_{(0,\nu)}(\mathcal{D}_\gamma^c) + \epsilon \mathbb{1}_{\{\nu\}}(\mathcal{D}_\gamma^c)$$

with $\epsilon \in \{0, 1\}$. The proof of Ghimenti and Lewin is based on the local convexity of the periodic HF functional. Since this property does not hold any longer here, we rather rely on a careful study of the second-order expansion of the periodic DF functional due to one of us [20].

2 Description of the periodic DF model and main results

The paragraph below is copied from [9] for the reader's convenience. 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 center 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 $z \in \mathbb{R}^+$ 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 modeled by a Q_ℓ -periodic function whose L^1 -norm over the elementary cell equals the “number of electrons” per cell $q \in \mathbb{R}^+ := (0, +\infty)$ (the electronic charge per cell is equal to $-q$).

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

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

where δ_x is the Dirac measure at $x \in \mathbb{R}^3$. By convention, we choose G_ℓ such that

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

With this convention, G_ℓ changes sign, but is bounded from below. With

$$C_0 := \ell \sup_{x \in Q_\ell} \left| G_\ell(x) - \frac{1}{|x|} \right|, \quad (2.3)$$

we have

$$G_\ell(x) \geq -\frac{C_0}{\ell}, \quad \forall x \in Q_\ell,$$

where C_0 is a positive constant that is independent of ℓ (see [9, Lemma A1, Appendix A]).

The Fourier series of G_ℓ writes

$$G_\ell(x) = \frac{1}{\pi\ell} \sum_{p \in \mathbb{Z}^3 \setminus \{0\}} \frac{e^{\frac{2i\pi}{\ell} p \cdot x}}{|p|^2}, \quad \text{for every } x \in \mathbb{R}^3. \quad (2.4)$$

The free Dirac operator is defined by

$$\mathcal{D}^c = -ic \sum_{r=1}^3 \alpha_r \partial_r + c^2 \beta, \quad (2.5)$$

with 4×4 complex matrices $\alpha_1, \alpha_2, \alpha_3$ and β , whose standard forms are $\beta = \begin{pmatrix} \mathbb{1}_2 & 0 \\ 0 & -\mathbb{1}_2 \end{pmatrix}$, $\alpha_r = \begin{pmatrix} 0 & \sigma_r \\ \sigma_r & 0 \end{pmatrix}$ where $\mathbb{1}_2$ is the 2×2 identity matrix and the σ_r 's, for $r \in \{1, 2, 3\}$, are the well-known 2×2 Pauli matrices $\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $\sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$ and $\sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$. Here $c > 0$ denotes the speed of light.

The operator \mathcal{D}^c acts on 4-spinors; that is, on functions from \mathbb{R}^3 to \mathbb{C}^4 . It is self-adjoint on $L^2(\mathbb{R}^3; \mathbb{C}^4)$, 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 $\sigma(\mathcal{D}^c) = (-\infty, -c^2] \cup [c^2, +\infty)$. Following the notation in [10, 21], we denote by Λ^+ and $\Lambda^- = \mathbb{1}_{L^2} - \Lambda^+$ the two orthogonal projectors on $L^2(\mathbb{R}^3; \mathbb{C}^4)$ corresponding to the positive and negative eigenspaces of \mathcal{D}^c , respectively; that is

$$\begin{cases} \mathcal{D}^c \Lambda^+ = \Lambda^+ \mathcal{D}^c = \Lambda^+ \sqrt{c^4 - c^2 \Delta} = \sqrt{c^4 - c^2 \Delta} \Lambda^+; \\ \mathcal{D}^c \Lambda^- = \Lambda^- \mathcal{D}^c = -\Lambda^- \sqrt{c^4 - c^2 \Delta} = -\sqrt{c^4 - c^2 \Delta} \Lambda^-. \end{cases}$$

According to the Floquet theory [22], the underlying Hilbert space $L^2(\mathbb{R}^3; \mathbb{C}^4)$ is unitarily equivalent to $L^2(Q_\ell^*) \otimes L^2(Q_\ell; \mathbb{C}^4)$, where $Q_\ell^* = [-\frac{\pi}{\ell}, \frac{\pi}{\ell}]^3$ is the reciprocal cell of the lattice, whose volume is $|Q_\ell^*| = (2\pi)^3/\ell^3$. (In the Physics literature Q_ℓ^* is known as the first Brillouin zone.) The Floquet unitary transform $\mathfrak{U} : L^2(\mathbb{R}^3; \mathbb{C}^4) \rightarrow L^2(Q_\ell^*) \otimes L^2(Q_\ell; \mathbb{C}^4)$ is given by

$$\mathfrak{U} : \phi \mapsto \int_{Q_\ell^*}^\oplus (\mathfrak{U}\phi)_\xi d\xi, \quad (2.6)$$

with the shorthand \int_Ω standing for $\frac{1}{|\Omega|} \int_\Omega$, and

$$(\mathfrak{U}\phi)_\xi := \sum_{k \in \mathbb{Z}^3} e^{-i\ell k \cdot \xi} \phi(\cdot + \ell k) \quad (2.7)$$

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 $(\mathfrak{U}\phi)_\xi$ belongs to the space

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

which will simply be denoted by L_ξ^2 in the sequel. We write $L^2(\mathbb{R}^3; \mathbb{C}^4) = \int_{Q_\ell^*}^\oplus L_\xi^2 d\xi \cong L^2(Q_\ell^*) \otimes L^2(Q_\ell; \mathbb{C}^4)$ to refer to this direct integral decomposition of L^2 w.r.t. the Floquet transform \mathfrak{U} . Functions ψ in L_ξ^2 are called Bloch waves or Q_ℓ -quasi-periodic functions with quasi-momentum $\xi \in Q_\ell^*$. They satisfy

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

In particular, when $\xi = 0$, ψ is Q_ℓ -periodic, and we denote

$$L_{\text{per}}^2(Q_\ell) := L_0^2(Q_\ell).$$

The free Dirac operator can be rewritten accordingly as

$$\mathcal{D}^c = \int_{Q_\ell^*}^{\oplus} \mathcal{D}_\xi^c d\xi, \quad (2.8)$$

where the \mathcal{D}_ξ^c 's are self-adjoint operators on $L_\xi^2(Q_\ell; \mathbb{C}^4)$ with domains $H_\xi^1(Q_\ell; \mathbb{C}^4)$ and form-domains $H_\xi^{1/2}(Q_\ell; \mathbb{C}^4)$ respectively. Note that

$$(\mathcal{D}_\xi^c)^2 = c^4 - c^2 \Delta_\xi,$$

where $-\Delta = \int_{Q_\ell^*}^{\oplus} -\Delta_\xi d\xi$.

For every $\xi \in Q_\ell^*$, the positive spectrum of \mathcal{D}_ξ^c is composed of a non-decreasing sequence of real eigenvalues $(d_{c,j}^+(\xi))_{j \geq 1}$ counted with multiplicity. Each function $\xi \mapsto d_{c,j}^+(\xi)$ is continuous and Q_ℓ^* -periodic, and one has $d_{c,j}^+(Q_\ell^*) = [d_{c,*}(j), d_c^*(j)]$ with

$$d_{c,*}(j) := \min_{\xi \in Q_\ell^*} d_{c,j}^+(\xi) \quad \text{and} \quad d_c^*(j) := \max_{\xi \in Q_\ell^*} d_{c,j}^+(\xi). \quad (2.9)$$

Note that

$$d_{c,*}(j) \geq c^2, \quad \lim_{j \rightarrow +\infty} d_c^*(j) = +\infty.$$

In the same manner, the negative spectrum of \mathcal{D}_ξ^c is composed of the non-increasing sequence of real eigenvalues $d_{c,j}^-(\xi) = -d_{c,j}^+(\xi)$. Finally, one has

$$\sigma(\mathcal{D}^c) = \bigcup_{\xi \in Q_\ell^*} \sigma(\mathcal{D}_\xi^c) = \bigcup_{j \geq 1} [-d_c^*(j), -d_{c,*}(j)] \cup [d_{c,*}(j), d_c^*(j)] = (-\infty, -c^2] \cup [c^2, +\infty). \quad (2.10)$$

2.1 Functional framework

As in [9], we now introduce various functional spaces for linear operators on $L^2(Q_\ell; \mathbb{C}^4)$ and for operators on $L^2(\mathbb{R}^3; \mathbb{C}^4)$ that commute with periodic translations. Let $\mathcal{B}(E)$ be the set of bounded operators on a Banach space E to itself. We use the shorthand $\mathcal{B}(L_\xi^2)$ for $\mathcal{B}(L_\xi^2(Q_\ell; \mathbb{C}^4))$. The space of bounded operators on $\int_{Q_\ell^*}^{\oplus} L_\xi^2 d\xi$ which commute with the translations of $\ell\mathbb{Z}^3$ is denoted by Y . It is isomorphic to $L^\infty(Q_\ell^*; \mathcal{B}(L_\xi^2))$, and, for every $h = \int_{Q_\ell^*} h_\xi d\xi \in Y$,

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

(see [22, Theorem XIII.83]). In this paper, we also use another norm on Y which is defined by

$$\|h\|_{\mathcal{Y}} = \sup_{\xi \in Q_\ell^*} \|h\|_{\mathcal{Y}(\xi)}, \quad (2.11)$$

with

$$\|h\|_{\mathcal{Y}(\xi)} = \sup_{\substack{k \in \mathbb{Z}^3 \\ |k|_\infty \leq 1}} \int_{Q_\ell^* + \frac{2\pi k}{\ell}} \frac{\|h_{\xi'}\|_{\mathcal{B}(L_{\xi'}^2)}}{|\xi - \xi'|^2} d\xi', \quad (2.12)$$

where $|k|_\infty := \max\{|k_1|; |k_2|; |k_3|\}$. This convolution-type norm plays a critical role in this paper (see for example the proof of Lemma 4.6). Let

$$C_Y := \sup_{\xi \in Q_\ell^*} \int_{Q_\ell^*} \frac{d\xi'}{|\xi - \xi'|^2} = \int_{Q_\ell^*} \frac{d\xi}{|\xi|^2}. \quad (2.13)$$

It is easy to see that for every $h \in Y$,

$$\|h\|_Y \leq C_Y \|h\|_Y, \quad (2.14)$$

since $|\xi|^{-2}$ lies in $L^1_{\text{loc}}(\mathbb{R}^3)$. In addition, we shall use the rescaled c -dependent norms $\|h\|_{Y_c} := c\|h\|_Y$ and $\|h\|_{Y_c} := c\|h\|_Y$.

For $s \in [1, \infty)$ and $\xi \in Q_\ell^*$, we now define

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

endowed with the norm

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

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

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

endowed with the usual norm of $L^\infty(Q_\ell^*; \mathfrak{S}_s(\xi))$ when $t = +\infty$ and with the following norm when $t < +\infty$:

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

We also define

$$X^\tau(\xi) := \left\{ h_\xi \in \mathcal{B}(L^2_\xi) \mid (1 - \Delta_\xi)^{\tau/4} h_\xi (1 - \Delta_\xi)^{\tau/4} \in \mathfrak{S}_1(\xi) \right\}$$

endowed with the norm

$$\|h_\xi\|_{X^\tau(\xi)} = \left\| (1 - \Delta_\xi)^{\tau/4} h_\xi (1 - \Delta_\xi)^{\tau/4} \right\|_{\mathfrak{S}_1(\xi)}$$

and

$$X_t^\tau := \left\{ h = \int_{Q_\ell^*}^\oplus h_\xi d\xi \mid h_\xi \in \mathfrak{S}_1(\xi) \text{ a.e. } \xi \in Q_\ell^*, (1 - \Delta)^{\tau/4} h (1 - \Delta)^{\tau/4} \in \mathfrak{S}_{1,t} \right\}$$

endowed with the norm

$$\|h\|_{X_t^\tau} = \left\| (1 - \Delta)^{\tau/4} h (1 - \Delta)^{\tau/4} \right\|_{\mathfrak{S}_{1,t}}.$$

The space $X := X_1^1$ plays an important role in the definition of periodic density matrices (see Definition 2.1 below). For convenience, we use the notation $X(\xi)$ for $X^1(\xi)$. On X , we will also use the norm (dependent on c)

$$\|\gamma\|_{X_c} := \left\| |\mathcal{D}^c|^{1/2} \gamma |\mathcal{D}^c|^{1/2} \right\|_{\mathfrak{S}_{1,1}}.$$

It is easy to see that

$$c\|\gamma\|_X \leq \|\gamma\|_{X_c} \leq c^2\|\gamma\|_X$$

since for $c \geq 1$,

$$c(1 - \Delta)^{1/2} \leq |\mathcal{D}^c| \leq c^2(1 - \Delta)^{1/2}. \quad (2.15)$$

The norm on the intersection of any two functional spaces A and B will be defined by

$$\|\gamma\|_{A \cap B} := \max\{\|\gamma\|_A; \|\gamma\|_B\}, \quad \forall \gamma \in A \cap B.$$

We are now in the position to set the DF model for crystals.

2.2 The periodic DF model

We start with the following.

Definition 2.1 (Periodic one-particle density matrices [9]). *We denote by Γ the set of Q_ℓ -periodic one-particle density matrices*

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

We are particularly interested in the following subsets

$$\Gamma_q := \left\{ \gamma \in \Gamma \mid \int_{Q_\ell^*} \text{Tr}_{L_\xi^2}(\gamma_\xi) d\xi = q \right\}$$

and

$$\Gamma_{\leq q} := \left\{ \gamma \in \Gamma \mid 0 \leq \int_{Q_\ell^*} \text{Tr}_{L_\xi^2}(\gamma_\xi) d\xi \leq q \right\},$$

for any $q \in [0, +\infty)$. When q is an integer, Γ_q (resp. $\Gamma_{\leq q}$) is the set of all periodic DF states of a system of exactly q (resp. at most q) electrons per unit cell. The density of $\gamma \in \mathfrak{S}_{1,1}$ is defined as follows

$$\rho_{\gamma_\xi}(x) := \text{Tr}_4[\gamma_\xi(x, x)] \quad \text{and} \quad \rho_\gamma(x) := \int_{Q_\ell^*} \rho_{\gamma_\xi}(x) d\xi, \quad (2.16)$$

for every $x \in \mathbb{R}^3$, where the notation Tr_4 stands for the usual trace of 4×4 matrices.

For $\gamma \in \Gamma_{\leq q}$, the periodic DF energy is defined by

$$\begin{aligned} \mathcal{E}(\gamma) := & \int_{Q_\ell^*} \text{Tr}_{L_\xi^2}[\mathcal{D}_\xi^c \gamma_\xi] d\xi - z \int_{Q_\ell} G_\ell(x) \rho_\gamma(x) dx + \frac{\alpha}{2} \iint_{Q_\ell \times Q_\ell} \rho_\gamma(x) G_\ell(x - y) \rho_\gamma(y) dx dy \\ & - \frac{\alpha}{2} \iint_{Q_\ell^* \times Q_\ell^*} d\xi d\xi' \iint_{Q_\ell \times Q_\ell} \text{Tr}_4[\gamma_\xi(x, y) \gamma_{\xi'}(y, x)] W_\ell^\infty(\xi - \xi', x - y) dx dy. \end{aligned} \quad (2.17)$$

In the above definition of the energy, the so-called fine structure constant α is a dimensionless positive constant. Throughout the paper, we make the abuse of notation $\text{Tr}_{L_\xi^2}[\mathcal{D}_\xi^c \gamma_\xi]$ for the quantity $\text{Tr}_{L_\xi^2}[|\mathcal{D}_\xi^c|^{1/2} \gamma_\xi |\mathcal{D}_\xi^c|^{1/2} \text{sign}(\mathcal{D}_\xi^c)]$.

The potential W_ℓ^∞ that enters the definition of the last term, the so-called ‘‘exchange term’’, is defined on $\mathbb{R}^3 \times \mathbb{R}^3$ by

$$W_\ell^\infty(\eta, x) = \sum_{k \in \mathbb{Z}^3} \frac{e^{i\ell k \cdot \eta}}{|x + \ell k|} = \frac{4\pi}{\ell^3} \sum_{p \in \mathbb{Z}^3} \frac{1}{\left| \frac{2\pi p}{\ell} - \eta \right|^2} e^{i\left(\frac{2\pi p}{\ell} - \eta\right) \cdot x}. \quad (2.18)$$

It is Q_ℓ^* -periodic w.r.t. η and quasi-periodic with quasi-momentum η w.r.t. x .

For every $\gamma \in \Gamma_{\leq q}$, we now define the mean-field periodic Dirac operator

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

where

$$V_{\gamma,\xi} = \rho_\gamma * G_\ell - W_{\gamma,\xi} \tag{2.19}$$

with

$$\rho_\gamma * G_\ell(x) = \int_{Q_\ell} G_\ell(x-y) \rho_\gamma(y) dy = \widetilde{\text{Tr}}_{L^2}[G_\ell(x-\cdot)\gamma] \tag{2.20}$$

and, for every ψ_ξ in L_ξ^2 ,

$$W_{\gamma,\xi}\psi_\xi(x) = \int_{Q_\ell^*} d\xi' \int_{Q_\ell} W_\ell^\infty(\xi' - \xi, x-y) \gamma_{\xi'}(x,y) \psi_\xi(y) dy. \tag{2.21}$$

In (2.20) we keep the notation $\cdot * \cdot$ for the convolution of periodic functions on Q_ℓ , and we define the trace per unit cell as follows

$$\widetilde{\text{Tr}}_{L^2}[\gamma] := \int_{Q_\ell^*} \text{Tr}_{L_\xi^2}[\gamma_\xi] d\xi,$$

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

Then, the periodic DF functional may be rewritten as follows

$$\mathcal{E}(\gamma) = \widetilde{\text{Tr}}_{L^2}[\mathcal{D}_\gamma^c \gamma] - \frac{\alpha}{2} \widetilde{\text{Tr}}_{L^2}[V_\gamma \gamma], \tag{2.22}$$

with $V_\gamma = \int_{Q_\ell^*}^\oplus V_{\gamma,\xi} d\xi$. In the standard DF theory, the system of units is chosen such that $m = c = \hbar = 1$, where m is the mass of the electron, c the speed of light and \hbar the Planck constant, and z in (2.17) should be replaced by αz . Consequently, with this choice, the fine structure constant $\alpha \approx \frac{1}{137}$.

In this paper, we rather consider the non-relativistic regime and the weak electron-electron interaction regime when q and z are kept fixed. The *non-relativistic regime* corresponds to the case $c \gg 1$, whereas the *weak coupling regime* means $\alpha \ll 1$. In both cases, we assume in the following, without loss of generality, that $c \geq 1$ and $0 < \alpha \leq 1$.

2.3 Preliminary estimates

In the two following lemmas, we recall some useful results proved in [9] that we adapt to the new norm \mathcal{Y} .

Lemma 2.2 (Some Hardy-type inequalities [9, Lemmas 4.1, 4.5 and 4.7]). *Let $\gamma \in X \cap Y$ with $\gamma^* = \gamma$. There exist positive constants $C_G := C_G(\ell) \geq 1$, $C_W := C_W(\ell) \geq 1$, $C_{EE} := C_{EE}(\ell) \geq 1$ ¹ and $C''_{EE} := C''_{EE}(\ell)$ that only depend on ℓ and such that for any $\xi \in Q_\ell^*$ and $\psi_\xi \in H_\xi^1$,*

$$\|W_{\gamma,\xi}\|_{\mathcal{B}(L_\xi^2)} \leq C_W \|\gamma\|_{X \cap \mathcal{Y}(\xi)} \leq \frac{C_W}{c} \|\gamma\|_{X_c \cap \mathcal{Y}_c(\xi)}, \tag{2.23}$$

¹Lemma 4.7 in [9] involves other constants C_H and C'_{EE} . Since $C_H \leq C_G$, C_H can be replaced by C_G in the bounds without loss of generality. Additionally, since $C_{EE} \leq C'_{EE}$ thanks to Eqs. (C5) and (C7) in [9], we may replace C_{EE} by C'_{EE} everywhere. For the sake of simplicity of notation, we next set $C_{EE} := C'_{EE}$.

$$\|G_\ell \psi_\xi\|_{L_\xi^2} \leq C_G \|(1 - \Delta_\xi)^{1/2} \psi_\xi\|_{L_\xi^2} \leq \frac{C_G}{c} \|\mathcal{D}_\xi^c \psi_\xi\|_{L_\xi^2}, \quad (2.24)$$

$$\|V_\gamma\|_Y \leq C_{EE} \|\gamma\|_{X \cap Y} \leq \frac{C_{EE}}{c} \|\gamma\|_{X_c \cap Y_c}, \quad (2.25)$$

$$\|V_\gamma\|_Y \leq \frac{C_{EE}}{(1 + C_Y)} \|\gamma\|_{X \cap Y} \leq \frac{C_{EE}}{(1 + C_Y)c} \|\gamma\|_{X_c \cap Y_c}, \quad (2.26)$$

$$\|V_\gamma (1 - \Delta)^{-1/2}\|_Y \leq C_{EE} \|\gamma\|_{\mathfrak{S}_{1,1} \cap Y} \quad (2.27)$$

and

$$-C_{EE}'' \|\gamma\|_{\mathfrak{S}_{1,1} \cap Y} \|\psi_\xi\|_{L_\xi^2}^2 \leq (\psi_\xi, V_{\gamma, \xi} \psi_\xi)_{L_\xi^2}. \quad (2.28)$$

Proof. Most estimates can be found in [9, Lemmas 4.5 and 4.7]. The estimate (2.23) is slightly different from its analog in [9] because of the change of the functional space (\mathcal{Y} instead of Y). As in [9], we introduce

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

(see also Eq. (4.1) below). According to [9, Eqs. (B.18) and (B.19)], we know that, for any $\xi \in Q_\ell^*$,

$$\begin{aligned} & \left\| \int_{Q_\ell^*} d\xi' \int_{Q_\ell} W_{<2, \ell}^\infty(\xi' - \xi, x - y) \gamma_{\xi'}(x, y) \psi_\xi(y) dy \right\|_{L_\xi^2} \\ & \leq \frac{4\pi \|\psi_\xi\|_{L_\xi^2}}{\ell^3} \sum_{\substack{p \in \mathbb{Z}^3 \\ |p|_\infty \leq 1}} \int_{Q_\ell^* + \frac{2\pi p}{\ell}} \frac{\|\gamma_{\xi'}\|_{\mathcal{B}(L_{\xi'}^2)}}{|\xi' - \xi|^2} d\xi' \leq \frac{108\pi}{\ell^3} \|\gamma\|_{\mathcal{Y}(\xi)} \|\psi_\xi\|_{L_\xi^2}, \end{aligned}$$

since $\|\gamma_{\xi'}\|_{\mathcal{B}(L_{\xi'}^2)} = \|\gamma_{\xi' + \frac{2\pi p}{\ell}}\|_{\mathcal{B}(L_{\xi' + \frac{2\pi p}{\ell}}^2)}$ for every $p \in \mathbb{Z}^3$. Repeating the proof of [9, Eq. (4.8)], that is given in [9, Appendix B], the estimate (2.23) follows. Then, (2.26) is a slight modification of (2.25) where we have replaced the estimates on the exchange term W_γ by (2.23). \square

Let now

$$P_\gamma^\pm = \int_{Q^*}^\oplus P_{\gamma, \xi}^\pm d\xi \quad \text{with} \quad P_{\gamma, \xi}^\pm := \mathbb{1}_{\mathbb{R}_\pm}(\mathcal{D}_{\gamma, \xi}^c)$$

denote the projection onto the positive and negative spectrum of \mathcal{D}_γ^c , respectively. Note that by definition $P_{0, \xi}^\pm = \mathbb{1}_{\mathbb{R}_\pm}(\mathcal{D}_\xi^c - zG_\ell)$.

We now introduce

$$\kappa(\alpha, c) := \frac{1}{c} (C_G z + C_{EE} \alpha q^+), \quad (2.29)$$

with C_G and C_{EE} being given by Lemma 2.2 and $q^+ = \max\{q; 1\}$.

Then, we have the following.

Lemma 2.3. [9, Lemma 4.10, Lemma 4.11 and Eq. (5.16)] Let $\gamma \in \Gamma_{\leq q}$ and $\kappa(\alpha, c) < 1$. Then,

$$(1 - \kappa(\alpha, c))^2 |\mathcal{D}^c|^2 \leq |\mathcal{D}_\gamma^c|^2 \leq (1 + \kappa(\alpha, c))^2 |\mathcal{D}^c|^2, \quad (2.30)$$

in the sense of operators. Consequently,

$$(1 - \kappa(\alpha, c)) |\mathcal{D}^c| \leq |\mathcal{D}_\gamma^c| \leq (1 + \kappa(\alpha, c)) |\mathcal{D}^c|. \quad (2.31)$$

Moreover,

$$\| |\mathcal{D}^c|^{1/2} P_\gamma^\pm |\mathcal{D}^c|^{-1/2} \|_Y \leq \frac{(1 + \kappa(\alpha, c))^{1/2}}{(1 - \kappa(\alpha, c))^{1/2}} \quad (2.32)$$

and

$$\inf \sigma(|\mathcal{D}_\gamma^c|) \geq c^2 \lambda_0(\alpha, c) > c^2 (1 - \kappa(\alpha, c)), \quad (2.33)$$

where

$$\lambda_0(\alpha, c) := 1 - c^{-1} \max \left\{ C_G z + C_{EE}'' \alpha q^+; \frac{C_0}{\ell} z + C_{EE} \alpha q^+ \right\}, \quad (2.34)$$

with C_0 being defined by Eq. (2.3) and C_{EE} and C_{EE}'' in Lemma 2.2.

In addition, we obtain new estimates on the positive eigenvalues of the family of operators $\mathcal{D}_{\gamma, \xi}^c$ for any $\gamma \in \Gamma_{\leq q}$ that are uniform in c , α , γ and $\xi \in Q_\ell^*$.

Lemma 2.4 (Properties of the positive eigenvalues of $\mathcal{D}_{\gamma, \xi}^c$). Assume $0 < \alpha \leq 1$, $c \geq 1$ and $\kappa(\alpha, c) \leq \frac{1}{2}$. Let $\gamma \in \Gamma_{\leq q}$. For $n \geq 1$, we denote by $\lambda_n^c(\xi)$ the n -th positive eigenvalue (counted with multiplicity) of the mean-field operator $\mathcal{D}_{\gamma, \xi}^c$. Then, there exist positive constants $\underline{\Lambda}_n(\alpha, c)$ and $\overline{\Lambda}_n(\alpha, c)$ independent of γ and $\xi \in Q_\ell^*$ and a positive constant Σ_n that is independent of γ , ξ , α and c such that

$$0 < \underline{\Lambda}_n(\alpha, c) \leq \lambda_n^c(\xi) \leq \overline{\Lambda}_n(\alpha, c) \leq c^2 + \Sigma_n, \quad \forall \xi \in Q_\ell^*, \forall n \geq 1, \quad (2.35)$$

with $\underline{\Lambda}_n(\alpha, c) \geq c(1 - \kappa(\alpha, c)) \geq \frac{c}{2}$ and $\overline{\Lambda}_n(\alpha, c) \rightarrow +\infty$ when $n \rightarrow +\infty$. The interval $[\underline{\Lambda}_n(\alpha, c), \overline{\Lambda}_n(\alpha, c)]$ is independent of γ in $\Gamma_{\leq q}$. In particular, for any $n \in \mathbb{N}^*$, there exists a positive integer \mathfrak{N}_n with $\mathfrak{N}_n \geq n$ that is independent of γ , ξ , α and c such that the operators $\mathcal{D}_{\gamma, \xi}^c$ have at most \mathfrak{N}_n positive eigenvalues in $(0, \overline{\Lambda}_n(\alpha, c)]$.

The proof of Lemma 2.4 is postponed until Appendix A. We provide in this proof explicit values for the constants $\underline{\Lambda}_n(\alpha, c)$ and $\overline{\Lambda}_n(\alpha, c)$ appearing in (2.35) (see Eqs. (A.1) and (A.2)). In addition, Σ_n and \mathfrak{N}_n are given by Eqs. (A.5) and (A.9).

We now define the positive constant

$$K_q := (1 + \Sigma_{[q]}) \sqrt{2 \left(1 + 4 (C_G z + C_{EE} q^+)^2 \right)}, \quad (2.36)$$

with $\Sigma_{[q]}$ being defined by Eqs. (2.35) and (A.5). Here we have used the standard notation $[q] := \min\{m \in \mathbb{N} \mid m \geq q\}$ for any $q \in \mathbb{R}^+$.

Then, we have the following *a priori* estimates on the H^1 norms of normalized eigenfunctions of the $\mathcal{D}_{\gamma, \xi}^c$'s.

Lemma 2.5. We assume $0 < \alpha \leq 1$, $c \geq 1$ and $\kappa(\alpha, c) \leq \frac{1}{2}$. Let $\xi \in Q_\ell^*$, $\gamma \in \Gamma_{\leq q}$ and ψ_ξ be a normalized eigenfunction of the operator $\mathcal{D}_{\gamma, \xi}^c$ with eigenvalue $\lambda(\xi) \in (0, c^2 + \Sigma_{[q]})$. Then,

$$\|\psi_\xi\|_{H_\xi^1(Q_\ell)} \leq K_q.$$

Furthermore, if $\gamma' \in \Gamma_{\leq q}$ satisfies $0 \leq \gamma' \leq \mathbb{1}_{(0, c^2 + \Sigma_{[q]})}(\mathcal{D}_\gamma^c)$, then

$$\|\gamma'\|_X \leq K_q q. \quad (2.37)$$

Proof. As $\mathcal{D}_{\gamma,\xi}^c \psi_\xi = \lambda(\xi) \psi_\xi$, we have

$$\|\mathcal{D}_\xi^c \psi_\xi\|_{L_\xi^2} = \|(\lambda(\xi) + zG_\ell - \alpha V_{\gamma,\xi}) \psi_\xi\|_{L_\xi^2}.$$

According to the Hardy inequalities (2.24) and (2.27) in Lemma 2.2 and since $|\lambda(\xi)| \leq c^2 + \Sigma_{[q]}$,

$$\begin{aligned} \|\mathcal{D}_\xi^c \psi_\xi\|_{L_\xi^2}^2 &= c^4 \|\psi_\xi\|_{L_\xi^2}^2 + c^2 \|\nabla_\xi \psi_\xi\|_{L_\xi^2}^2 \\ &\leq (c^4 + 2c^2 \Sigma_{[q]} + \Sigma_{[q]}^2) \|\psi_\xi\|_{L_\xi^2}^2 \\ &\quad + 2(C_G z + \alpha C_{EE} q^+) (c^2 + \Sigma_{[q]}) \|(1 - \Delta_\xi)^{1/2} \psi_\xi\|_{L_\xi^2} \|\psi_\xi\|_{L_\xi^2} \\ &\quad + c^2 \kappa(\alpha, c)^2 \|(1 - \Delta_\xi)^{1/2} \psi_\xi\|_{L_\xi^2}^2, \end{aligned}$$

where we used the definition (2.29) of $\kappa(\alpha, c)$ in the last inequality. As $\|\psi\|_{L_\xi^2} = 1$, $c \geq 1$, and $\kappa(\alpha, c) \leq \frac{1}{2}$ and by using the Cauchy–Schwarz and the Young’s inequalities, we obtain

$$\begin{aligned} \|\nabla_\xi \psi_\xi\|_{L_\xi^2}^2 &\leq 2 \Sigma_{[q]} + \frac{1}{c^2} \Sigma_{[q]}^2 + \kappa^2(\alpha, c) \|(1 - \Delta_\xi)^{1/2} \psi_\xi\|_{L_\xi^2}^2 \\ &\quad + 2(C_G z + \alpha C_{EE} q^+) (1 + \frac{1}{c^2} \Sigma_{[q]}) \|(1 - \Delta_\xi)^{1/2} \psi_\xi\|_{L_\xi^2} \\ &\leq 2 \Sigma_{[q]} + \Sigma_{[q]}^2 + \frac{1}{4} \|(1 - \Delta_\xi)^{1/2} \psi_\xi\|_{L_\xi^2}^2 \\ &\quad + 4(C_G z + \alpha C_{EE} q^+)^2 (1 + \Sigma_{[q]})^2 + \frac{1}{4} \|(1 - \Delta_\xi)^{1/2} \psi_\xi\|_{L_\xi^2}^2 \\ &\leq \frac{1}{2} + 2 \Sigma_{[q]} + \Sigma_{[q]}^2 + 4(C_G z + C_{EE} q^+)^2 (1 + \Sigma_{[q]})^2 + \frac{1}{2} \|\nabla_\xi \psi_\xi\|_{L_\xi^2}^2, \end{aligned}$$

since $\alpha \leq 1$. Thus, with the definition (2.36) of K_q

$$\|\psi_\xi\|_{H_\xi^1(Q_\ell)}^2 \leq K_q^2.$$

For the second estimate, we express γ' as

$$\gamma'_\xi = \sum_{i=1}^{+\infty} \mu_i(\xi) |\psi_i(\xi)\rangle \langle \psi_i(\xi)|$$

where $0 \leq \mu_i(\xi) \leq 1$, $\sum_{i=1}^{+\infty} \int_{Q_\ell^*} \mu_i(\xi) d\xi \leq q$ and $\psi_i(\xi)$ is a normalized eigenfunction of $\mathcal{D}_{\gamma,\xi}^c$ with eigenvalue $\lambda_i(\xi) \in (0, c^2 + \Sigma_{[q]})$. Thus, by interpolation,

$$\|\gamma'\|_X = \sum_{i=1}^{+\infty} \int_{Q_\ell^*} \mu_i(\xi) \|\psi_i(\xi)\|_{H_\xi^{1/2}}^2 d\xi \leq \sum_{i=1}^{+\infty} \int_{Q_\ell^*} \mu_i(\xi) \|\psi_i(\xi)\|_{H_\xi^1} \|\psi_i(\xi)\|_{L_\xi^2} d\xi \leq K_q q.$$

This concludes the proof. \square

2.4 The periodic DF ground state

We recall that

$$P_\gamma^\pm = \int_{Q^*}^\oplus P_{\gamma,\xi}^\pm d\xi \quad \text{with} \quad P_{\gamma,\xi}^\pm := \mathbb{1}_{\mathbb{R}^\pm}(\mathcal{D}_{\gamma,\xi}^c)$$

denote the projection onto the positive and negative spectrum of \mathcal{D}_γ^c , respectively. We define

$$\Gamma_q^+ := \{\gamma \in \Gamma_q \mid \gamma = P_\gamma^+ \gamma P_\gamma^+\}, \quad \Gamma_{\leq q}^+ := \{\gamma \in \Gamma_{\leq q} \mid \gamma = P_\gamma^+ \gamma P_\gamma^+\}$$

and the ground state energy

$$I_q := \inf_{\gamma \in \Gamma_q^+} \mathcal{E}(\gamma). \quad (2.38)$$

Existence of a ground state has been proved in [9] under the following assumption.

Assumption 2.6. *Let $q, z \in \mathbb{R}^+$. We recall that $\kappa(\alpha, c) := c^{-1}(C_G z + C_{EE} \alpha q^+)$ with C_G and C_{EE} being given by Lemma 2.2. We assume that α and c are chosen in such a way that*

1. $\kappa(\alpha, c) < 1 - \frac{\alpha}{2c} C_{EE} q^+$;
2. $\frac{\alpha}{c} \sqrt{\max \left\{ \left(1 - \kappa(\alpha, c) - \frac{\alpha}{2c} C_{EE} q^+\right)^{-1} c^{-2} \overline{\Lambda_{|q|}}(\alpha, c) q; 1 \right\} q^+} < \left(1 - \kappa(\alpha, c)\right)^{1/2} \lambda_0(\alpha, c)^{1/2}$

where $\lambda_0(\alpha, c) \geq 1 - \kappa(\alpha, c) > 0$ is given by Lemma 2.3, and $\overline{\Lambda_{|q|}}(\alpha, c)$ is defined by Eq. (2.35) in Lemma 2.4.

In the statement of Assumption 2.6, Condition 1 is necessary to ensure that minimizers of the corresponding relaxed minimization problem $J_{\leq q}$ on $\Gamma_{\leq q}^+$ (see (3.1) below) are not 0. Condition 2 is a rather technical assumption that arises from the retraction method that is used in [9] to prove the existence of minimizers of I_q .

Theorem 2.7 (Existence of minimizers [9, Theorem 2.6]). *Under Assumption 2.6, the minimization problem I_q admits a minimizer $\gamma_* \in \Gamma_q^+$. Furthermore, γ_* solves the following nonlinear self-consistent equation:*

$$\gamma_* = \mathbb{1}_{[0, \nu]}(\mathcal{D}_{\gamma_*}^c) + \delta \quad (2.39)$$

where $0 \leq \delta \leq \mathbb{1}_{\{\nu\}}(\mathcal{D}_{\gamma_*}^c)$ and ν is the Lagrange multiplier due to the charge constraint $\int_{Q_\ell^*} \text{Tr}_{L_\xi^2}(\gamma_\xi) d\xi = q$ satisfying $\nu \in [c^2 \lambda_0(\alpha, c), \overline{\Lambda_{|q|}}(\alpha, c)]$.

2.5 Main result

We now introduce further assumptions on α and c that imply that α is small or c is large.

Assumption 2.8. *Let $z, q \in \mathbb{R}^+$ be fixed. We assume that $0 < \alpha \leq 1$ and $c \geq 1$ are chosen such that*

1. Assumption 2.6 is satisfied ;
2. $c \geq 2(C_G z + C_{EE} q^+)$;
3. $\frac{\alpha}{c} < \frac{2\pi}{C_{\text{cri}}(q, z)}$ where $C_{\text{cri}}(q, z)$ is a large enough positive constant that is independent of α and c and that is given explicitly in the statement of Lemma 4.6 below.

Remark 2.9. *Assumption 2.6 is not empty. According to [9, Remark 2.8], for $c = 1$, $\alpha = \frac{1}{137}$ and $\ell \approx 1000$, Assumption 2.6 is satisfied for $q = z \leq 17$. It is necessary to guarantee the existence of minimizers of I_q that satisfy (2.39). Condition 2 in Assumption 2.8 is used to guarantee that $1 - \kappa(\alpha, c)$ stays away from 0 uniformly; actually, it ensures that $1 - \kappa(\alpha, c) \geq \frac{1}{2}$. As we consider the case $c \gg 1$, we can choose $c \geq 2(C_G z + C_{EE} q^+)$ without loss of generality. Note that In the non-relativistic limit $c \rightarrow +\infty$, we have $\kappa(\alpha, c) \rightarrow 0$. In the same manner, in the weak coupling limit $\alpha \rightarrow 0^+$, we have $\kappa(\alpha, c) \rightarrow C_G \frac{z}{c}$.*

The purpose of this paper is to show that, under above conditions on α and c , we have the following.

Theorem 2.10 (Properties of the last shell). *Under Assumption 2.8, for any minimizer γ_* of (2.38), the density matrix δ given in the Euler–Lagrange equation (2.39) satisfies either $\delta = 0$ or $\delta = \mathbb{1}_{\{\nu\}}(\mathcal{D}_{\gamma_*}^c)$. As a result, γ_* is a projector.*

Remark 2.11. *We point out the fact that this is the first time that an explicit upper bound on $\frac{\alpha}{c}$ is given which ensures that any DF minimizer is a projector. (In the DF model for atoms and molecules [20], the same result is not available.)*

As in the HF model, the molecular and the crystal cases rely on totally different arguments: for atoms and molecules, the positive definiteness of the nonlinear term is used, whereas for crystals, the proof is based on a careful analysis of the singularity w.r.t. $\xi \in Q_\ell^$ of the nonlinear term which provides a quantitative estimate that is independent of α and c . This estimate gives the upper bound $C_{\text{cri}}(q, z)$.*

Remark 2.12. *When $\alpha = 0$, the nonlinear term V_γ disappears. In the non-relativistic case, the proof that any minimizer is a projector relies on the absolute continuity of the spectrum of the linear periodic operator $-\frac{1}{2}\Delta - zG_\ell$: by [15, Theorem 1.9, Chapter 7.1] $G_\ell(-\Delta)^{-1}$ is compact. On the contrary, the operator $G_\ell(\mathcal{D}^c)^{-1}$ is not compact, and we do not know whether the spectrum of the periodic Dirac–Coulomb operator $\mathcal{D}^c - zG_\ell$ is absolutely continuous.*

The proof of Theorem 2.10 adapts the ideas of Ghimenti and Lewin [12] for the periodic HF model. Their proof is based on the local convexity and the second-order expansion of the periodic HF functional on the constraint set. In the DF case, 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. Both observations lead to the failure of the direct study of the second-order expansion of the periodic DF model on Γ_q^+ .

Following our previous work [9], instead of studying directly the DF model on Γ_q^+ , we consider a penalized DF model; namely, $\mathcal{E}(\gamma) - \epsilon_P \widetilde{\text{Tr}}_{L^2}[\gamma]$ for $\epsilon_P \in \mathbb{R}^+$, on $\Gamma_{\leq q}^+$. Then, using a retraction technique developed by Séré [23] (see also Catto-Meng-Paturel-Séré [9] for the adaptation to the periodic setting), we construct a retraction mapping θ onto an open subset $\mathcal{U}_R \subset \Gamma_{\leq q}^+$, such that any minimizer of I_q is situated in \mathcal{U}_R , and such that we have $\theta(\gamma) \in \Gamma_{\leq q}^+$ for any $\gamma \in \mathcal{U}_R$. As shown in [9, Lemma 3.2 and Theorem 3.3], we have

$$\begin{aligned} I_q - \epsilon_P q &= \inf_{\gamma \in \Gamma_{\leq q}^+} \left(\mathcal{E}(\gamma) - \epsilon_P \widetilde{\text{Tr}}_{L^2}[\gamma] \right) = \inf_{\gamma \in \Gamma_{\leq q}^+ \cap \mathcal{U}_R} \left(\mathcal{E}(\gamma) - \epsilon_P \widetilde{\text{Tr}}_{L^2}[\gamma] \right) \\ &= \inf_{\gamma \in \mathcal{U}_R} \left(\mathcal{E}(\theta(\gamma)) - \epsilon_P \widetilde{\text{Tr}}_{L^2}[\theta(\gamma)] \right). \end{aligned}$$

Therefore, we investigate in this paper the second-order expansion of the new DF functional $\gamma \mapsto \mathcal{E}(\theta(\gamma)) - \epsilon_P \widetilde{\text{Tr}}_{L^2}[\theta(\gamma)]$ on \mathcal{U}_R . This latter property can be obtained by mimicking the proof of Meng [20].

With these results in hand, Theorem 2.10 is obtained by following the lines of the proof in [12].

Organisation of this paper: In Section 3, we first study the penalized DF model on $\Gamma_{\leq q}^+$, the retraction θ and the second-order expansion for the new DF functional. In Section 4, we adapt the ideas of [12] to prove our main result Theorem 2.10. In Section 5, we adapt the proof of the existence of the retraction (Lemma 3.2) to our new functional framework. In Section 6, we give the details about the proof of the second-order expansion for the new DF functional in our new functional space \mathcal{Y}_c . Finally, Appendix A is devoted to the proof of Lemma 2.4.

3 New DF functional and its second-order expansion

It is shown in [9] that, under Assumption 2.6, existence of minimizers for problem I_q is equivalent to the following penalized minimization problem

$$J_{\leq q} := \inf_{\gamma \in \Gamma_{\leq q}^+} (\mathcal{E}(\gamma) - \epsilon_P \widetilde{\text{Tr}}_{L^2}[\gamma]) + \epsilon_P q, \quad (3.1)$$

for some real number ϵ_P large enough. More precisely, the following holds.

Theorem 3.1 (Minimizers of the penalized problem [9, Theorem 3.3]). *We assume that Assumption 2.6 holds. Then there is a positive constant ϵ_0 small enough independent of α, c such that for $\epsilon_P := \overline{\Lambda_{[q]}}(\alpha, c) + \epsilon_0$ with $\overline{\Lambda_{[q]}}(\alpha, c)$ given in Lemma 2.4, the penalized minimization problem $J_{\leq q}$ admits a minimizer $\gamma_* \in \Gamma_{\leq q}^+$ with $\int_{Q_\ell^*} \text{Tr}_{L_\xi^2}(\gamma_{*, \xi}) d\xi = q$. As a result, $I_q = J_{\leq q}$. Moreover, any minimizer γ_* of $J_{\leq q}$ is a minimizer of I_q and vice versa.*

In addition, γ_ solves the following nonlinear self-consistent equation:*

$$\gamma_* = \mathbb{1}_{[0, \nu]}(\mathcal{D}_{\gamma_*}^c) + \delta \quad (3.2)$$

where $0 \leq \delta \leq \mathbb{1}_{\{\nu\}}(\mathcal{D}_{\gamma_*}^c)$ and $\nu \in [c^2 \lambda_0(\alpha, c), \overline{\Lambda_{[q]}}(\alpha, c)]$ is the Lagrange multiplier due to the charge constraint $\int_{Q_\ell^*} \text{Tr}_{L_\xi^2}(\gamma_{*, \xi}) d\xi \leq q$.

The proof of existence of minimizers of (3.1) relies on the construction of a regular retraction θ defined on an open subset \mathcal{U}_R of $\Gamma_{\leq q}$ such that

$$\theta : \mathcal{U}_R \rightarrow \mathcal{U}_R \cap \Gamma_{\leq q}^+, \quad \text{and} \quad \theta(\mathcal{U}_R \cap \Gamma_{\leq q}^+) = \mathcal{U}_R \cap \Gamma_{\leq q}^+. \quad (3.3)$$

For $\gamma \in \Gamma_{\leq q}$, the retraction is defined by

$$\theta(\gamma) := \lim_{n \rightarrow +\infty} T^n(\gamma), \quad (3.4)$$

with

$$T(\gamma) = P_\gamma^+ \gamma P_\gamma^+, \quad T^n(\gamma) = T(T^{n-1}(\gamma)), \quad T^0(\gamma) = \gamma.$$

According to the Floquet decomposition, we have

$$T(\gamma) = \int_{Q_\ell^*}^{\oplus} T_\xi(\gamma) d\xi = \int_{Q_\ell^*}^{\oplus} P_{\gamma, \xi}^+ \gamma_\xi P_{\gamma, \xi}^+ d\xi.$$

With θ in hand, if a minimizer γ_* of $J_{\leq q}$ is in \mathcal{U}_R , the penalized minimization problem $J_{\leq q}$ reduces to a simpler one, where the nonlinear constraint $P_\gamma^+ \gamma P_\gamma^+ = \gamma$ is incorporated in the new functional; namely,

$$J_{\leq q} = \min_{\gamma \in \mathcal{U}_R} E(\gamma) + \epsilon_P q, \quad (3.5)$$

where the new DF functional $E(\cdot)$ is defined by

$$E(\gamma) := \mathcal{E}(\theta(\gamma)) - \epsilon_P \widetilde{\text{Tr}}_{L^2}[\theta(\gamma)], \quad \text{for any } \gamma \in \mathcal{U}_R. \quad (3.6)$$

Note that $\theta(\gamma) \in \mathcal{U}_R \cap \Gamma_{\leq q}^+$ by construction (see Eq.(3.3)). The following lemma guarantees the existence of the retraction θ in our setting where the norm Y in [9, Proposition 5.3] is replaced by \mathcal{Y}_c .

Lemma 3.2. *Assume $\kappa(\alpha, c) < 1$ and define $A(\alpha, c) := \frac{\alpha}{2c} C_{EE} (1 - \kappa(\alpha, c))^{-1}$. Given $1 < R < \frac{1}{2A(\alpha, c)}$, let $M(\alpha, c) := \max\left(\frac{1+A(\alpha, c)q^+}{2}; \frac{1}{1-2A(\alpha, c)R}\right)$, and let*

$$\mathcal{U}_R := \left\{ \gamma \in \Gamma_{\leq q} \mid \frac{1}{c} \max\left\{ \|\gamma\|_{\mathcal{D}^c}^{1/2} \|g_{\mathfrak{S}_{1,1}}\|; \|\gamma\|_{\mathcal{Y}} \right\} + \frac{M(\alpha, c)}{c^2} \|T(\gamma) - \gamma\|_{X_c \cap \mathcal{Y}_c} < R \right\}. \quad (3.7)$$

Then, \mathcal{U}_R is a open subset in $\Gamma_{\leq q}$, T maps continuously \mathcal{U}_R into \mathcal{U}_R , and, for any $\gamma \in \mathcal{U}_R$, the sequence $(T^n(\gamma))_{n \geq 0}$ converges to a limit $\theta(\gamma) \in \Gamma_{\leq q}^+$. Moreover, for all $\gamma \in \mathcal{U}_R$,

$$\|T^{n+1}(\gamma) - T^n(\gamma)\|_{X_c \cap \mathcal{Y}_c} \leq L(\alpha, c) \|T^n(\gamma) - T^{n-1}(\gamma)\|_{X_c \cap \mathcal{Y}_c} \quad (3.8)$$

and

$$\|\theta(\gamma) - T^n(\gamma)\|_{X_c \cap \mathcal{Y}_c} \leq \frac{L^n(\alpha, c)}{1 - L(\alpha, c)} \|T(\gamma) - \gamma\|_{X_c \cap \mathcal{Y}_c}, \quad (3.9)$$

with $0 < L(\alpha, c) := 2A(\alpha, c)R < 1$.

This result is collected in [9, Proposition 5.4] and can be proved by adapting [9, Proposition 5.8] and [23, Proposition 2.1] to our new functional space \mathcal{Y} . For the reader's convenience, the proof of Lemma 3.2 in this context is provided in Section 5.

The main ingredient of the proof of Theorem 2.10 is the following.

Theorem 3.3 (Second-order expansion for the new DF energy). *Let $\kappa(\alpha, c) < 1$ and $A(\alpha, c)$ be given as in Lemma 3.2. Let $1 < R < \frac{1}{2A(\alpha, c)}$ be fixed, and let $L(\alpha, c) := 2A(\alpha, c)R < 1$. Given any $\gamma \in \mathcal{U}_R \cap \Gamma_{\leq q}^+$ and $h \in X \cap Y$ such that $P_\gamma^+ h P_\gamma^+ = h$, and given any $t \in \mathbb{R}$ such that $\gamma + th \in \mathcal{U}_R$, we have*

$$E(\gamma + th) = E(\gamma) + t \widetilde{\text{Tr}}_{L^2}[(\mathcal{D}_\gamma^c - \epsilon_P)h] + \frac{\alpha t^2}{2} \widetilde{\text{Tr}}_{L^2}[V_h h] + t^2 \frac{\alpha^2}{c^2} \text{Err}(t, \gamma, h) \quad (3.10)$$

where $|\text{Err}(t, \gamma, h)| \leq (2 + \frac{\epsilon_P}{c^2}) \mathcal{N}_{\gamma+th}(h)$ with

$$\begin{aligned} \mathcal{N}_g(h) := & \frac{C_{EE}^2}{2(1 - \kappa(\alpha, c))^2 \lambda_0(\alpha, c)} \int_{Q_\ell^*} \|h\|_{X \cap \mathcal{Y}(\xi)}^2 \|g_\xi\|_{\mathfrak{S}_1(\xi)} d\xi \\ & + \left(q \frac{\alpha^2}{c^2} + R \frac{\alpha^2}{c^2} + \frac{\alpha}{c} \right) \frac{10 C_{EE}^4}{(1 - \kappa(\alpha, c))^4 \lambda_0(\alpha, c)^{5/2} (1 - L(\alpha, c))^2} \\ & \times \left(\frac{1}{c} \int_{Q_\ell^*} \|h\|_{X \cap \mathcal{Y}(\xi)} \|g_\xi\|_{\mathcal{D}_\xi^c}^{1/2} \|g_{\mathfrak{S}_1(\xi)}\| d\xi + \frac{1}{c} \sup_{\xi \in Q_\ell^*} \sup_{\substack{k \in \mathbb{Z}^3 \\ |k|_\infty \leq 1}} \int_{Q_\ell^* + \frac{2\pi k}{\ell}} \frac{\|h\|_{X \cap \mathcal{Y}(\xi')}}{|\xi - \xi'|^2} d\xi' \right)^2. \end{aligned} \quad (3.11)$$

The proof of Theorem 3.3 is postponed until Section 6.

Remark 3.4. *For $q \in \mathbb{R}^+$, it is not difficult to see that*

$$\mathcal{N}_\gamma(h) \leq (R + q) \|h\|_{X \cap Y}$$

by using $\gamma \in \mathcal{U}_R$ as in [20]. As a result, $\text{Err}(t, \gamma, h)$ is uniformly bounded with respect to t if $\gamma + th \in \mathcal{U}_R$. However, in this paper, we can not simplify (3.11). This complicated formula will be used in Lemma 4.6 to control the singular behavior with respect to the ξ variable.

We now embark on the proof of Theorem 2.10.

4 Properties of the last shell

In this section, we are going to mimic the proof in [12] to prove Theorem 2.10 with the help of Theorem 3.3. Throughout the section, we assume that γ_* is a minimizer of $J_{\leq q}$ with $J_{\leq q}$ being given by (3.1).

4.1 Continuity of the eigenfunctions of $\mathcal{D}_{\gamma_*, \xi}^c$ w.r.t. ξ

We recall that W_ℓ^∞ is defined by (2.18). We may separate the singularities of W_ℓ^∞ w.r.t. $\eta \in 2Q_\ell^*$ and $x \in 2Q_\ell$ as follows

$$W_\ell^\infty(\eta, x) = W_{\geq 2, \ell}^\infty(\eta, x) + W_{< 2, \ell}^\infty(\eta, x), \quad (4.1)$$

with

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

and

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

Here we recall that $|p|_\infty := \max\{|p_1|; |p_2|; |p_3|\}$.

It is convenient to study $\mathcal{D}_{\gamma_*}^c$ on the fixed Hilbert space $L_{\text{per}}^2(Q_\ell)$. Thus we introduce the unitary operator defined in each Bloch fiber by

$$U_\xi : L_{\text{per}}^2(Q_\ell) \rightarrow L_\xi^2(Q_\ell), \quad u \mapsto e^{i\xi \cdot x} u(\cdot).$$

When A_ξ is an operator on $L_\xi^2(Q_\ell)$, we shall use the notation $\tilde{A}_\xi := U_\xi^* A_\xi U_\xi$ for the unitarily equivalent operator on $L_{\text{per}}^2(Q_\ell)$. For the operator $W_{\gamma_*, \xi}$ defined by (2.21), we get the operator $\tilde{W}_{\gamma_*, \xi}$ defined by its kernel

$$\begin{aligned} \tilde{W}_{\gamma_*, \xi}(x, y) &= [U_\xi^* W_{\gamma_*, \xi} U_\xi](x, y) \\ &= \int_{Q_\ell^*} \left[\tilde{W}_{\geq 2, \ell}^\infty(\xi - \xi', x - y) + \tilde{W}_{< 2, \ell}^\infty(\xi - \xi', x - y) \right] \tilde{\gamma}_{*, \xi'}(x, y) d\xi', \end{aligned} \quad (4.2)$$

where, for every x and $\xi \in \mathbb{R}^3$, $\tilde{W}_{\geq 2, \ell}^\infty(\eta, x) = e^{i\eta \cdot x} W_{\geq 2, \ell}^\infty(\eta, x)$, $\tilde{W}_{< 2, \ell}^\infty(\eta, x) = e^{i\eta \cdot x} W_{< 2, \ell}^\infty(\eta, x)$ and $\tilde{\gamma}_{*, \xi'}(x, y) = e^{-i\xi' \cdot x} \gamma_{*, \xi'}(x, y) e^{i\xi' \cdot y}$.

Lemma 4.1 (Hölder continuity of \tilde{W}). *Let $0 < a < 1$. The family $(\tilde{W}_{\gamma_*, \xi})_{\xi \in Q_\ell^*}$ is bounded and a -Hölder continuous in $\mathcal{B}(L_{\text{per}}^2(Q_\ell))$ w.r.t. $\xi \in Q_\ell^*$. Moreover, for every ξ_1 and ξ_2 in Q_ℓ^* ,*

$$\|\tilde{W}_{\gamma_*, \xi_1} - \tilde{W}_{\gamma_*, \xi_2}\|_{\mathcal{B}(L_{\text{per}}^2(Q_\ell))} \leq C_a |\xi_1 - \xi_2|^a,$$

with C_a being a positive constant which is independent of ξ_1 and ξ_2 .

Proof. The boundedness of $\tilde{W}_{\gamma_*, \xi}$ follows from (2.23). Indeed,

$$\text{ess sup}_{\xi \in Q_\ell^*} \|\tilde{W}_{\gamma_*, \xi}\|_{\mathcal{B}(L_{\text{per}}^2(Q_\ell))} = \text{ess sup}_{\xi \in Q_\ell^*} \|U_\xi^* W_{\gamma_*, \xi} U_\xi\|_{\mathcal{B}(L_{\text{per}}^2(Q_\ell))} = \|W_{\gamma_*}\|_Y \leq C \|\gamma_*\|_{X \cap \mathcal{Y}}.$$

¹It is claimed in [8, Page 745] and [12, Lemma 1] that the function $f(\eta, x) := W_\ell^\infty(\eta, x) - e^{-i\eta \cdot x} G_\ell(x) - \frac{4\pi}{\ell^3} \frac{e^{-i\eta \cdot x}}{|\eta|^2}$ is harmonic which is not true.

Using (4.1) and (4.2), for any $u, v \in L^2_{\text{per}}(Q_\ell)$, we have

$$\begin{aligned} & \left(u, (\widetilde{W}_{\gamma_*, \xi_1} - \widetilde{W}_{\gamma_*, \xi_2})v \right)_{L^2_{\text{per}}} \\ &= \int_{Q_\ell^*} \iint_{Q_\ell \times Q_\ell} \left(\widetilde{W}_{\geq 2, \ell}^\infty(\xi_1 - \xi', x - y) - \widetilde{W}_{\geq 2, \ell}^\infty(\xi_2 - \xi', x - y) \right) \tilde{\gamma}_{*, \xi'}(x, y) u(y) v(x) dx dy d\xi' \\ &+ \int_{Q_\ell^*} \iint_{Q_\ell \times Q_\ell} \left(\widetilde{W}_{< 2, \ell}^\infty(\xi_1 - \xi', x - y) - \widetilde{W}_{< 2, \ell}^\infty(\xi_2 - \xi', x - y) \right) \tilde{\gamma}_{*, \xi'}(x, y) u(y) v(x) dx dy d\xi'. \end{aligned}$$

Since $\widetilde{W}_{\geq 2, \ell}^\infty(\eta, z) = e^{i\eta \cdot z} W_{\geq 2, \ell}^\infty(\eta, z)$, we have

$$\begin{aligned} & \widetilde{W}_{\geq 2, \ell}^\infty(\eta_1, z) - \widetilde{W}_{\geq 2, \ell}^\infty(\eta_2, z) \\ &= \int_0^1 i(\eta_1 - \eta_2) \cdot z e^{i(\eta_2 + t(\eta_1 - \eta_2)) \cdot z} W_{\geq 2, \ell}^\infty(\eta_2 + t(\eta_1 - \eta_2), z) dt \\ &+ \int_0^1 e^{i(\eta_2 + t(\eta_1 - \eta_2)) \cdot z} \nabla_\eta W_{\geq 2, \ell}^\infty(\eta_2 + t(\eta_1 - \eta_2), z) \cdot (\eta_1 - \eta_2) dt, \end{aligned}$$

by the Taylor formula. Therefore, using (4.1), we have, for any $u, v \in L^2_{\text{per}}(Q_\ell)$,

$$\begin{aligned} & \left| \left(u, (\widetilde{W}_{\gamma_*, \xi_1} - \widetilde{W}_{\gamma_*, \xi_2})v \right)_{L^2_{\text{per}}} \right| \\ &\leq C |\xi_1 - \xi_2| \sup_{\xi \in 2Q_\ell^*} \iint_{Q_\ell \times Q_\ell} \int_{Q_\ell^*} |\widetilde{W}_{\geq 2, \ell}^\infty(\xi - \xi', x - y)| |\tilde{\gamma}_{*, \xi'}(x, y)| |u(y)| |v(x)| d\xi' dx dy \\ &+ |\xi_1 - \xi_2| \left(\int_{Q_\ell^*} \sup_{\xi \in 2Q_\ell^*} \|\nabla_\xi W_{\geq 2, \ell}^\infty \tilde{\gamma}_{*, \xi'}\|_{L^2(Q_\ell \times Q_\ell)} d\xi' \right) \|u\|_{L^2_{\text{per}}(Q_\ell)} \|v\|_{L^2_{\text{per}}(Q_\ell)} \\ &+ \frac{4\pi}{\ell^3} \sum_{\substack{p \in \mathbb{Z}^3 \\ |p|_\infty < 2}} \int_{Q_\ell^*} d\xi' \left| \frac{1}{|\xi' - \xi_1 - \frac{2\pi p}{\ell}|^2} - \frac{1}{|\xi' - \xi_2 - \frac{2\pi p}{\ell}|^2} \right| \left| (\tilde{\gamma}_{*, \xi'} U_{2\pi p} u, U_{2\pi p} v)_{L^2_{\text{per}}} \right|. \end{aligned}$$

It is shown in [9, Corollary B.2 and Lemma B.3] that

$$\sup_{\xi \in 2Q_\ell^*} \| |W_{\geq 2, \ell}^\infty|^{1/2}(\xi, \cdot) |\mathcal{D}_\xi^c|^{-1/2} \|_{\mathcal{B}(L_\xi^2)} \leq C, \quad \sup_{\xi \in 2Q_\ell^*} \|\nabla_\xi W_{\geq 2, \ell}^\infty\|_{L^\infty(Q_\ell)} \leq C.$$

Then as $\|\gamma\|_Y \leq 1$, and arguing as for [9, Eq. (B.9)] for the first term on the right-hand side, we get, from (2.23),

$$\begin{aligned} & \left| \left((\widetilde{W}_{\gamma_*, \xi_1} - \widetilde{W}_{\gamma_*, \xi_2})u, v \right)_{L^2_{\text{per}}} \right| \leq C |\xi_1 - \xi_2| \|\gamma_*\|_X \|u\|_{L^2_{\text{per}}(Q_\ell)} \|v\|_{L^2_{\text{per}}(Q_\ell)} \\ &+ C |\xi_1 - \xi_2| \left(\int_{Q_\ell^*} \iint_{Q_\ell \times Q_\ell} |\tilde{\gamma}_{*, \xi'}(x, y)|^2 d\xi' dx dy \right)^{1/2} \|u\|_{L^2_{\text{per}}(Q_\ell)} \|v\|_{L^2_{\text{per}}(Q_\ell)} \\ &+ C \left(\sum_{\substack{p \in \mathbb{Z}^3 \\ |p|_\infty < 2}} \int_{Q_\ell^*} \left| \frac{1}{|\xi' - \xi_1 - \frac{2\pi p}{\ell}|^2} - \frac{1}{|\xi' - \xi_2 - \frac{2\pi p}{\ell}|^2} \right| d\xi' \right) \|u\|_{L^2_{\text{per}}(Q_\ell)} \|v\|_{L^2_{\text{per}}(Q_\ell)}. \end{aligned}$$

Observe that

$$\int_{Q_\ell^*} \iint_{Q_\ell \times Q_\ell} |\tilde{\gamma}_{*, \xi'}(x, y)|^2 d\xi' dx dy = \int_{Q_\ell^*} \text{Tr}_{L^2_{\text{per}}(Q_\ell)} [\tilde{\gamma}_{*, \xi'}^2] d\xi' \leq \int_{Q_\ell^*} \text{Tr}_{L^2_{\text{per}}(Q_\ell)} [\tilde{\gamma}_{*, \xi'}] d\xi' = q,$$

since $0 \leq \gamma_* \leq 1$. Then

$$\left\| \widetilde{W}_{\gamma_*, \xi_1} - \widetilde{W}_{\gamma_*, \xi_2} \right\|_{\mathcal{B}(L^2_{\text{per}}(Q_\ell))} \leq C |\xi_1 - \xi_2| + C \sum_{\substack{p \in \mathbb{Z}^3 \\ |p|_\infty < 2}} \int_{Q_\ell^*} \left| \frac{1}{|\xi' - \xi_1 - \frac{2\pi p}{\ell}|^2} - \frac{1}{|\xi' - \xi_2 - \frac{2\pi p}{\ell}|^2} \right| d\xi'.$$

The Hölder continuity follows since the function $\xi \mapsto f_{Q_\ell^*} \frac{d\xi'}{|\xi - \xi'|^2}$ is locally a -Hölder continuous w.r.t. ξ for any $0 < a < 1$. \square

We also need the following, which adapts [12, Lemma 4] to the periodic Dirac operator. We recall that for any operator A_ξ , we have $\widetilde{A}_\xi := U_\xi^* A_\xi U_\xi$ with $U_\xi u(x) = e^{i\xi \cdot x} u(x)$ for any $x \in \mathbb{R}^3$ and u Q_ℓ -periodic.

Lemma 4.2. *Let $0 < \kappa(\alpha, c) < 1$. Consider an open subset Ω of Q_ℓ^* . Let $\epsilon > 0$ and let K be a compact set in \mathbb{C} such that $\inf_{\xi \in \Omega} d\left(K; \sigma(\widetilde{\mathcal{D}}_{\gamma_*, \xi}^c) \cap \mathbb{R}^+\right) \geq \epsilon$. Then,*

1. $\mathcal{D}^c(\widetilde{\mathcal{D}}_{\gamma_*, \xi}^c - z)^{-1}$ is bounded on $L^2_{\text{per}}(Q_\ell)$, uniformly w.r.t. $\xi \in \Omega$ and $z \in K$;
2. The map $\xi \mapsto \mathcal{D}^c(\widetilde{\mathcal{D}}_{\gamma_*, \xi}^c - z)^{-1}$ is Hölder continuous w.r.t. $\xi \in \Omega$ with values in $\mathcal{B}(L^2_{\text{per}}(Q_\ell))$, uniformly in $z \in K$.

Proof. As $\widetilde{\mathcal{D}}_\xi^c = \mathcal{D}^c + c \sum_{r=1}^3 \alpha_r \xi_r$ thanks to (2.5) and (2.8), we have, for every $\xi \in \Omega \subset Q_\ell^*$ and $z \in K$,

$$\begin{aligned} & \left\| \mathcal{D}^c(\widetilde{\mathcal{D}}_{\gamma_*, \xi}^c - z)^{-1} \right\|_{\mathcal{B}(L^2_{\text{per}}(Q_\ell))} \\ & \leq \left\| \widetilde{\mathcal{D}}_\xi^c(\widetilde{\mathcal{D}}_{\gamma_*, \xi}^c - z)^{-1} \right\|_{\mathcal{B}(L^2_{\text{per}}(Q_\ell))} + c \left\| |\xi|(\widetilde{\mathcal{D}}_{\gamma_*, \xi}^c - z)^{-1} \right\|_{\mathcal{B}(L^2_{\text{per}}(Q_\ell))} \\ & \leq \left\| \mathcal{D}_\xi^c(\mathcal{D}_{\gamma_*, \xi}^c - z)^{-1} \right\|_{\mathcal{B}(L^2_\xi(Q_\ell))} + \frac{C}{\epsilon} c. \end{aligned}$$

Thanks to (2.30) in Lemma 2.3, we have, for all $\xi \in \Omega$ and $z \in K$,

$$\begin{aligned} \left\| \mathcal{D}_\xi^c(\mathcal{D}_{\gamma_*, \xi}^c - z)^{-1} \right\|_{\mathcal{B}(L^2_\xi(Q_\ell))} & \leq \frac{1}{1 - \kappa(\alpha, c)} \left\| \mathcal{D}_{\gamma_*, \xi}^c(\mathcal{D}_{\gamma_*, \xi}^c - z)^{-1} \right\|_{\mathcal{B}(L^2_\xi(Q_\ell))} \\ & \leq \frac{1}{1 - \kappa(\alpha, c)} + \frac{|z|}{\epsilon(1 - \kappa(\alpha, c))}, \end{aligned}$$

which implies

$$\left\| \mathcal{D}^c(\widetilde{\mathcal{D}}_{\gamma_*, \xi}^c - z)^{-1} \right\|_{\mathcal{B}(L^2_{\text{per}}(Q_\ell))} \leq C, \quad \text{uniformly w.r.t. } \xi \in \Omega, z \in K.$$

The Hölder continuity follows from the fact that

$$\begin{aligned} & \mathcal{D}^c[(\mathcal{D}_{\gamma_*, \xi}^c - z)^{-1} - (\mathcal{D}_{\gamma_*, \xi'}^c - z)^{-1}] \\ & = \mathcal{D}^c(\mathcal{D}_{\gamma_*, \xi}^c - z)^{-1} [\mathcal{D}_{\gamma_*, \xi}^c - \mathcal{D}_{\gamma_*, \xi'}^c] (\mathcal{D}_{\gamma_*, \xi'}^c - z)^{-1} \\ & = [\mathcal{D}^c(\mathcal{D}_{\gamma_*, \xi}^c - z)^{-1}] \left[-ic \sum_{r=1}^3 \alpha_r (\xi_r - \xi'_r) - \widetilde{W}_{\gamma_*, \xi} + \widetilde{W}_{\gamma_*, \xi'} \right] (\mathcal{D}_{\gamma_*, \xi'}^c - z)^{-1}. \end{aligned}$$

Here $\mathcal{D}^c(\mathcal{D}_{\gamma_*, \xi}^c - z)^{-1}$ and $(\mathcal{D}_{\gamma_*, \xi'}^c - z)^{-1}$ are bounded on $L^2_{\text{per}}(Q_\ell)$, and $\xi \mapsto \widetilde{W}_{\gamma_*, \xi}$ is Hölder continuous as shown in Lemma 4.1. \square

We denote by $(\lambda_n(\xi))_{n \geq 1}$ the positive eigenvalues of $\tilde{\mathcal{D}}_{\gamma_*, \xi}^c$ counted with multiplicity, which are the same ones as the eigenvalues of the $\mathcal{D}_{\gamma_*, \xi}^c$'s since U_ξ is unitary. We may assume that the $\lambda_n(\xi)$'s are counted in nondecreasing order: $\lambda_1(\xi) \leq \lambda_2(\xi) \leq \dots$.

Arguing as in [12, Lemmas 5 and 6] and using Cauchy's formula [15], we immediately obtain the following lemma.

Lemma 4.3. *Let $0 < \kappa(\alpha, c) < 1$. For any $n \in \mathbb{N}^*$, the positive eigenvalues $(\lambda_n(\xi))_n$ of $\mathcal{D}_{\gamma_*, \xi}^c$ are Hölder continuous with respect to $\xi \in Q_\ell^*$. Moreover, let Ω be an open subset of Q_ℓ^* and $I = (a, b)$ a bounded interval of \mathbb{R}^+ such that $\sigma(\tilde{\mathcal{D}}_{\gamma_*, \xi}^c) \cap \{a, b\} = \emptyset$ for all $\xi \in \Omega$. Then, the map*

$$\Omega \ni \xi \mapsto \mathcal{D}^c \mathbb{1}_I(\tilde{\mathcal{D}}_{\gamma_*, \xi}^c) \in \mathcal{B}(L_{\text{per}}^2(Q_\ell))$$

is Hölder continuous. In particular, there exists $N \in \mathbb{N}$ independent of $\xi \in \Omega$ and an orthonormal basis $(u_1(\xi), \dots, u_N(\xi))$ of the range of $\mathbb{1}_I(\tilde{\mathcal{D}}_{\gamma_, \xi}^c)$ such that $\Omega \ni \xi \mapsto u_n(\xi) \in H_{\text{per}}^1(Q_\ell)$ is Hölder continuous w.r.t. $\xi \in \Omega$ for every $n \in \{1, \dots, N\}$.*

Indeed, as in [12], the existence of $\epsilon > 0$ and of the compact K in the statement of Lemma 4.2 is ensured by the fact that the positive eigenvalues of $\mathcal{D}_{\gamma_*, \xi}^c$ go to infinity uniformly with respect to $\xi \in Q_\ell^*$ in virtue of Lemma 2.4.

4.2 The Fermi level is either empty or totally filled.

Recall that γ_* is a minimizer of $J_{\leq q}$ satisfying the Euler–Lagrange equation (2.39) with $J_{\leq q}$ being given by (3.1) (or, equivalently (3.5)).

We argue by contradiction and assume as in [12] that $\delta \neq 0$ and $\delta \neq \mathbb{1}_{\{\nu\}}(\mathcal{D}_{\gamma_*}^c)$, and that the Lagrange multiplier ν defined in Theorem 2.7 is an eigenvalue of $\mathcal{D}_{\gamma_*}^c$ (otherwise, $\delta_\xi = 0$ for almost every $\xi \in Q_\ell^*$). Then,

$$\left| \{ \xi \in Q_\ell^* \mid \exists n \geq 1, \lambda_n(\xi) = \nu \} \right| \neq 0.$$

As in [12], we have the following lemma which is obtained without difficulty by replacing the HF operator H_{γ_*} by the DF operator $\mathcal{D}_{\gamma_*}^c$ in the proof of [12, Lemma 7].

Lemma 4.4. *Let $0 < \kappa(\alpha, c) < 1$. Assume that $\nu > 0$ is an eigenvalue of $\mathcal{D}_{\gamma_*}^c$ such that $\delta \neq 0$ and $\delta \neq \mathbb{1}_{\{\nu\}}(\mathcal{D}_{\gamma_*}^c)$. Then, there exists a constant $0 < \epsilon \leq 1$, a Borel set $\omega \subset Q_\ell^*$ with $|\omega| \neq 0$ and two continuous functions $\omega \ni \xi \mapsto u(\xi) \in H_{\text{per}}^1(Q_\ell)$ and $\omega \ni \xi \mapsto u'(\xi) \in H_{\text{per}}^1(Q_\ell)$ such that*

$$u(\xi), u'(\xi) \in \ker \left(\tilde{\mathcal{D}}_{\gamma_*, \xi}^c - \nu \right), \quad \|u(\xi)\|_{L_{\text{per}}^2(Q_\ell)} = \|u'(\xi)\|_{L_{\text{per}}^2(Q_\ell)} = 1,$$

and, denoting $\psi_\xi := U_\xi u(\xi)$ and $\psi'_\xi := U_\xi u'(\xi)$ in $H_\xi^1(Q_\ell)$, we have

$$0 \leq \delta_\xi + t |\psi_\xi\rangle \langle \psi_\xi| - t' |\psi'_\xi\rangle \langle \psi'_\xi| \leq 1 \tag{4.3}$$

on $L_\xi^2(Q_\ell)$ for all $\xi \in \omega$ and all $t, t' \in [0, \epsilon)$, where $|\psi\rangle \langle \psi|$ denotes the projector onto the vector space spanned by the function ψ .

Recall that $V_{\gamma, \xi}$ is defined in (2.19); that is,

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

The desired contradiction is based on the positivity of the second-order term shown in Theorem 3.3.

Lemma 4.5. *Let $0 < \alpha \leq 1$ and $c \geq 1$. Assume that ν is an eigenvalue of $\mathcal{D}_{\gamma_*}^c$ given by (3.2), that $\delta \neq 0$ and $\delta \neq \mathbb{1}_{\{\nu\}}(\mathcal{D}_{\gamma_*}^c)$, and let ω , ψ_ξ and ψ'_ξ be as in Lemma 4.4. Then, there exists $R > 1$ such that if α and c satisfy*

$$c \geq 2(C_G z + C_{EE} q) \quad \text{and} \quad \frac{\alpha}{c} \leq \frac{1}{4C_{EE}R}, \quad (4.4)$$

we have

$$\gamma_*, \gamma_* + th \in \mathcal{U}_R, \quad \text{provided} \quad |t| \leq \min \left\{ \frac{\epsilon}{\max\{\|\eta\|_{L^\infty}; \|\eta'\|_{L^\infty}\}}; 1 \right\}$$

where the periodic density matrix $h = \int_{Q_\ell^*}^\oplus h_\xi d\xi$ is defined by

$$h_\xi = \eta(\xi) |\psi_\xi\rangle \langle \psi_\xi| - \eta'(\xi) |\psi'_\xi\rangle \langle \psi'_\xi|,$$

with η and $\eta' \in L^\infty(\omega, \mathbb{R}^+)$ satisfying $\int_\omega \eta = \int_\omega \eta'$ and $\psi|_{Q_\ell^* \setminus \omega} = \psi'|_{Q_\ell^* \setminus \omega} = 0$.

Furthermore, for $|t| \leq \min \left\{ \frac{\epsilon}{\max\{\|\eta\|_{L^\infty}; \|\eta'\|_{L^\infty}\}}; 1 \right\}$, we also have

$$\frac{\alpha}{2} \widetilde{\text{Tr}}_{L^2}[V_h h] + \frac{\alpha^2}{c^2} \text{Err}(t, \gamma_*, h) \geq 0. \quad (4.5)$$

In above inequality, $\text{Err}(t, \gamma_*, h)$ is defined in Theorem 3.3 and satisfies

$$|\text{Err}(t, \gamma_*, h)| \leq \left(2 + \frac{\epsilon P}{c^2}\right) \mathcal{N}_{\gamma_* + th}(h).$$

Proof. In this proof, we denote by C various positive constants that are independent of α and c . Let $t_0 := \min \left\{ \frac{\epsilon}{\max\{\|\eta\|_{L^\infty}; \|\eta'\|_{L^\infty}\}}; 1 \right\}$ where ϵ is defined in Lemma 4.4. Let

$$R := 1 + K_q^{1/2} q + C_Y + 16 C_{EE} (1 + C_Y)^2 K_q^{3/2} q^+ \quad (4.6)$$

with K_q being defined in Lemma 2.5 and C_Y in Eq. (2.14). Before going further, we shall point out that (4.4) implies that

$$\kappa(\alpha, c) \leq \frac{C_G z + C_{EE} \alpha q}{c} \leq \frac{1}{2}$$

and

$$L(\alpha, c) = 2A(\alpha, c)R = \frac{\alpha}{c} \frac{C_{EE}}{(1 - \kappa(\alpha, c))} R \leq \frac{1}{2},$$

since $\alpha \leq 1$ and $c \geq 1$. In particular, the assumptions of Lemma 2.5 are satisfied with $\gamma = \gamma' = \gamma_*$, and we have

$$\|\gamma_*\|_X \leq K_q q. \quad (4.7)$$

We first check that $\gamma_* \in \mathcal{U}_R$. Recall that \mathcal{U}_R is defined by Eq. (3.7). Thanks to (4.7) and using the Cauchy–Schwarz inequality in $\mathfrak{S}_{2,2}$, we obtain

$$\frac{1}{c} \|\gamma_* |\mathcal{D}^c|^{1/2}\|_{\mathfrak{S}_{1,1}} \leq \frac{1}{c} \|\gamma_*\|_{\mathfrak{S}_{1,1}}^{1/2} \|\gamma_*\|_{X_c}^{1/2} \leq \|\gamma_*\|_{\mathfrak{S}_{1,1}}^{1/2} \|\gamma_*\|_X^{1/2} \leq K_q^{1/2} q \quad (4.8)$$

and

$$\|\gamma_*\|_Y \leq \|\gamma_*\|_Y \int_{Q_\ell^*} \frac{d\xi}{|\xi|^2} \leq C_Y.$$

Thus, since $T(\gamma_*) = \gamma_*$,

$$\begin{aligned} \frac{1}{c} \max \left\{ \|\gamma_* | \mathcal{D}^c |^{1/2} \|_{\mathfrak{S}_{1,1}}; \|\gamma_*\|_{\mathcal{Y}} \right\} + \frac{M}{c^2} \|T(\gamma_*) - \gamma_*\|_{X_c \cap \mathcal{Y}_c} \\ = \frac{1}{c} \max \left\{ \|\gamma_* | \mathcal{D}^c |^{1/2} \|_{\mathfrak{S}_{1,1}}; \|\gamma_*\|_{\mathcal{Y}} \right\} \leq K_q^{1/2} q + C_{\mathcal{Y}} < R. \end{aligned}$$

This implies $\gamma_* \in \mathcal{U}_R$.

We now show that $\gamma_* + th \in \mathcal{U}_R$. For any $t \in [-t_0, t_0]$, $\gamma_* + th \in \Gamma_{\leq q}$ and $0 \leq \gamma_* + th \leq \mathbb{1}_{(0, \nu]}(\mathcal{D}_{\gamma_*}^c)$ with $\nu \leq c^2 + \Sigma([q])$ thanks to Lemma 2.4. In particular, in virtue of Eq. (2.37) in Lemma 2.5,

$$\|\gamma_* + th\|_X \leq K_q q.$$

By repeating the above estimate for γ_* , we obtain

$$\frac{1}{c} \|(\gamma_* + th) | \mathcal{D}^c |^{1/2} \|_{\mathfrak{S}_{1,1}} \leq K_q^{1/2} q \quad \text{and} \quad \|\gamma_* + th\|_{\mathcal{Y}} \leq C_{\mathcal{Y}}.$$

Note that $P_{\gamma_*}^+(\gamma_* + th)P_{\gamma_*}^+ = \gamma_* + th$ from the definition of h . Applying Lemma 6.5 below with $g = \gamma_*$ and $\gamma = \gamma_* + th$ then leads to

$$\begin{aligned} \frac{1}{c^2} \|T(\gamma_* + th) - \gamma_* - th\|_{X_c} &\leq 4C_{EE} |t| \frac{\alpha}{c^3} \int_{Q_\ell^*} \|h\|_{X \cap \mathcal{Y}(\xi)} \|\gamma_{*, \xi} | \mathcal{D}_\xi^c |^{1/2} \|_{\mathfrak{S}_1(\xi)} d\xi \\ &\leq 4C_{EE} t_0 \frac{\alpha}{c^3} \|h\|_{X \cap \mathcal{Y}} \|\gamma_* | \mathcal{D}^c |^{1/2} \|_{\mathfrak{S}_{1,1}} \\ &\leq 8C_{EE} (1 + C_{\mathcal{Y}}) K_q^{3/2} \frac{\alpha}{c^2} q, \end{aligned}$$

since $\lambda_0(\alpha, c) \geq 1 - \kappa(\alpha, c) \geq \frac{1}{2}$, and

$$\frac{1}{c^2} \|T(\gamma_* + th) - \gamma_* - th\|_{\mathcal{Y}_c} \leq 4C_{EE} C_{\mathcal{Y}} t_0 \frac{\alpha}{c^3} \|h\|_{X \cap \mathcal{Y}} \leq 8C_{EE} C_{\mathcal{Y}} (1 + C_{\mathcal{Y}}) K_q \frac{\alpha}{c^2},$$

since, according to Lemma 2.5 and because $K_q \geq 1$, we have

$$|t| \|h\|_{X \cap \mathcal{Y}(\xi)} \leq (1 + C_{\mathcal{Y}}) |t| \|h\|_{X \cap \mathcal{Y}} \leq 2(1 + C_{\mathcal{Y}}) t_0 \max \{ \|\eta\|_{L^\infty}; \|\eta'\|_{L^\infty} \} K_q \leq 2(1 + C_{\mathcal{Y}}) K_q.$$

According to the definition of $M(\alpha, c)$ in Lemma 3.2, it is easy to see that $M(\alpha, c) \leq 2$. Thus,

$$\frac{M(\alpha, c)}{c^2} \|T(\gamma_* + th) - \gamma_* - th\|_{X_c \cap \mathcal{Y}_c} \leq 16C_{EE} (1 + C_{\mathcal{Y}})^2 K_q^{3/2} q^+ \frac{\alpha}{c^2}. \quad (4.9)$$

We conclude that

$$\begin{aligned} \frac{1}{c} \max \left\{ \|(\gamma_* + th) | \mathcal{D}^c |^{1/2} \|_{\mathfrak{S}_{1,1}}; \|\gamma_* + th\|_{\mathcal{Y}} \right\} + \frac{M(\alpha, c)}{c^2} \|T(\gamma_* + th) - \gamma_* - th\|_{X_c \cap \mathcal{Y}_c} \\ \leq K_q^{1/2} q + C_{\mathcal{Y}} + 16C_{EE} (1 + C_{\mathcal{Y}})^2 K_q^{3/2} q^+ \frac{\alpha}{c^2} < R. \end{aligned} \quad (4.10)$$

Thus, $\gamma_* + th \in \mathcal{U}_R$.

Next, from Lemma 3.2, the limit $\theta(\gamma)$ exists for any $\gamma \in \mathcal{U}_R$. Hence $E(\gamma_*)$ and $E(\gamma_* + th)$ are well-defined. Then, from Eq. (3.5) and Theorem 3.1, we have, for any $t \in [-t_0, t_0]$,

$$E(\gamma_* + th) \geq \min_{\gamma \in \mathcal{U}_R} E(\gamma) = E(\gamma_*).$$

By definition of γ_* and h , we also have

$$\int_{Q_\ell^*} \text{Tr}_{L_\xi^2} [(\mathcal{D}_{\gamma_*, \xi}^c - \epsilon_P) h_\xi] d\xi = 0.$$

Finally, we deduce from Theorem 3.3 that

$$\frac{\alpha}{2} \widetilde{\text{Tr}}_{L^2}[V_h h] + \frac{\alpha^2}{c^2} \text{Err}(t, \gamma_*, h) \geq 0$$

with $|\text{Err}(t, \gamma_*, h)| \leq (2 + \frac{\epsilon_P}{c^2}) \mathcal{N}_{\gamma_*+th}(h)$. This ends the proof. \square

Let $B(\xi, \lambda)$ denote the ball of radius $\lambda > 0$ centered at $\xi \in \mathbb{R}^3$. As $|\omega| \neq 0$, we may find two points ξ_1 and ξ_2 in ω such that $|\omega \cap B(\xi_j, \lambda)| \neq 0$ for $j = 1, 2$. In particular, for λ small enough, we have $\omega \cap B(\xi_j, \lambda) = B(\xi_j, \lambda)$. As in [12], we introduce the operator $h^\lambda = \int_{Q_\ell^*}^\oplus h_\xi^\lambda d\xi$ defined by

$$h_\xi^\lambda := \eta_\lambda(\xi) |\psi_\xi\rangle \langle \psi_\xi| - \eta'_\lambda(\xi) |\psi'_\xi\rangle \langle \psi'_\xi|$$

for every $\xi \in Q_\ell^*$, where

$$\eta_\lambda = \frac{\mathbb{1}_{\omega \cap B(\xi_1, \lambda)}}{|\omega \cap B(\xi_1, \lambda)|} \quad \text{and} \quad \eta'_\lambda = \frac{\mathbb{1}_{\omega \cap B(\xi_2, \lambda)}}{|\omega \cap B(\xi_2, \lambda)|}.$$

As shown in the proof of [12, Lemma 9], for λ small enough we have

$$\widetilde{\text{Tr}}_{L^2}[V_{h^\lambda} h^\lambda] \leq C - \frac{4\pi}{\lambda^2}. \quad (4.11)$$

On the other hand, we have the following.

Lemma 4.6. *Let*

$$C_{\text{cri}}(q, z) := \max \left\{ 16\pi C_{EE} R; \right. \\ \left. 48 C_{EE}^2 (4 + \Sigma_{[q]}) \left(|Q_\ell^*|^{-1} \mathfrak{N}_{[q]} (|Q_\ell^*|^{-1} K_q + C_y) + 2^{13/2} \times 15\pi^6 (C_{EE} + 1) C_{EE} \right) \right\}$$

with the constants $\Sigma_{[q]} \in \mathbb{R}^+$ and $\mathfrak{N}_{[q]} \in \mathbb{N}^*$ being given in Lemma 2.4, $K_q \in \mathbb{R}^+$ being given by (2.36), and R being given as in (4.6).

Then there exists a constant $C > 0$ such that for any $\frac{\alpha}{c} \leq \frac{2\pi}{C_{\text{cri}}}$, $c \geq 2(C_G z + C_{EE} q)$ and any λ small enough,

$$\limsup_{t \rightarrow 0} |\text{Err}(t, \gamma_*, h^\lambda)| \leq \left(2 + \frac{\epsilon_P}{c^2} \right) \mathcal{N}_{\gamma_*}(h^\lambda) \leq C + \frac{C_{\text{cri}}(q, z)}{\lambda^2}$$

where Err and \mathcal{N} are defined by Eqs. (3.10) and (3.11) respectively.

Proof. In this proof, C denotes various positive constants that are independent of α , c , and λ .

As $C_{\text{cri}}(q, z) \geq 16\pi C_{EE} R$, we have

$$\frac{\alpha}{c} \leq \frac{4\pi}{C_{\text{cri}}(q, z)} \leq \frac{1}{4C_{EE} R}. \quad (4.12)$$

Thus Lemma 4.5 holds, and $\kappa(\alpha, c) \leq \frac{1}{2}$ and $L(\alpha, c) \leq \frac{1}{2}$. As a result, from Lemma 4.5, we infer $\limsup_{t \rightarrow 0} |\text{Err}(t, \gamma_*, h^\lambda)| \leq (2 + \frac{\epsilon_P}{c^2}) \mathcal{N}_{\gamma_*}(h^\lambda)$ for any $\lambda > 0$. In addition, according to Theorem 3.1 and Lemma 2.4, $(2 + \frac{\epsilon_P}{c^2}) \leq 4 + \Sigma_{[q]}$. Hence,

$$\limsup_{t \rightarrow 0} |\text{Err}(t, \gamma_*, h^\lambda)| \leq (2 + \frac{\epsilon_P}{c^2}) \mathcal{N}_{\gamma_*}(h^\lambda) \leq (4 + \Sigma_{[q]}) \mathcal{N}_{\gamma_*}(h^\lambda).$$

We then prove that the three terms appearing in $\mathcal{N}_{\gamma_*}(h^\lambda)$ satisfy respectively

$$\frac{1}{c} \int_{Q_\ell^*} \|h^\lambda\|_{X \cap \mathcal{Y}(\xi)} \|\gamma_{*, \xi}\|_{\mathcal{D}_\xi^c}^{1/2} \|\mathfrak{S}_1(\xi)\| d\xi \leq 2 K_q \mathfrak{N}_{[q]} (|Q_\ell^*|^{-1} K_q + C_y), \quad (4.13)$$

$$\int_{Q_\ell^*} \|h^\lambda\|_{X \cap \mathcal{Y}(\xi)}^2 \|\gamma_{*,\xi}\|_{\mathfrak{S}_1(\xi)} d\xi \leq 12 |Q_\ell^*|^{-1} \mathfrak{N}_{[q]} (|Q_\ell^*|^{-1} K_q + C_Y) \lambda^{-2} \quad (4.14)$$

and

$$\sup_{\xi \in Q_\ell^*} \sup_{\substack{k \in \mathbb{Z}^3 \\ |k|_\infty \leq 1}} \int_{Q_\ell^* + \frac{2\pi k}{\ell}} \frac{\|h^\lambda\|_{X \cap \mathcal{Y}(\xi')}}{|\xi - \xi'|^2} d\xi' \leq 3\pi^3 \lambda^{-1}, \quad (4.15)$$

for λ small enough. Once the above estimates are established, using Eq. (4.12) to get $4 R_c^\alpha C_{EE} \leq 1$ and the hypothesis $2 C_{EE} q c^{-1} \leq 1$, a tedious but easy calculation leads to

$$\mathcal{N}_{\gamma_*}(h^\lambda) \leq C + 48 C_{EE}^2 \left(|Q_\ell^*|^{-1} \mathfrak{N}_{[q]} (|Q_\ell^*|^{-1} K_q + C_Y) + 2^{13/2} \times 15\pi^6 (C_{EE} + 1) C_{EE} \right) \lambda^{-2}$$

since $\frac{1}{2} \leq 1 - L(\alpha, c) \leq 1$ and $\frac{1}{2} \leq 1 - \kappa(\alpha, c) \leq \lambda_0(\alpha, c) \leq 1$ independently of α and c . We therefore focus on the proof of Eqs. (4.13)–(4.15).

According to Theorem 3.1, $0 \leq \gamma_* \leq 1_{(0,\nu]}(\mathcal{D}_{\gamma_*}^c)$. As $\nu \leq \overline{\Lambda_{[q]}}$, we have $\text{Rank}(\gamma_{*,\xi}) \leq \mathfrak{N}_{[q]}$ by Lemma 2.4. Thus,

$$\|\gamma_{*,\xi}\|_{\mathfrak{S}_1(\xi)} \leq \text{Rank}(\gamma_{*,\xi}) \leq \mathfrak{N}_{[q]}. \quad (4.16)$$

On the other hand, we write $\gamma_{*,\xi} = \sum_{n=1}^{\mathfrak{N}_{[q]}} \mu_n(\xi) |\psi_n(\xi)\rangle \langle \psi_n(\xi)|$ with $0 \leq \mu_n(\xi) \leq 1$ and with $\psi_n(\xi)$ being a normalized eigenfunction of $\mathcal{D}_{\gamma_{*,\xi}}^c$ associated to the eigenvalue $0 \leq \lambda_n(\xi) \leq \overline{\Lambda_{[q]}}$. By Eq. (2.30) and Lemma 2.5, we finally get

$$\frac{1}{c} \|\gamma_{*,\xi} |\mathcal{D}_\xi^c|^{1/2}\|_{\mathfrak{S}_1(\xi)} \leq \|\gamma_{*,\xi} (1 - \Delta_\xi)^{1/4}\|_{\mathfrak{S}_1(\xi)} \leq \sum_{n=1}^{\mathfrak{N}_{[q]}} \|\psi_n(\xi)\|_{H_\xi^{1/2}(Q_\ell)}^2 \leq K_q \mathfrak{N}_{[q]} \quad (4.17)$$

by the interpolation inequality to obtain the $H^{1/2}$ norm. It is easy to see that

$$\|h^\lambda\|_X \leq |Q_\ell^*|^{-1} \int_{\omega \cap B(\xi_1, \lambda)} \|\psi_\xi\|_{H_\xi^{1/2}}^2 d\xi + |Q_\ell^*|^{-1} \int_{\omega \cap B(\xi_2, \lambda)} \|\psi'_\xi\|_{H_\xi^{1/2}}^2 d\xi. \quad (4.18)$$

By Lemma 2.5 again, this leads to

$$\|h^\lambda\|_X \leq 2|Q_\ell^*|^{-1} K_q. \quad (4.19)$$

We now turn to the study of the term $\|h^\lambda\|_{\mathcal{Y}(\xi)}$. First, as $\omega \cap B(\xi_j, \lambda) = B(\xi_j, \lambda)$ for λ small enough, and by (2.13) and the rearrangement inequality,

$$\|h^\lambda\|_{\mathcal{Y}(\xi)} = \sup_{\substack{k \in \mathbb{Z}^3 \\ |k|_\infty \leq 1}} \int_{Q_\ell^* + \frac{2\pi k}{\ell}} \frac{\|h_{\xi'}^\lambda\|_{\mathcal{B}(L_{\xi'}^2)}}{|\xi - \xi'|^2} d\xi' \leq |Q_\ell^*|^{-1} \sum_{j=1,2} \int_{\omega \cap B(\xi_j, \lambda)} \frac{d\xi'}{|\xi - \xi'|^2} \quad (4.20)$$

$$= 2|Q_\ell^*|^{-1} \int_{B(0, \lambda)} \frac{d\xi'}{|\xi'|^2} = 6|Q_\ell^*|^{-1} \lambda^{-2}. \quad (4.21)$$

Thus by (2.13), (4.17), (4.19) and (4.20), we know that

$$\begin{aligned} & \frac{1}{c} \int_{Q_\ell^*} \|h\|_{X \cap \mathcal{Y}(\xi)} \|\gamma_{*,\xi} |\mathcal{D}_\xi^c|^{1/2}\|_{\mathfrak{S}_1(\xi)} d\xi \\ & \leq 2|Q_\ell^*|^{-1} K_q^2 \mathfrak{N}_{[q]} + K_q \mathfrak{N}_{[q]} \sum_{k=1,2} \int_{\omega \cap B(\xi_k, \lambda)} \int_{Q_\ell^*} \frac{1}{|\xi - \xi'|^2} d\xi d\xi' \\ & = 2 K_q \mathfrak{N}_{[q]} (|Q_\ell^*|^{-1} K_q + C_Y). \end{aligned}$$

This gives (4.13) for λ small enough.

Analogously, arguing as above and using Eq.(4.16) instead of Eq.(4.17),

$$\int_{Q_\ell^*} \|h^\lambda\|_{X \cap \mathcal{Y}(\xi)} \|\gamma_{*,\xi}\|_{\mathfrak{S}_1(\xi)} d\xi \leq 2\mathfrak{N}_{|q|} (|Q_\ell^*|^{-1}K_q + C_\mathcal{Y}).$$

To prove (4.14), we observe that, for λ small enough, by (4.19) and (4.21),

$$\|h^\lambda\|_{X \cap \mathcal{Y}(\xi)} \leq \|h^\lambda\|_{X \cap \mathcal{Y}} \leq 6|Q_\ell^*|^{-1}\lambda^{-2}, \quad (4.22)$$

for λ small enough and for all $\xi \in Q_\ell^*$. Therefore,

$$\begin{aligned} \int_{Q_\ell^*} \|h^\lambda\|_{X \cap \mathcal{Y}(\xi)}^2 \|\gamma_{*,\xi}\|_{\mathfrak{S}_1(\xi)} d\xi &\leq \|h^\lambda\|_{X \cap \mathcal{Y}} \int_{Q_\ell^*} \|h^\lambda\|_{X \cap \mathcal{Y}(\xi)} \|\gamma_{*,\xi}\|_{\mathfrak{S}_1(\xi)} d\xi \\ &\leq 12|Q_\ell^*|^{-1}\mathfrak{N}_{|q|} (|Q_\ell^*|^{-1}K_q + C_\mathcal{Y})\lambda^{-2}. \end{aligned}$$

We now turn to the last estimate, i.e., Eq. (4.15). From (4.19), we have

$$\sup_{\xi \in Q_\ell^*} \int_{Q_\ell^* + \frac{2\pi k}{\ell}} \frac{\|h^\lambda\|_X}{|\xi - \xi'|^2} d\xi' \leq 2|Q_\ell^*|^{-1}C_\mathcal{Y}K_q.$$

On the other hand, according to [17, Chapter 5.10, Formula (3)],

$$\int_{\mathbb{R}^3} \frac{d\xi'}{|\xi - \xi'|^2 |\xi' - \xi''|^2} = \frac{\pi^3}{|\xi - \xi''|}.$$

Hence, for λ small enough,

$$\begin{aligned} &\sup_{\xi \in Q_\ell^*} \sup_{\substack{k \in \mathbb{Z}^3 \\ |k|_\infty \leq 1}} \int_{Q_\ell^* + \frac{2\pi k}{\ell}} \frac{\|h^\lambda\|_{\mathcal{Y}(\xi')} }{|\xi - \xi'|^2} d\xi' \\ &\leq \sum_{j=1,2} \sup_{\xi \in Q_\ell^*} \int_{\omega \cap B(\xi_j, \lambda)} d\xi'' \int_{Q_\ell^*} \frac{d\xi'}{|\xi - \xi'|^2 |\xi' - \xi''|^2} \\ &\leq \pi^3 \sum_{j=1,2} \sup_{\xi \in Q_\ell^*} \int_{\omega \cap B(\xi_j, \lambda)} \frac{d\xi''}{|\xi - \xi''|} \leq 2\pi^3 \int_{B(0, \lambda)} \frac{d\xi}{|\xi_j|} \leq 3\pi^3 \lambda^{-1}. \end{aligned}$$

Thus for λ small enough, we deduce

$$\sup_{\xi \in Q_\ell^*} \int_{Q_\ell^*} \frac{\|h^\lambda\|_{X \cap \mathcal{Y}(\xi')}}{|\xi - \xi'|^2} d\xi' \leq 3\pi^3 \lambda^{-1}.$$

This ends the proof of Lemma 4.6. \square

We turn now to the proof of Theorem 2.10.

Proof of Theorem 2.10. Indeed, by using Eq. (4.11) and Lemma 4.6, under Assumption 2.8 we get

$$\limsup_{t \rightarrow 0} \left(\frac{\alpha}{2} \widetilde{\text{Tr}}_{L^2} [V_{h^\lambda} h^\lambda] + \frac{\alpha^2}{c^2} \text{Err}(t, \gamma_*, h^\lambda) \right) \leq C + \frac{C_{\text{cri}}(q, z) \alpha^2 c^{-2} - 2\pi\alpha}{\lambda^2}.$$

Thus, for $\alpha > 0$ and $\frac{\alpha}{c}$ small enough satisfying

$$\frac{\alpha}{c} < \frac{2\pi}{C_{\text{cri}}(q, z)}, \quad (4.23)$$

we have

$$\lim_{\lambda \rightarrow 0} \lim_{t \rightarrow 0} \left(\frac{\alpha}{2} \widetilde{\text{Tr}}_{L^2} [V_{h^\lambda} h^\lambda] + \frac{\alpha^2}{c^2} \text{Err}(t, \gamma_*, h^\lambda) \right) \leq C + \lim_{\lambda \rightarrow 0} \frac{(C_{\text{cri}}(q, z) \frac{\alpha}{c} - 2\pi) \alpha}{\lambda^2} = -\infty.$$

We reach a contradiction with (4.5) whenever Assumption 2.8 is satisfied. The proof of Theorem 2.10 is now complete. \square

5 Existence of the retraction

In this section, we argue as in [9, Proposition 5.8] and [23] to give a sketch of the proof of Lemma 3.2. It is based on the following result.

Lemma 5.1. *Let $0 < \kappa(\alpha, c) < 1$. Recall that $A(\alpha, c) := \frac{\alpha}{2c} C_{EE} (1 - \kappa(\alpha, c))^{-1/2} \lambda_0(\alpha, c)^{-1/2}$. Then for any $\gamma, \gamma' \in \Gamma_{\leq q}$ and $\xi \in Q_\ell^*$, we have*

$$\| |\mathcal{D}_\xi^c|^{1/2} (P_{\gamma, \xi}^+ - P_{\gamma', \xi}^+) \|_{\mathcal{B}(L_\xi^2)} \leq \frac{A(\alpha, c)}{(1 + C_Y)} \|\gamma - \gamma'\|_{X \cap \mathcal{Y}(\xi)} \leq \frac{A(\alpha, c)}{c(1 + C_Y)} \|\gamma - \gamma'\|_{X_c \cap \mathcal{Y}_c(\xi)} \quad (5.1)$$

and

$$\begin{aligned} \|T^2(\gamma) - T(\gamma)\|_{X_c \cap \mathcal{Y}_c} &\leq 2A(\alpha, c) \left(\frac{1}{c} \max \left\{ \|T(\gamma) |\mathcal{D}^c|^{1/2}\|_{\mathfrak{S}_{1,1}}; \|\gamma\|_{\mathcal{Y}} \right\} \right. \\ &\quad \left. + \frac{A(\alpha, c) q^+}{c^2} \|T(\gamma) - \gamma\|_{X_c \cap \mathcal{Y}_c} \right) \|\gamma - \gamma'\|_{X_c \cap \mathcal{Y}_c}. \end{aligned} \quad (5.2)$$

Proof. By Taylor's formula, we have

$$P_\gamma^\pm = \frac{1}{2} \pm \frac{1}{2\pi} \int_{-\infty}^{+\infty} (\mathcal{D}_\gamma^c - iz)^{-1} dz. \quad (5.3)$$

Thus,

$$P_\gamma^\pm - P_{\gamma'}^\pm = \pm \frac{\alpha}{2\pi} \int_{-\infty}^{+\infty} (\mathcal{D}_\gamma^c - iz)^{-1} V_{\gamma - \gamma'} (\mathcal{D}_{\gamma'}^c - iz)^{-1} dz.$$

Now, according to Eqs. (2.26), (2.31) and (2.33) and by using the formula

$$\int_{-\infty}^{+\infty} \frac{B}{B^2 + z^2} dz = \pi, \quad \text{when } B > 0, \quad (5.4)$$

we obtain, for any $\psi_\xi, \phi_\xi \in L_\xi^2$,

$$\begin{aligned} &\left| \left(\psi_\xi, |\mathcal{D}_\xi^c|^{1/2} (P_{\gamma, \xi}^+ - P_{\gamma', \xi}^+) \phi_\xi \right)_{L_\xi^2} \right| \\ &= \frac{\alpha}{2\pi} \left| \int_{-\infty}^{+\infty} \left(\psi_\xi, |\mathcal{D}_\xi^c|^{1/2} (\mathcal{D}_{\gamma, \xi}^c - iz)^{-1} V_{\gamma - \gamma', \xi} (\mathcal{D}_{\gamma', \xi}^c - iz)^{-1} \phi_\xi \right)_{L_\xi^2} dz \right| \\ &\leq \frac{\alpha}{2\pi} \|V_{\gamma - \gamma', \xi}\|_{\mathcal{B}(L_\xi^2)} \left(\int_{-\infty}^{+\infty} \|(\mathcal{D}_{\gamma, \xi}^c - iz)^{-1} |\mathcal{D}_\xi^c|^{1/2} \psi_\xi\|_{L_\xi^2}^2 dz \right)^{1/2} \\ &\quad \times \left(\int_{-\infty}^{+\infty} \|(\mathcal{D}_{\gamma', \xi}^c - iz)^{-1} \phi_\xi\|_{L_\xi^2}^2 dz \right)^{1/2} \\ &\leq \frac{\alpha}{2} \|V_{\gamma - \gamma'}\|_Y \| |\mathcal{D}^c|^{1/2} |\mathcal{D}_\gamma^c|^{-1/2} \|_Y \| |\mathcal{D}_{\gamma'}^c|^{-1/2} \|_Y \|\psi_\xi\|_{L_\xi^2} \|\phi\|_{L_\xi^2} \\ &\leq \frac{C_{EE}}{2(1 + C_Y)} (1 - \kappa(\alpha, c))^{-1/2} \lambda_0(\alpha, c)^{-1/2} \frac{\alpha}{c} \|\gamma - \gamma'\|_{X \cap \mathcal{Y}} \|\psi\|_{L_\xi^2} \|\phi\|_{L_\xi^2} \end{aligned}$$

$$\leq \frac{C_{EE}}{2(1+C_Y)} (1 - \kappa(\alpha, c))^{-1/2} \lambda_0(\alpha, c)^{-1/2} \frac{\alpha}{c^2} \|\gamma - \gamma'\|_{X_c \cap \mathcal{Y}_c} \|\psi\|_{L_\xi^2} \|\phi\|_{L_\xi^2}.$$

Then Eq. (5.1) follows. We now turn to the proof of (5.2). We have

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

Hence,

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

Since $c^2 \leq |\mathcal{D}^c|$, we have

$$\|T(\gamma) (P_{T(\gamma)}^+ - P_\gamma^+)\|_{X_c \cap \mathcal{Y}_c} \leq \|\mathcal{D}^c\|^{1/2} (P_{T(\gamma)}^+ - P_\gamma^+)\|_Y \max \left\{ \|T(\gamma)\|_{\mathfrak{S}_{1,1}} \|\mathcal{D}^c\|^{1/2}; \|T(\gamma)\|_{\mathcal{Y}} \right\}$$

and

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

Observe from (2.14) that $\|T(\gamma)\|_{\mathfrak{S}_{1,1}} \leq \|\gamma\|_{\mathfrak{S}_{1,1}} \leq q$ and $\|T(\gamma)\|_{\mathcal{Y}} \leq \|\gamma\|_{\mathcal{Y}} \leq C_Y$, from which we deduce that $\|T(\gamma)\|_{\mathfrak{S}_{1,1} \cap \mathcal{Y}} \leq (1 + C_Y) q^+$. Then, using (5.1), we obtain

$$\begin{aligned} \|T^2(\gamma) - T(\gamma)\|_{X_c \cap \mathcal{Y}_c} &\leq 2 A(\alpha, c) \left(\frac{1}{c} \max \left\{ \|T(\gamma)\|_{\mathfrak{S}_{1,1}} \|\mathcal{D}^c\|^{1/2}; \|T(\gamma)\|_{\mathcal{Y}} \right\} \right. \\ &\quad \left. + \frac{A(\alpha, c) q^+}{2c^2} \|\gamma - T(\gamma)\|_{X_c \cap \mathcal{Y}_c} \right) \|\gamma - T(\gamma)\|_{X_c \cap \mathcal{Y}_c}. \end{aligned}$$

□

We turn now to the following.

Proof of Lemma 3.2. First of all, we observe that $T(\gamma) \leq \gamma \leq \mathbb{1}_{L^2(\mathbb{R}^3)}$, $\|T(\gamma)\|_{\mathfrak{S}_{1,1}} \leq \|\gamma\|_{\mathfrak{S}_{1,1}} \leq q$ and $\|T(\gamma)\|_{\mathcal{Y}} \leq \|\gamma\|_{\mathcal{Y}}$. Then, from (2.32),

$$\|T(\gamma)\|_X \leq \frac{1 - \kappa(\alpha, c)}{1 + \kappa(\alpha, c)} \|\gamma\|_X.$$

Therefore, $T(\gamma) \in \Gamma_{\leq q}$. We are going to prove that T maps \mathcal{U}_R into \mathcal{U}_R . For $\gamma \in \mathcal{U}_R$, we have

$$\|T(\gamma)\|_{\mathfrak{S}_{1,1}} \|\mathcal{D}^c\|^{1/2} \leq \|\gamma\|_{\mathfrak{S}_{1,1}} \|\mathcal{D}^c\|^{1/2} + \frac{1}{c} \|\gamma - T(\gamma)\|_{X_c}. \quad (5.5)$$

As $M(\alpha, c) \geq \frac{1 + A(\alpha, c) q^+}{2}$, (5.2) implies

$$\|T^2(\gamma) - T(\gamma)\|_{X_c} \leq L(\alpha, c) \|T(\gamma) - \gamma\|_{X_c} \quad (5.6)$$

with $L(\alpha, c) = 2A(\alpha, c)R$ and

$$\frac{1}{c} \|T(\gamma)\|_{\mathcal{Y}} \leq \frac{1}{c} \|\gamma\|_{\mathcal{Y}} + \frac{1}{c^2} \|T(\gamma) - \gamma\|_{\mathcal{Y}_c}. \quad (5.7)$$

Moreover, as $M(\alpha, c) \geq \frac{1}{1 - 2A(\alpha, c)R}$, we have $1 + M(\alpha, c) L(\alpha, c) \leq M$. Then, from Eqs. (5.5)-(5.7) and the fact that $\gamma \in \mathcal{U}_R$,

$$\frac{1}{c} \max \left\{ \|T(\gamma)\|_{\mathfrak{S}_{1,1}} \|\mathcal{D}^c\|^{1/2}; \|T(\gamma)\|_{\mathcal{Y}} \right\} + \frac{M(\alpha, c)}{c^2} \|T^2(\gamma) - T(\gamma)\|_{X_c \cap \mathcal{Y}_c}$$

$$\leq \frac{1}{c} \max \left\{ \|\gamma|D^c|^{1/2}\|_{\mathfrak{S}_{1,1}}; \|\gamma\|_{\mathcal{Y}} \right\} + \frac{1 + M(\alpha, c) L(\alpha, c)}{c^2} \|\gamma - T(\gamma)\|_{X_c \cap \mathcal{Y}_c} < R.$$

Therefore, $T(\gamma) \in \mathcal{U}_R$. Thus, T maps \mathcal{U}_R into \mathcal{U}_R , and so does T^n for any $n \in \mathbb{N}$.

Next, we prove the existence of θ . From (5.2), we know

$$\|T^n(\gamma) - T^{n-1}(\gamma)\|_{X_c \cap \mathcal{Y}_c} \leq L(\alpha, c) \|T^{n-1}(\gamma) - T^{n-2}(\gamma)\|_{X_c \cap \mathcal{Y}_c} \quad (5.8)$$

and

$$\|T^n(\gamma)\|_{X_c \cap \mathcal{Y}_c} \leq \sum_{i=1}^n \|T^i(\gamma) - T^{i-1}(\gamma)\|_{X_c \cap \mathcal{Y}_c} + \|\gamma\|_X \leq \frac{1}{1 - L(\alpha, c)} \|T(\gamma) - \gamma\|_{X_c \cap \mathcal{Y}_c} + \|\gamma\|_{X_c \cap \mathcal{Y}_c}.$$

This implies that $\|T^n(\gamma)\|_{X_c \cap \mathcal{Y}_c}$ is uniformly bounded with respect to $n \in \mathbb{N}$, and $(T^n(\gamma))_n$ is a Cauchy sequence in $X_c \cap \mathcal{Y}_c$. Thus, for any $\gamma \in \mathcal{U}_R$, the retraction $\theta(\gamma) := \lim_{n \rightarrow +\infty} T^n(\gamma)$ exists in $X_c \cap \mathcal{Y}_c$. Furthermore, we have

$$\|\theta(\gamma) - T^n(\gamma)\|_{X_c \cap \mathcal{Y}_c} \leq \frac{L(\alpha, c)^n}{1 - L(\alpha, c)} \|T(\gamma) - \gamma\|_{X_c \cap \mathcal{Y}_c}.$$

It can be deduced directly from (5.1) that T is continuous on \mathcal{U}_R . Finally, the fact that $\theta(\gamma) \in \Gamma_{\leq q}^+$ for any $\gamma \in \mathcal{U}_R$ follows from the fact that

$$\|T(\theta(\gamma)) - \theta(\gamma)\|_{X_c \cap \mathcal{Y}_c} = \lim_{n \rightarrow +\infty} \|T^{n+1}(\gamma) - T^n(\gamma)\|_{X_c \cap \mathcal{Y}_c} = 0.$$

This ends the proof. \square

6 Second-order expansion of $E(\gamma)$

This section is devoted to the proof of Theorem 3.3. We fix α and c . To simplify the notation, we denote $L := L(\alpha, c)$, $\kappa := \kappa(\alpha, c)$ and $\lambda_0 := \lambda_0(\alpha, c)$ throughout this section. The main ingredient is the following proposition, which is essentially the same as in [20], but with a more delicate study.

Proposition 6.1. *Let $R > 1$ be fixed, and let $\kappa < 1$ and $L < 1$ be given as in Lemma 3.2. For any $\gamma \in \mathcal{U}_R$ and any $g \in \Gamma_{\leq q}$, if $P_g^+ \gamma P_g^+ = \gamma$, we have*

$$\left| E(\gamma) - (\mathcal{E}(\gamma) - \epsilon_P \widetilde{\text{Tr}}_{L^2}[\gamma]) \right| \leq \left(2 + \frac{\epsilon_P}{c^2}\right) \frac{\alpha^2}{c^2} \mathcal{N}_\gamma(\gamma - g), \quad (6.1)$$

where $\mathcal{N}_\gamma(h)$ is given in Eq. (3.11).

Remark 6.2. *Actually, for atoms and molecules, using a finer version of this estimate, it is shown in [20] that the DF model is an approximation of the electron-positron Hartree–Fock model (see, e.g., [5] for this model).*

We first use Proposition 6.1 to prove Theorem 3.3.

Proof of Theorem 3.3. Let

$$\text{Err}(t, \gamma, h) := \frac{c^2}{\alpha^2 t^2} \left(E(\gamma + th) - (\mathcal{E}(\gamma + th) - \epsilon_P \widetilde{\text{Tr}}_{L^2}[\gamma]) \right).$$

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

$$E(\gamma + th) = E(\gamma) + \mathcal{E}(\gamma + th) - (\mathcal{E}(\gamma) - \epsilon_P \widetilde{\text{Tr}}_{L^2}(\gamma)) + t^2 \frac{\alpha^2}{c^2} \text{Err}(t, \gamma, h).$$

This is precisely Eq. (3.10). Then, by replacing g by γ and γ by $\gamma + th$ in Proposition 6.1, we finally get

$$|\text{Err}(t, \gamma, h)| \leq \left(2 + \frac{\epsilon_P}{c^2}\right) t^{-2} \mathcal{N}_{\gamma+th}(th) = \left(2 + \frac{\epsilon_P}{c^2}\right) \mathcal{N}_{\gamma+th}(h). \quad (6.2)$$

\square

6.1 Proof of Proposition 6.1

We first consider the error bound between $E(\gamma)$ and $\mathcal{E}(\gamma)$ for any $\gamma \in \mathcal{U}_R$.

Lemma 6.3. *Let $R \geq 1$ be fixed. Assume that $\kappa < 1$ and $L < 1$ as in Lemma 3.2. Let $C_{\kappa,L} := \frac{5C_{EE}^2}{(1-\kappa)^2\lambda_0^{3/2}(1-L)^2}$. Then, for any $\gamma \in \mathcal{U}_R$,*

$$\begin{aligned} & \left| E(\gamma) - (\mathcal{E}(\gamma) - \epsilon_P \widetilde{\text{Tr}}_{L^2}[\gamma]) \right| \\ & \leq \frac{2c^2 + \epsilon_P}{c^2} \left[C_{\kappa,L} \left(R \frac{\alpha}{c} + q \frac{\alpha}{c} + 1 \right) \frac{\alpha}{c^3} \|T(\gamma) - \gamma\|_{X_c \cap \mathcal{Y}_c}^2 + \|P_\gamma^- \gamma P_\gamma^-\|_{X_c} \right]. \end{aligned} \quad (6.3)$$

This is an immediate result of the following.

Lemma 6.4. *Let $\kappa \leq 1$ and $L < 1$. For any $\gamma \in \mathcal{U}_R$,*

$$\|P_\gamma^+(\theta(\gamma) - T(\gamma))P_\gamma^+\|_{X_c \cap \mathcal{Y}_c} \leq C_{\kappa,L} R \frac{\alpha^2}{c^4} \|T(\gamma) - \gamma\|_{X_c \cap \mathcal{Y}_c}^2 \quad (6.4)$$

and

$$\|P_\gamma^-\theta(\gamma)P_\gamma^-\|_{X_c \cap \mathcal{Y}_c} \leq C_{\kappa,L} q \frac{\alpha^2}{c^4} \|T(\gamma) - \gamma\|_{X_c \cap \mathcal{Y}_c}^2. \quad (6.5)$$

We first use it to prove Lemma 6.3 and we postpone the proof of 6.4 until Section 6.2.

Proof of Lemma 6.3. Notice that

$$\begin{aligned} & E(\gamma) - (\mathcal{E}(\gamma) - \epsilon_P \widetilde{\text{Tr}}_{L^2}[\gamma]) \\ & = \widetilde{\text{Tr}}_{L^2}[\mathcal{D}_\gamma^c(\theta(\gamma) - \gamma)] + \frac{\alpha}{2} \widetilde{\text{Tr}}_{L^2}[V_{\theta(\gamma) - \gamma}(\theta(\gamma) - \gamma)] - \epsilon_P \widetilde{\text{Tr}}_{L^2}[\theta(\gamma) - \gamma]. \end{aligned} \quad (6.6)$$

We calculate each term on the right-hand side of Eq. (6.6) separately.

Estimate on $\widetilde{\text{Tr}}_{L^2}[\mathcal{D}_\gamma^c(\theta(\gamma) - \gamma)]$. We consider the first term on the right-hand side of (6.6). Notice that $T(\gamma) = P_\gamma^+ \gamma P_\gamma^+$. We have

$$\begin{aligned} \widetilde{\text{Tr}}_{L^2}[\mathcal{D}_\gamma^c(\theta(\gamma) - \gamma)] & = \widetilde{\text{Tr}}_{L^2}[\mathcal{D}_\gamma^c(P_\gamma^+ + P_\gamma^-)(\theta(\gamma) - \gamma)(P_\gamma^+ + P_\gamma^-)] \\ & = \widetilde{\text{Tr}}_{L^2}[|\mathcal{D}_\gamma^c|P_\gamma^+(\theta(\gamma) - T(\gamma))P_\gamma^+] - \widetilde{\text{Tr}}_{L^2}[|\mathcal{D}_\gamma^c|P_\gamma^-(\theta(\gamma) - \gamma)P_\gamma^-]. \end{aligned}$$

Thanks to (2.31), (6.4) and since $\kappa < 1$, we have

$$\begin{aligned} \left| \widetilde{\text{Tr}}_{L^2}[|\mathcal{D}_\gamma^c|P_\gamma^+(\theta(\gamma) - T(\gamma))P_\gamma^+] \right| & \leq \| |\mathcal{D}_\gamma^c|^{1/2} P_\gamma^+(\theta(\gamma) - T(\gamma))P_\gamma^+ |\mathcal{D}_\gamma^c|^{1/2} \|_{\mathfrak{S}_{1,1}} \\ & \leq 2 \|P_\gamma^+(\theta(\gamma) - T(\gamma))P_\gamma^+\|_{X_c} \leq 2 C_{\kappa,L} R \frac{\alpha^2}{c^4} \|T(\gamma) - \gamma\|_{X_c \cap \mathcal{Y}_c}^2. \end{aligned}$$

On the other hand, from (2.31) and (6.5), we infer

$$\begin{aligned} \left| \widetilde{\text{Tr}}_{L^2}[|\mathcal{D}_\gamma^c|P_\gamma^-(\theta(\gamma) - \gamma)P_\gamma^-] \right| & \leq \| |\mathcal{D}_\gamma^c|^{1/2} P_\gamma^-(\theta(\gamma) - \gamma)P_\gamma^- |\mathcal{D}_\gamma^c|^{1/2} \|_{\mathfrak{S}_{1,1}} + \| |\mathcal{D}_\gamma^c|^{1/2} P_\gamma^- \gamma P_\gamma^- |\mathcal{D}_\gamma^c|^{1/2} \|_{\mathfrak{S}_{1,1}} \\ & \leq 2 \left(\|P_\gamma^-(\theta(\gamma) - \gamma)P_\gamma^-\|_{X_c} + \|P_\gamma^- \gamma P_\gamma^-\|_{X_c} \right) \\ & \leq 2 C_{\kappa,L} q \frac{\alpha^2}{c^4} \|T(\gamma) - \gamma\|_{X_c \cap \mathcal{Y}_c}^2 + 2 \|P_\gamma^- \gamma P_\gamma^-\|_{X_c}. \end{aligned}$$

Then we conclude that

$$\left| \widetilde{\text{Tr}}_{L^2}[\mathcal{D}_\gamma^c(\theta(\gamma) - \gamma)] \right| \leq 2 C_{\kappa,L} (R + q) \frac{\alpha^2}{c^4} \|T(\gamma) - \gamma\|_{X_c \cap \mathcal{Y}_c}^2 + 2 \|P_\gamma^- \gamma P_\gamma^-\|_{X_c \cap \mathcal{Y}_c}.$$

Estimate on $\epsilon_P \widetilde{\text{Tr}}_{L^2}[\theta(\gamma) - \gamma]$. This term can be treated analogously. Actually, as $c^2 \leq |\mathcal{D}^c|$, we have

$$\begin{aligned} \epsilon_P \left| \widetilde{\text{Tr}}_{L^2}[\theta(\gamma) - \gamma] \right| &\leq \epsilon_P \left| \widetilde{\text{Tr}}_{L^2}[P_\gamma^+(\theta(\gamma) - \gamma)P_\gamma^+] + \widetilde{\text{Tr}}_{L^2}[P_\gamma^-(\theta(\gamma) - \gamma)P_\gamma^-] \right| \\ &\leq \frac{\epsilon_P}{c^2} \left(\|P_\gamma^+(\theta(\gamma) - T(\gamma))P_\gamma^+\|_{X_c} + \|P_\gamma^-\theta(\gamma)P_\gamma^-\|_{X_c} + \|P_\gamma^-\gamma P_\gamma^-\|_{X_c} \right). \end{aligned}$$

Then proceeding as for the term $\text{Tr}[\mathcal{D}_\gamma^c(\theta(\gamma) - \gamma)]$, we obtain

$$\epsilon_P \left| \widetilde{\text{Tr}}_{L^2}[\theta(\gamma) - \gamma] \right| \leq \frac{\epsilon_P}{c^2} C_{\kappa, L} q \frac{\alpha^2}{c^4} \|T(\gamma) - \gamma\|_{X_c \cap \mathcal{Y}_c}^2 + \frac{\epsilon_P}{c^2} \|P_\gamma^-\gamma P_\gamma^-\|_{X_c \cap \mathcal{Y}_c}.$$

Estimate on $\frac{\alpha}{2} \widetilde{\text{Tr}}_{L^2}[V_{\theta(\gamma) - \gamma}(\theta(\gamma) - \gamma)]$. Using (2.26) and (3.9), we infer

$$\begin{aligned} \alpha \left| \widetilde{\text{Tr}}_{L^2}[V_{\theta(\gamma) - \gamma}(\theta(\gamma) - \gamma)] \right| &\leq \frac{C_{EE}}{(1 + C_Y)} \frac{\alpha}{c} \|\theta(\gamma) - \gamma\|_{X_c \cap \mathcal{Y}_c} \|\theta(\gamma) - \gamma\|_{\mathfrak{S}_{1,1}} \\ &\leq \frac{C_{EE}}{(1 + C_Y)} \frac{\alpha}{c^3} \|\theta(\gamma) - \gamma\|_{X_c \cap \mathcal{Y}_c} \|\theta(\gamma) - \gamma\|_{X_c} \\ &\leq \frac{C_{EE}}{(1 + C_Y)(1 - L)^2} \frac{\alpha}{c^3} \|T(\gamma) - \gamma\|_{X_c \cap \mathcal{Y}_c}^2 \leq C_{\kappa, L} \frac{\alpha}{c^3} \|T(\gamma) - \gamma\|_{X_c \cap \mathcal{Y}_c}. \end{aligned}$$

Conclusion. We then deduce the following estimate :

$$\begin{aligned} \left| E(\gamma) - (\mathcal{E}(\gamma) - \epsilon_P \widetilde{\text{Tr}}_{L^2}[\gamma]) \right| &\leq \frac{2c^2 + \epsilon_P}{c^2} \left[C_{\kappa, L} \left(R \frac{\alpha}{c} + q \frac{\alpha}{c^2} + 1 \right) \frac{\alpha}{c^2} \|T(\gamma) - \gamma\|_{X_c \cap \mathcal{Y}_c}^2 + \|P_\gamma^-\gamma P_\gamma^-\|_{X_c \cap \mathcal{Y}_c} \right]. \end{aligned}$$

□

We now consider the term $T(\gamma) - \gamma$ and $P_\gamma^-\gamma P_\gamma^-$ under the condition $\gamma = P_g^+ \gamma P_g^-$.

Lemma 6.5. *Let $0 < \kappa < 1$ and $g, \gamma \in \Gamma_{\leq q}$. If $P_g^+ \gamma P_g^- = \gamma$, we have*

$$\|T(\gamma) - \gamma\|_{X_c} \leq \frac{\sqrt{2} C_{EE}}{\lambda_0^{1/2} (1 - \kappa)} \frac{\alpha}{c} \int_{Q_\ell^*} \|\gamma - g\|_{X \cap \mathcal{Y}(\xi)} \|\gamma_\xi |\mathcal{D}_\xi^c|^{1/2}\|_{\mathfrak{S}_1(\xi)} d\xi,$$

$$\|T(\gamma) - \gamma\|_{\mathcal{Y}_c} \leq \frac{\sqrt{2} C_{EE}}{\lambda_0^{1/2} (1 - \kappa)} \frac{\alpha}{c} \sup_{\xi \in Q_\ell^*} \int_{Q_\ell^*} \frac{\|\gamma - g\|_{X \cap \mathcal{Y}(\xi')}}{|\xi - \xi'|^2} d\xi'$$

and

$$\|P_\gamma^-\gamma P_\gamma^-\|_{X_c} \leq \frac{C_{EE}^2}{2(1 - \kappa)^2 \lambda_0} \frac{\alpha^2}{c^2} \int_{Q_\ell^*} \|g - \gamma\|_{X \cap \mathcal{Y}(\xi)}^2 \|\gamma_\xi\|_{\mathfrak{S}_1(\xi)} d\xi.$$

Proof. Indeed, we have

$$T(\gamma) - \gamma = (P_\gamma^+ - P_g^+) \gamma P_\gamma^+ + P_g^+ \gamma (P_\gamma^+ - P_g^+).$$

Then, according to (5.1) and (2.32) and as $0 < \kappa < 1$,

$$\|T_\xi(\gamma) - \gamma_\xi\|_{X_c(\xi)} \leq \frac{2(1 + \kappa)^{1/2}}{(1 - \kappa)^{1/2}} \|\mathcal{D}_\xi^c|^{1/2} (P_{\gamma, \xi}^+ - P_{g, \xi}^+)\|_{\mathcal{B}(L_\xi^2)} \|\gamma_\xi |\mathcal{D}_\xi^c|^{1/2}\|_{\mathfrak{S}_1(\xi)}$$

$$\leq \frac{\sqrt{2}C_{EE}}{(1+C_{\mathcal{Y}})\lambda_0^{1/2}(1-\kappa)} \frac{\alpha}{c} \|\gamma - g\|_{X \cap \mathcal{Y}(\xi)} \|\gamma_\xi |D_\xi^c|^{1/2}\|_{\mathfrak{S}_1(\xi)}.$$

Thus,

$$\|T(\gamma) - \gamma\|_{X_c} \leq \frac{\sqrt{2}C_{EE}}{\lambda_0^{1/2}(1-\kappa)} \frac{\alpha}{c} \int_{Q_\ell^*} \|\gamma - g\|_{X \cap \mathcal{Y}(\xi)} \|\gamma_\xi |D_\xi^c|^{1/2}\|_{\mathfrak{S}_1(\xi)} d\xi.$$

Analogously for the second estimate, the bounds $\|\gamma_\xi\|_{\mathcal{B}(L_\xi^2)} \leq 1$, $c^2 \leq |D^c|$ together with (2.14) yield

$$\begin{aligned} \|T(\gamma) - \gamma\|_{\mathcal{Y}_c} &\leq \sup_{\xi \in Q_\ell^*} \sup_{\substack{k \in \mathbb{Z}^3 \\ |k|_\infty \leq 1}} \int_{Q_\ell^* + \frac{2\pi k}{\ell}} \frac{2}{|\xi - \xi'|^2} \| |D_{\xi'}^c|^{1/2} (P_{\gamma, \xi'}^+ - P_{g, \xi'}^+) \|_{\mathcal{B}(L_{\xi'}^2)} \|\gamma_{\xi'}\|_{\mathcal{B}(L_{\xi'}^2)} d\xi' \\ &\leq \frac{\sqrt{2}C_{EE}}{\lambda_0^{1/2}(1-\kappa)} \frac{\alpha}{c} \sup_{\xi \in Q_\ell^*} \sup_{\substack{k \in \mathbb{Z}^3 \\ |k|_\infty \leq 1}} \int_{Q_\ell^* + \frac{2\pi k}{\ell}} \frac{\|\gamma - g\|_{X \cap \mathcal{Y}(\xi')}}{|\xi - \xi'|^2} d\xi'. \end{aligned}$$

We now turn to the last estimate. Obviously,

$$P_\gamma^- \gamma P_\gamma^- = P_\gamma^- (P_g^+ - P_\gamma^+) \gamma (P_g^+ - P_\gamma^+) P_\gamma^-.$$

Then using Eqs. (5.1) and (2.32) twice, we get

$$\begin{aligned} \|P_{\gamma, \xi}^- \gamma_\xi P_{\gamma, \xi}^- \|_{X_c(\xi)} &= \| |D_\xi^c| P_{\gamma, \xi}^- (P_{g, \xi}^+ - P_{\gamma, \xi}^+) \gamma_\xi (P_{g, \xi}^+ - P_{\gamma, \xi}^+) P_{\gamma, \xi}^- |D_\xi^c| \|_{\mathfrak{S}_1(\xi)} \\ &\leq \frac{1 + \kappa(\alpha, c)}{1 - \kappa(\alpha, c)} \| |D_\xi^c|^{1/2} (P_{g, \xi}^+ - P_{\gamma, \xi}^+) \|_{\mathcal{B}(L_\xi^2)}^2 \|\gamma_\xi\|_{\mathfrak{S}_1(\xi)} \\ &\leq \frac{C_{EE}^2}{2(1-\kappa)^2 \lambda_0} \frac{\alpha^2}{c^2} \|g - \gamma\|_{X \cap \mathcal{Y}(\xi)}^2 \|\gamma_\xi\|_{\mathfrak{S}_1(\xi)}. \end{aligned}$$

Thus,

$$\|P_\gamma^- \gamma P_\gamma^- \|_{X_c} \leq \frac{C_{EE}^2}{2(1-\kappa)^2 \lambda_0} \frac{\alpha^2}{c^2} \int_{Q_\ell^*} \|g - \gamma\|_{X \cap \mathcal{Y}(\xi)}^2 \|\gamma_\xi\|_{\mathfrak{S}_1(\xi)} d\xi.$$

This ends the proof. \square

Inserting Lemma 6.5 into Eq. (6.3), we get immediately

$$\left| E(\gamma) - (\mathcal{E}(\gamma) - \epsilon_P \widetilde{\text{Tr}}_{L^2}[\gamma]) \right| \leq \left(2 + \frac{\epsilon_P}{c^2}\right) \frac{\alpha^2}{c^2} \mathcal{N}_\gamma(\gamma - g),$$

where $\mathcal{N}_\gamma(h)$ is given by (3.11); namely,

$$\begin{aligned} \mathcal{N}_\gamma(h) &= \frac{C_{EE}^2}{2(1-\kappa)^2 \lambda_0} \int_{Q_\ell^*} \|h\|_{X \cap \mathcal{Y}(\xi)}^2 \|\gamma_\xi\|_{\mathfrak{S}_1(\xi)} d\xi \\ &\quad + \left(q \frac{\alpha^2}{c^2} + R \frac{\alpha^2}{c^2} + \frac{\alpha}{c} \right) \frac{10C_{EE}^4}{(1-\kappa)^4 \lambda_0^{5/2} (1-L)^2} \\ &\quad \times \left(\frac{1}{c} \int_{Q_\ell^*} \|h\|_{X \cap \mathcal{Y}(\xi)} \|\gamma_\xi |D_\xi^c|^{1/2}\|_{\mathfrak{S}_1(\xi)} d\xi + \frac{1}{c} \sup_{\xi \in Q_\ell^*} \sup_{\substack{k \in \mathbb{Z}^3 \\ |k|_\infty \leq 1}} \int_{Q_\ell^* + \frac{2\pi k}{\ell}} \frac{\|h\|_{X \cap \mathcal{Y}(\xi')}}{|\xi - \xi'|^2} d\xi' \right)^2. \end{aligned}$$

6.2 Proof of Lemma 6.4

To complete the proof of Proposition 6.1, Lemma 6.4 remains to be proved. Before going further, we need the following.

Proposition 6.6. *Let $\kappa < 1$. For any $\gamma, \gamma' \in \Gamma_{\leq q}$ and $h \in X$,*

$$P_\gamma^+(dP_\gamma^+h)P_\gamma^+ = 0 \quad (6.7)$$

where dP_γ^+h is the Gateaux derivative of P_γ^+ at $\gamma \in \Gamma_{\leq q}$ in the direction h . In addition, we have

$$\left\| |\mathcal{D}^c|^{1/2} [P_\gamma^+ - P_{\gamma'}^+ - dP_{\gamma'}^+(\gamma - \gamma')] \right\|_Y \leq \frac{C_{EE}^2}{2(1-\kappa)^{1/2}(1+C_Y)^2\lambda_0^{3/2}} \frac{\alpha^2}{c^5} \|\gamma - \gamma'\|_{X_c \cap \mathcal{Y}_c}^2. \quad (6.8)$$

Proof. The proof is essentially the same as in [20]. As $P_{\gamma+th}^+ = (P_{\gamma+th}^+)^2$ for any $h \in X$, we have

$$dP_\gamma^+h = P_\gamma^+(dP_\gamma^+h) + (dP_\gamma^+h)P_\gamma^+.$$

Thus,

$$P_\gamma^+(dP_\gamma^+h)P_\gamma^+ = 2P_\gamma^+(dP_\gamma^+h)P_\gamma^+,$$

hence (6.7). Recall that

$$P_\gamma^+ - P_{\gamma'}^+ = \frac{\alpha}{2\pi} \int_{-\infty}^{+\infty} (\mathcal{D}_\gamma^c - iz)^{-1} V_{\gamma'-\gamma} (\mathcal{D}_{\gamma'}^c - iz)^{-1} dz$$

and

$$dP_\gamma^+(\gamma - \gamma') = \frac{\alpha}{2\pi} \int_{-\infty}^{+\infty} (\mathcal{D}_\gamma^c - iz)^{-1} V_{\gamma'-\gamma} (\mathcal{D}_\gamma^c - iz)^{-1} dz.$$

Thus,

$$P_\gamma^+ - P_{\gamma'}^+ - dP_\gamma^+(\gamma - \gamma') = -\frac{\alpha^2}{2\pi} \int_{-\infty}^{+\infty} (\mathcal{D}_\gamma^c - iz)^{-1} V_{\gamma'-\gamma} (\mathcal{D}_{\gamma'}^c - iz)^{-1} V_{\gamma'-\gamma} (\mathcal{D}_\gamma^c - iz)^{-1} dz.$$

Analogously to (5.1), using (2.26), (2.31), (5.4) and (2.33) again, for any $\phi_\xi, \psi_\xi \in L_\xi^2$,

$$\begin{aligned} & \left| \left(\phi_\xi, |\mathcal{D}_\xi^c|^{1/2} [P_{\gamma,\xi}^+ - P_{\gamma',\xi}^+ - (dP_\gamma^+(\gamma - \gamma'))_\xi] \psi_\xi \right) \right| \\ & \leq \frac{\alpha^2}{2\pi} \|V_{\gamma'-\gamma}\|_Y \|\mathcal{D}_{\gamma'}^c\|_Y^{-1} \\ & \times \left(\int_{-\infty}^{+\infty} \|(\mathcal{D}_{\gamma,\xi}^c - iz)^{-1} |\mathcal{D}_\xi^c|^{1/2} \phi_\xi\|_{L_\xi^2} \right)^{1/2} \left(\int_{-\infty}^{+\infty} \|(\mathcal{D}_{\gamma,\xi}^c - iz)^{-1} \psi_\xi\|_{L_\xi^2} \right)^{1/2} \\ & \leq \frac{C_{EE}^2}{2(1-\kappa)^{1/2}(1+C_Y)^2\lambda_0^{3/2}} \frac{\alpha^2}{c^5} \|\gamma - \gamma'\|_{X_c \cap \mathcal{Y}_c}^2 \|\phi_\xi\|_{L_\xi^2} \|\psi_\xi\|_{L_\xi^2}. \end{aligned}$$

This gives (6.8). Hence the proposition. \square

Proof of Lemma 6.4. We first prove (6.4). Indeed, it suffices to prove

$$\begin{aligned} & \|P_\gamma^+(T^n(\gamma) - T^{n-1}(\gamma))P_\gamma^+\|_{X_c \cap \mathcal{Y}_c} \\ & \leq C_{\kappa,L}(1-L)R \frac{\alpha^2}{c^4} \|T(\gamma) - \gamma\|_{X_c \cap \mathcal{Y}_c} \|T^{n-1}(\gamma) - T^{n-2}(\gamma)\|_{X_c \cap \mathcal{Y}_c}. \end{aligned}$$

Then, by Lemma 3.2,

$$\begin{aligned}
\|P_\gamma^+(\theta(\gamma) - T(\gamma))P_\gamma^+\|_{X_c \cap \mathcal{Y}_c} &\leq \sum_{n=2}^{+\infty} \|P_\gamma^+(T^n(\gamma) - T^{n-1}(\gamma))P_\gamma^+\|_{X_c \cap \mathcal{Y}_c} \\
&\leq C_{\kappa,L}(1-L)R\frac{\alpha^2}{c^4} \|T(\gamma) - \gamma\|_{X_c \cap \mathcal{Y}_c} \sum_{n=2}^{+\infty} \|T^{n-1}(\gamma) - T^{n-2}(\gamma)\|_{X_c \cap \mathcal{Y}_c} \\
&\leq C_{\kappa,L}R\frac{\alpha^2}{c^4} \|T(\gamma) - \gamma\|_{X_c \cap \mathcal{Y}_c}^2.
\end{aligned}$$

Let $\gamma_n := T^n(\gamma)$ and $\gamma_0 := \gamma$. Then for $n \geq 2$, $\gamma_n = P_{\gamma_{n-1}}^+ \gamma_{n-1} P_{\gamma_{n-1}}^+$ and $\gamma_{n-1} = P_{\gamma_{n-2}}^+ \gamma_{n-1} P_{\gamma_{n-2}}^+$. Hence, for $n \geq 2$

$$\begin{aligned}
P_\gamma^+(\gamma_n - \gamma_{n-1})P_\gamma^+ &= P_\gamma^+(P_{\gamma_{n-1}}^+ - P_{\gamma_{n-2}}^+)P_{\gamma_{n-2}}^+ \gamma_{n-1} P_{\gamma_{n-1}}^+ P_\gamma^+ \\
&\quad + P_\gamma^+ \gamma_{n-1} P_{\gamma_{n-2}}^+ (P_{\gamma_{n-1}}^+ - P_{\gamma_{n-2}}^+) P_\gamma^+. \tag{6.9}
\end{aligned}$$

We only need to consider the first term on the right-hand side ; the second term can be treated in the same manner. According to (6.7), we have

$$\begin{aligned}
&P_\gamma^+(P_{\gamma_{n-1}}^+ - P_{\gamma_{n-2}}^+)P_{\gamma_{n-2}}^+ \gamma_{n-1} P_{\gamma_{n-1}}^+ P_\gamma^+ \\
&= P_{\gamma_{n-2}}^+ (P_{\gamma_{n-1}}^+ - P_{\gamma_{n-2}}^+ - dP_{\gamma_{n-2}}^+(\gamma_{n-1} - \gamma_{n-2})) P_{\gamma_{n-2}}^+ \gamma_{n-1} P_{\gamma_{n-1}}^+ P_\gamma^+ \\
&\quad + (P_\gamma^+ - P_{\gamma_{n-2}}^+) (P_{\gamma_{n-1}}^+ - P_{\gamma_{n-2}}^+) P_{\gamma_{n-2}}^+ \gamma_{n-1} P_{\gamma_{n-1}}^+ P_\gamma^+. \tag{6.10}
\end{aligned}$$

Thus, according to (6.8) and (2.32), for the first term on the right-hand side

$$\begin{aligned}
&\|P_{\gamma_{n-2}}^+ (P_{\gamma_{n-1}}^+ - P_{\gamma_{n-2}}^+ - dP_{\gamma_{n-2}}^+(\gamma_{n-1} - \gamma_{n-2})) P_{\gamma_{n-2}}^+ \gamma_{n-1} P_{\gamma_{n-1}}^+ P_\gamma^+\|_{X_c \cap \mathcal{Y}_c} \\
&\leq \frac{(1+\kappa)^{1/2}}{(1-\kappa)^{1/2}} \|\mathcal{D}^c\|^{1/2} \|P_{\gamma_{n-1}}^+ - P_{\gamma_{n-2}}^+ - dP_{\gamma_{n-2}}^+(\gamma_{n-1} - \gamma_{n-2})\|_Y \\
&\quad \times \max \{ \|\gamma_{n-1} P_{\gamma_{n-1}}^+ P_\gamma^+ | \mathcal{D}^c |^{1/2} \|_{\mathfrak{S}_1}; \|\gamma_{n-1}\|_{\mathcal{Y}} \} \\
&\leq \frac{C_{EE}^2 (1+\kappa)^{3/2}}{2(1-\kappa)^2 (1+C_{\mathcal{Y}})^2 \lambda_0^{3/2}} \frac{\alpha^2}{c^5} \|\gamma_{n-1} - \gamma_{n-2}\|_{X_c \cap \mathcal{Y}_c}^2 \max \{ \|\gamma_{n-1} | \mathcal{D}^c |^{1/2} \|_{\mathfrak{S}_{1,1}}; \|\gamma_{n-1}\|_{\mathcal{Y}} \}.
\end{aligned}$$

As $\gamma \in \mathcal{U}_R$ and according to Lemma 3.2, we get, for any $n \geq 2$,

$$\|\gamma_{n-1} - \gamma_{n-2}\|_{X_c \cap \mathcal{Y}_c} \leq \|\gamma - T(\gamma)\|_{X_c \cap \mathcal{Y}_c}, \quad \frac{1}{c} \max \{ \|\gamma_{n-1} | \mathcal{D}^c |^{1/2} \|_{\mathfrak{S}_{1,1}}; \|\gamma_{n-1}\|_{\mathcal{Y}} \} \leq R.$$

Then, as $\kappa \leq 1$ and $C_{\mathcal{Y}} \geq 0$, we have

$$\begin{aligned}
&\|P_{\gamma_{n-2}}^+ (P_{\gamma_{n-1}}^+ - P_{\gamma_{n-2}}^+ - dP_{\gamma_{n-2}}^+(\gamma_{n-1} - \gamma_{n-2})) P_{\gamma_{n-2}}^+ \gamma_{n-1} P_{\gamma_{n-1}}^+ P_\gamma^+\|_{X_c \cap \mathcal{Y}_c} \\
&\leq C'_{\kappa,L} R \frac{\alpha^2}{c^4} \|T(\gamma) - \gamma\|_{X_c \cap \mathcal{Y}_c} \|\gamma_{n-1} - \gamma_{n-2}\|_{X_c \cap \mathcal{Y}_c},
\end{aligned}$$

with $C'_{\kappa,L} := \frac{2C_{EE}^2}{(1-\kappa)^2 \lambda_0^{3/2}}$.

We now consider the second term in the right-hand side of (6.10). By (3.8) we have $\|\gamma_n - \gamma\|_{X_c \cap \mathcal{Y}_c} \leq \frac{1}{1-L} \|T(\gamma) - \gamma\|_{X_c \cap \mathcal{Y}_c}$. Thus, by (5.1),

$$\begin{aligned}
&\|(P_\gamma^+ - P_{\gamma_{n-2}}^+) (P_{\gamma_{n-1}}^+ - P_{\gamma_{n-2}}^+) P_{\gamma_{n-2}}^+ \gamma_{n-1} P_{\gamma_{n-1}}^+ P_\gamma^+\|_{X_c \cap \mathcal{Y}_c} \\
&\leq \frac{(1+\kappa)}{(1-\kappa)} \|\mathcal{D}^c\|^{1/2} \|P_\gamma^+ - P_{\gamma_{n-2}}^+\|_Y \|\mathcal{D}^c\|^{-1/2} \|P_{\gamma_{n-1}}^+ - P_{\gamma_{n-2}}^+\|_Y
\end{aligned}$$

$$\begin{aligned}
& \times \max \{ \|\gamma_{n-1}\|_{\mathfrak{S}_1}^{1/2} \|\mathcal{D}^c\|_{\mathfrak{S}_1}; \|\gamma_{n-1}\|_{\mathcal{Y}} \} \\
& \leq \frac{C_{EE}^2(1+\kappa)}{4(1-\kappa)^2(1+C_{\mathcal{Y}})^2\lambda_0^{3/2}} R \frac{\alpha^2}{c^4} \|\gamma_{n-2} - \gamma\|_{X_c \cap \mathcal{Y}_c} \|\gamma_{n-1} - \gamma_{n-2}\|_{X_c \cap \mathcal{Y}_c} \\
& \leq C''_{\kappa,L} R \frac{\alpha^2}{c^4} \|T(\gamma) - \gamma\|_{X_c \cap \mathcal{Y}_c} \|\gamma_{n-1} - \gamma_{n-2}\|_{X_c \cap \mathcal{Y}_c},
\end{aligned}$$

with $C''_{\kappa,L} := \frac{C_{EE}^2}{2(1-\kappa)^2\lambda_0^{3/2}(1-L)}$. Thus by (6.10),

$$\begin{aligned}
& \|P_{\gamma}^+(P_{\gamma_{n-1}}^+ - P_{\gamma_{n-2}}^+)P_{\gamma_{n-2}}^+\gamma_{n-1}P_{\gamma_{n-1}}^+P_{\gamma}^+\|_{X_c \cap \mathcal{Y}_c} \\
& \leq (C'_{\kappa,L} + C''_{\kappa,L})R \frac{\alpha^2}{c^4} \|T(\gamma) - \gamma\|_{X_c \cap \mathcal{Y}_c} \|T^{n-1}(\gamma) - T^{n-2}(\gamma)\|_{X_c \cap \mathcal{Y}_c}.
\end{aligned}$$

The second term in the right-hand side of (6.9) can be treated analogously, thus

$$\|P_{\gamma}^+(\gamma_n - \gamma_{n-1})P_{\gamma}^+\|_{X_c \cap \mathcal{Y}_c} \leq C_{\kappa,L}(1-L)R \frac{\alpha^2}{c^4} \|T(\gamma) - \gamma\|_{X_c \cap \mathcal{Y}_c} \|T^{n-1}(\gamma) - T^{n-2}(\gamma)\|_{X_c \cap \mathcal{Y}_c},$$

where $C_{\kappa,L} := \frac{5C_{EE}^2}{(1-\kappa)^2\lambda_0^{3/2}(1-L)^2} \geq 2(1-L)^{-1}(C'_{\kappa,L} + C''_{\kappa,L})$. Hence (6.4).

Finally, we consider the term $P_{\gamma}^-\theta(\gamma)P_{\gamma}^-$. As $\theta(\gamma) = P_{\theta(\gamma)}^+\theta(\gamma)P_{\theta(\gamma)}^+$, we have

$$P_{\gamma}^-\theta(\gamma)P_{\gamma}^- = P_{\gamma}^-(P_{\theta(\gamma)}^+ - P_{\gamma}^+)\theta(\gamma)(P_{\theta(\gamma)}^+ - P_{\gamma}^+)P_{\gamma}^-,$$

from which we deduce

$$\begin{aligned}
\|P_{\gamma}^-\theta(\gamma)P_{\gamma}^-\|_{X_c \cap \mathcal{Y}_c} & \leq \frac{1+\kappa}{1-\kappa} \|\mathcal{D}^c\|_{\mathfrak{S}_1}^{1/2} \|P_{\theta(\gamma)}^+ - P_{\gamma}^+\|_Y^2 \max \{ \|\theta(\gamma)\|_{\mathfrak{S}_{1,1}}; \|\theta(\gamma)\|_{\mathcal{Y}} \} \\
& \leq \frac{C_{EE}^2(1+\kappa)}{4(1-\kappa)^2(1+C_{\mathcal{Y}})^2\lambda_0(1-L)^2} (q+C_{\mathcal{Y}}) \frac{\alpha^2}{c^4} \|T(\gamma) - \gamma\|_{X_c \cap \mathcal{Y}_c}^2 \\
& \leq C_{\kappa,L} q \frac{\alpha^2}{c^4} \|T(\gamma) - \gamma\|_{X_c \cap \mathcal{Y}_c}^2.
\end{aligned}$$

In the last inequality, we use $(1+C_{\mathcal{Y}})^{-2}(q+C_{\mathcal{Y}}) \leq q(1+C_{\mathcal{Y}})^{-1} \leq 1$. This ends the proof. \square

A Proof of Lemma 2.4

Before going further, we introduce the following technical lemma which will be used in the proof of Lemma 2.4

Lemma A.1. *Let $c \geq 1$ and $A > 0$ such that $\max\{1; 2A\} \leq c$. Let $f : [0, +\infty) \rightarrow \mathbb{R}$ be defined by $f(x) := c^2\sqrt{1+c^{-2}x^2} - A\sqrt{1+x^2}$. Then*

1. We define $x_{0,c} \in [0, +\infty)$ by

$$x_{0,c} := \sqrt{\frac{\max\{A^2 - 1; 0\}}{1 - c^{-2}A^2}}.$$

Then, the function f is decreasing for $x \in [0, x_{0,c})$ and is increasing for $x \in [x_{0,c}, \infty)$ with In addition, $f(x) \rightarrow +\infty$ as $x \rightarrow +\infty$.

2. For any $x_1, x_2 \geq 0$, if $x_1 > \sqrt{18A^2 + \frac{21}{2} + 10x_2^2}$, then

$$f(x_1) > c^2\sqrt{1+c^{-2}x_2^2} + A\sqrt{1+x_2^2}.$$

Proof. Claim 1 follows directly from an easy calculation. Then we focus on Claim 2.

We first assume that $x_1 > x_2$. Then it suffices to show that

$$c^2 \left(\sqrt{1 + c^{-2}x_1^2} - \sqrt{1 + c^{-2}x_2^2} \right) > A \left(\sqrt{1 + x_1^2} + \sqrt{1 + x_2^2} \right).$$

Note that

$$\sqrt{1 + c^{-2}x_1^2} - \sqrt{1 + c^{-2}x_2^2} = c^{-2} \frac{x_1^2 - x_2^2}{\sqrt{1 + c^{-2}x_1^2} + \sqrt{1 + c^{-2}x_2^2}}.$$

Thus, it suffices to show that

$$\begin{aligned} x_1^2 - x_2^2 &> A \left(\sqrt{1 + c^{-2}x_1^2} + \sqrt{1 + c^{-2}x_2^2} \right) \left(\sqrt{1 + x_1^2} + \sqrt{1 + x_2^2} \right) \\ &= A \sum_{j,k=1,2} \sqrt{1 + c^{-2}x_j^2} \sqrt{1 + x_k^2}. \end{aligned}$$

Before going further, we first estimate $A\sqrt{1 + c^{-2}x_j^2}\sqrt{1 + x_k^2}$. Note that if $j = k$,

$$\begin{aligned} A\sqrt{1 + x_j^2}\sqrt{1 + c^{-2}x_j^2} &\leq \sqrt{1 + x_j^2} \sqrt{A^2 + \frac{1}{4}x_j^2} \\ &= \sqrt{A^2 + \frac{4A^2 + 1}{4}x_j^2 + \frac{1}{4}x_j^4} \leq 1 + A^2 + \frac{1}{2}x_j^2; \end{aligned}$$

if $j = 1$ and $k = 2$, by the Young inequality

$$A\sqrt{1 + c^{-2}x_1^2}\sqrt{1 + x_2^2} \leq \frac{A^2}{2}(1 + c^{-2}x_1^2) + \frac{1}{2}(1 + x_2^2) \leq \frac{A^2 + 1}{2} + \frac{1}{8}x_1^2 + \frac{1}{2}x_2^2;$$

and if $j = 2$ and $k = 1$, by the Young inequality

$$A\sqrt{1 + c^{-2}x_2^2}\sqrt{1 + x_1^2} \leq 2A^2(1 + c^{-2}x_2^2) + \frac{1}{8}(1 + x_1^2) \leq \frac{16A^2 + 1}{8} + \frac{1}{8}x_1^2 + \frac{1}{2}x_2^2.$$

Thus,

$$A \left(\sqrt{1 + c^{-2}x_1^2} + \sqrt{1 + c^{-2}x_2^2} \right) \left(\sqrt{1 + x_1^2} + \sqrt{1 + x_2^2} \right) \leq \frac{36A^2 + 21}{8} + \frac{3}{4}x_1^2 + \frac{3}{2}x_2^2.$$

Now it suffices to show that

$$x_1^2 - x_2^2 > \frac{36A^2 + 21}{8} + \frac{3}{4}x_1^2 + \frac{3}{2}x_2^2,$$

from which we get

$$x_1 > \sqrt{18A^2 + \frac{21}{2} + 10x_2^2}.$$

This also implies that $x_1 > x_2$. This proves Claim 2. \square

We are now able to prove Lemma 2.4.

Proof of Lemma 2.4. The proof is in the very same spirit as in [9, Lemma 4.12]. Additionally, we show here that there exists Σ_n independent of α , c , ξ and γ such that (2.35) holds. We also establish the existence of \mathfrak{N}_n . We adapt the proof of Lemma 4.12 in [9] by using the Hardy-type inequalities involving the operator $(1 - \Delta_\xi)^{1/2}$ in Lemma 2.2. We split the proof into three steps.

Step 1. Construction of $\underline{\Lambda}_n(\alpha, c)$ and $\overline{\Lambda}_n(\alpha, c)$. By monotonicity, from Eqs. (2.24) and (2.27), we have

$$|G_\ell| \leq C_G (1 - \Delta)^{1/2} \quad \text{and} \quad |V_\gamma| \leq C_{EE} q^+ (1 - \Delta)^{1/2}.$$

Then, by the Courant–Fisher formulas, for every $\xi \in Q_\ell^*$,

$$\lambda_n^c(\xi) \geq \sigma_n^+ (|\mathcal{D}_\xi^c| - (C_G z + \alpha C_{EE} q^+) (1 - \Delta_\xi)^{1/2}),$$

where $\sigma_n^+(A)$ is the n -th positive eigenvalue (counted with multiplicity) of the operator A . Hence, by the Courant–Fisher formulas, we have

$$\begin{aligned} \underline{\Lambda}_n(\alpha, c) &:= \inf_{\xi \in Q_\ell^*} \sigma_n^+ (|\mathcal{D}_\xi^c| - (C_G z + \alpha C_{EE} q^+) (1 - \Delta_\xi)^{1/2}) \\ &= \min_{\xi \in Q_\ell^*} \sigma_n^+ (|\mathcal{D}_\xi^c| - (C_G z + \alpha C_{EE} q^+) (1 - \Delta_\xi)^{1/2}) \\ &\geq c (1 - \kappa(\alpha, c)), \end{aligned} \tag{A.1}$$

thanks to (2.15). Obviously, $\underline{\Lambda}_n(\alpha, c) \rightarrow +\infty$ when $n \rightarrow +\infty$, since $\sigma_j^+((1 - \Delta_\xi)^{1/2})$ goes to infinity with j . We recall that $d_{c,n}^+(\xi)$ is the n -th positive value of \mathcal{D}_ξ^c introduced in Section 2. A similar argument yields to

$$\begin{aligned} \lambda_n^c(\xi) &\leq \sigma_n^+ (\mathcal{D}_\xi^c + (C_G z + \alpha C_{EE} q^+) (1 - \Delta_\xi)^{1/2}) \\ &\leq d_{c,n}^+(\xi) + (C_G z + \alpha C_{EE} q^+) \sigma_n^+ ((1 - \Delta_\xi)^{1/2}), \end{aligned}$$

where the second inequality holds by using the Courant–Fisher formula. We may then set

$$\overline{\Lambda}_n(\alpha, c) := \max_{\xi \in Q_\ell^*} \left(d_{c,n}^+(\xi) + (C_G z + \alpha C_{EE} q^+) \sigma_n^+ ((1 - \Delta_\xi)^{1/2}) \right) \tag{A.2}$$

Step 2. Independence of Σ_n in (2.35). Let $\mathfrak{M}_n(\xi)$ be the n -th eigenvalue of the operator $(-\Delta_\xi)^{1/2}$ (counted with multiplicity) with $\mathfrak{M}_1(\xi) \leq \mathfrak{M}_2(\xi) \leq \dots$ for every $\xi \in Q_\ell^*$. Since $(\mathcal{D}_\xi^c)^2 = c^4 - c^2 \Delta_\xi$, we have

$$d_{c,n}^+(\xi) = c^2 \sqrt{1 + \frac{1}{c^2} \mathfrak{M}_n^2(\xi)} \leq c^2 + \frac{1}{2} \mathfrak{M}_n^2(\xi), \tag{A.3}$$

whereas

$$\sigma_n^+ ((1 - \Delta_\xi)^{1/2}) = \sqrt{1 + \mathfrak{M}_n^2(\xi)}. \tag{A.4}$$

Therefore, since $\alpha \leq 1$, (2.35) holds with

$$\Sigma_n := \max_{\xi \in Q_\ell^*} \left(\frac{1}{2} \mathfrak{M}_n^2(\xi) + (C_G z + C_{EE} q^+) \sqrt{1 + \mathfrak{M}_n^2(\xi)} \right). \tag{A.5}$$

Step 3. Estimates on \mathfrak{N}_n . Now we set $A := c \kappa(1, c) = C_G z + C_{EE} q^+$. According to (2.35) and since $\underline{\Lambda}_n(\alpha, c) \rightarrow +\infty$ when $n \rightarrow +\infty$, $J_n(\alpha, c) := \min\{j \in \mathbb{N}^* | \underline{\Lambda}_j(\alpha, c) > \overline{\Lambda}_n(\alpha, c)\}$

exists, and $\mathcal{D}_{\gamma,\xi}^c$ has at most $J_n(\alpha, c)$ positive eigenvalues in $(0, \overline{\Lambda}_n(\alpha, c)]$. To end the proof, it suffices to find a bound on $J_n(\alpha, c)$ that is independent on α, c, γ and ξ .

According to (A.1) and (A.2), it suffices to find some integer $\mathfrak{N}_n \geq n$ independent of α, c, γ and ξ such that for any $j \geq \mathfrak{N}_n$ and any $\xi_1, \xi_2 \in \overline{Q_\ell^*}$,

$$\begin{aligned} \min_{\xi_1 \in \overline{Q_\ell^*}} \sigma_j^+ (|\mathcal{D}_{\xi_1}^c| - A(1 - \Delta_{\xi_1})^{1/2}) &> \max_{\xi_2 \in \overline{Q_\ell^*}} \left(d_{c,n}^+(\xi_2) + A\sigma_n^+((1 - \Delta_{\xi_2})^{1/2}) \right) \\ &= \max_{\xi_2 \in \overline{Q_\ell^*}} \left(c^2 \sqrt{1 + c^{-2} \mathfrak{M}_n^2(\xi_2)} + A\sqrt{1 + \mathfrak{M}_n^2(\xi_2)} \right). \end{aligned} \quad (\text{A.6})$$

where the last identity follows from (A.3)-(A.4). Indeed, for any $j \geq \mathfrak{N}_n$ and $\alpha \leq 1$, Eq.(A.6) implies

$$\begin{aligned} \underline{\Lambda}_j(\alpha, c) &\geq \underline{\Lambda}_j(1, c) = \min_{\xi_1 \in \overline{Q_\ell^*}} \sigma_j^+ (|\mathcal{D}_{\xi_1}^c| - A(1 - \Delta_{\xi_1})^{1/2}) \\ &> \max_{\xi_2 \in \overline{Q_\ell^*}} \left(d_{c,n}^+(\xi_2) + A\sigma_n^+((1 - \Delta_{\xi_2})^{1/2}) \right) = \overline{\Lambda}_n(1, c) \geq \overline{\Lambda}_n(\alpha, c). \end{aligned}$$

This shows that $J_n(\alpha, c) \leq \mathfrak{N}_n$ is independent of α, c, γ and ξ .

Let $\xi \in \overline{Q_\ell^*}$. We first study the eigenvalues $\sigma_j^+ (|\mathcal{D}_\xi^c| - A(1 - \Delta_\xi)^{1/2})$. By definition of the function f defined in Lemma A.1,

$$\sigma^+ (|\mathcal{D}_\xi^c| - A(1 - \Delta_\xi)^{1/2}) = \{f(\mathfrak{M}_j(\xi)) | j \in \mathbb{N}^*\}.$$

According to Lemma A.1, f is a not monotone function. So there may exist $j \in \mathbb{N}^*$ such that $\sigma_j^+ (|\mathcal{D}_\xi^c| - A(1 - \Delta_\xi)^{1/2}) \neq f(\mathfrak{M}_j(\xi))$. Nevertheless, we claim that there exists $j_* \in \mathbb{N}^*$ large enough such that for any $j \geq j_*$, $\sigma_j^+ (|\mathcal{D}_\xi^c| - A(1 - \Delta_\xi)^{1/2}) = f(\mathfrak{M}_j(\xi))$. We first apply Claim 2 in Lemma A.1 with $x_2 = 0$. We define

$$j_* := \min \left\{ j \in \mathbb{N}^* \mid \min_{\xi \in \overline{Q_\ell^*}} \mathfrak{M}_j(\xi) > \sqrt{\frac{21}{2} + 18A^2} \right\}.$$

The integer j_* is well-defined because $\min_{\xi \in \overline{Q_\ell^*}} \mathfrak{M}_j(\xi)$ is increasing and goes to infinity with respect to j . For any $\xi \in \overline{Q_\ell^*}$, from Lemma A.1, we have

$$f(\mathfrak{M}_{j_*}(\xi)) > c^2 + A > c^2 - A = f(0) = \max_{x \in [0, x_{0,c}]} f(x) \quad (\text{A.7})$$

with $x_{0,c}$ being defined in Lemma A.1. This also implies that

$$\min_{\xi \in \overline{Q_\ell^*}} \mathfrak{M}_{j_*}(\xi) \in [x_{0,c}, \infty).$$

As $f(x)$ is non-decreasing in $[x_{0,c}, \infty)$, for any $\xi \in \overline{Q_\ell^*}$, we have, using also (A.7) and the fact that $j \mapsto \mathfrak{M}_j(\cdot)$ is non-decreasing,

$$f(\mathfrak{M}_{j_*}(\xi)) \geq \max_{x \in [0, \mathfrak{M}_{j_*}(\xi)]} f(x) \geq \max_{j \leq j_*} f(\mathfrak{M}_j(\xi)).$$

Next, according to the monotonicity of f in $[x_{0,c}, \infty)$, we know that for any $j \geq j_*$,

$$\sigma_j^+ (|\mathcal{D}_\xi^c| - A(1 - \Delta_\xi)^{1/2}) = f(\mathfrak{M}_j(\xi)).$$

Let $\xi_2 \in Q_\ell^*$. With Claim 2 in Lemma A.1 again, applied this time with $x_2 = \max_{\xi_2 \in Q_\ell^*} \mathfrak{M}_n(\xi_2)$, we know that if $j \geq j_*$ satisfies

$$\min_{\xi_1 \in Q_\ell^*} \mathfrak{M}_j(\xi_1) > \max_{\xi_2 \in Q_\ell^*} \sqrt{\frac{21}{2} + 18A^2 + 10\mathfrak{M}_n^2(\xi_2)}, \quad (\text{A.8})$$

then Eq. (A.6) holds. In other words, Eq. (A.6) holds for any $j \geq \mathfrak{N}_n$, with \mathfrak{N}_n being defined by

$$\mathfrak{N}_n := \inf \left\{ j \geq j_* \mid \inf_{\xi_1 \in Q_\ell^*} \mathfrak{M}_j(\xi_1) > \sup_{\xi_2 \in Q_\ell^*} \sqrt{\frac{21}{2} + 18(C_{GZ} + C_{EEQ^+})^2 + 10\mathfrak{M}_n^2(\xi_2)} \right\}. \quad (\text{A.9})$$

Obviously $\mathfrak{N}_n \geq n$ and is independent of α, c, γ and ξ . The proof is complete. \square

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