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THÈSE DE DOCTORAT

Discipline : Mathématiques

présentée par

Ling-Ling CAO

Analyse mathématique de modèles de structures électroniques de matériaux avec défauts

Thèse dirigée par ÉRIC CANCÈS et GABRIEL STOLTZ
préparée au CERMICS, ENPC et Université Paris-Est

Soutenue le 29 octobre 2019 devant le Jury composé de :

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"..... 古人之观于天地、山川、草木、虫鱼、鸟兽，往往有得；以其求思之深，而无不在也。夫夷以近，则游者众；险以远，则至者少；而世之奇伟瑰怪非常之观，常在于险远，而人之所罕至焉；故非有志者，不能至也。有志矣，不随以止也，然力不足者，亦不能至也；有志与力，而又不随以怠，至于幽暗昏惑，而无物以相之，亦不能至也。然力足以至焉而不至，于人为可讥，而在己为有悔；尽吾志也，而不能至者，可以无悔矣....."

——《游褒禅山记》宋 王安石

"... Ancient people learned so much from watching sky and earth, mountains and streams, grass and trees, fish, insects, birds and beasts, because their deep curiosity extended everywhere. Flat places close at hand attract travelers aplenty, but few go where it is dangerous and far. Yet the strangest, grandest, most grotesque and unusual sights of this world are often found in those dangerous, far places that people seldom reach. People without a strong will cannot reach those places. Nor can those who do have the will, do not stop just because others stop, but lack of the physical strength. Nor can those who have both will and strength, do not turn sluggish just because others do, but have nothing to guide them once they reach the dark, confusing depths. When it is someone else who does not reach those places even though he has the strength, we might laugh at him; when it is our own self, we fell regret. However, if we have fully used our will, even if we do not actually reach the goal, regret can be absent ..."

— <Record of an excursion into BaoChan Mountain>, Song Dynasty (1054 AD), WANG Anshi. Translated by Jonathan Pease, <No Going Back, or, Youthful Bravado at the Baochan Mountain Cave>, *Journal of the American Oriental Society*, 2006.

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Résumé

Cette thèse porte sur l'analyse mathématique de modèles de structures électroniques de matériaux présentant des défauts, elle contient trois sujets différents. Dans le chapitre 2, nous étudions l'état fondamental d'un défaut étendu dans une mer de Fermi. Dans le chapitre 3, nous nous intéressons à la description mathématique de la jonction de deux matériaux quasi unidimensionnels. Dans le chapitre 4, nous construisons un cadre mathématique pour la dynamique d'un réseau cristallin de taille infinie, dans l'approximation de Born-Oppenheimer, dans laquelle l'électron est couplé à la dynamique nucléaire.

Abstract

This thesis focuses on the mathematical analysis of electronic structure models for materials with defects. It contains three different topics. In Chapter 2 we study the ground state of an extended defect in a Fermi sea. In Chapter 3 we are interested in the mathematical description of the junction of two perfect quasi one dimensional materials. In Chapter 4 we construct a mathematical framework for a lattice dynamics under the Born-Oppenheimer approximation, where electrons are coupled with the nuclear dynamics.

List of publications

Here is a list of articles that were written during this thesis:

- [CCS18] (with Éric Cancès and Gabriel Stoltz) *Removing a slab from the Fermi sea: the reduced Hartree-Fock model* (Nonlinearity (accepted), 2019).
- [Cao19] *Mean-field stability for the junction of quasi 1D systems with Coulomb interactions* (submitted, arxiv:1903.01127v2).
- [CCS19] (with Éric Cancès and Gabriel Stoltz) *Lattice dynamics in an adiabatic Born-Oppenheimer approximation* (in preparation).

Notation

Let us introduce some notation that will be used throughout this manuscript. We work in atomic units, where all physical constants, such as the elementary charge and the electron mass are taken to be equal to one. Unless otherwise specified, the functions on \mathbb{R}^d considered in this thesis are complex-valued. We denote respectively by $\mathcal{S}(\mathbb{R}^d)$ the Schwartz space of rapidly decreasing functions on \mathbb{R}^d , and by $\mathcal{S}'(\mathbb{R}^d)$ the space of tempered distributions on \mathbb{R}^d .

For a separable Hilbert space \mathfrak{H} , we denote by $\mathcal{L}(\mathfrak{H})$ the space of bounded (linear) operators, by $\mathcal{S}(\mathfrak{H})$ the space of bounded self-adjoint operators, and by $\mathcal{K}(\mathfrak{H})$ the space of compact operators on \mathfrak{H} . For an orthonormal basis $(\phi_n)_{n \geq 1}$ of \mathfrak{H} , the trace of a positive operator A acting on \mathfrak{H} is defined as

$$\mathrm{Tr}(A) := \sum_{n=1}^{\infty} (\phi_n, A\phi_n)_{\mathfrak{H}},$$

where $(\cdot, \cdot)_{\mathfrak{H}}$ is the inner product of the Hilbert space \mathfrak{H} . For $1 \leq p < \infty$, we denote by $\mathfrak{S}_p(\mathfrak{H})$ the p -Schatten class on \mathfrak{H} :

$$A \in \mathfrak{S}_p(\mathfrak{H}) \text{ if and only if } \|A\|_{\mathfrak{S}_p} = (\mathrm{Tr}(|A|^p))^{1/p} < \infty.$$

Operators in $\mathfrak{S}_1(\mathfrak{H})$ and $\mathfrak{S}_2(\mathfrak{H})$ are respectively called *trace-class* and *Hilbert–Schmidt*.

In this thesis the Hilbert space $L^2(\mathbb{R}^d)$ is frequently used. If $A \in \mathfrak{S}_1(L^2(\mathbb{R}^d))$, there exists a unique function $\rho_A \in L^1(\mathbb{R}^d)$ such that

$$\forall W \in L^\infty(\mathbb{R}^d), \quad \mathrm{Tr}(AW) = \int_{\mathbb{R}^d} \rho_A W.$$

The function ρ_A is called the *density of the operator* A . If the integral kernel $A(\mathbf{r}, \mathbf{r}')$ of A is continuous on $\mathbb{R}^d \times \mathbb{R}^d$, then $\rho_A(\mathbf{r}) = A(\mathbf{r}, \mathbf{r})$ for all $\mathbf{r} \in \mathbb{R}^d$. An operator $A \in \mathcal{L}(L^2(\mathbb{R}^d))$ is called *locally trace-class* if the operator $\chi A \chi$ is trace-class for any $\chi \in C_c^\infty(\mathbb{R}^d)$. The density of a locally trace-class operator $A \in \mathcal{L}(L^2(\mathbb{R}^d))$ is the unique function $\rho_A \in L^1_{\mathrm{loc}}(\mathbb{R}^d)$ such that

$$\forall W \in C_c^\infty(\mathbb{R}^d), \quad \mathrm{Tr}(AW) = \int_{\mathbb{R}^d} \rho_A W.$$

We denote respectively by \hat{u} and \check{u} the Fourier transform and the inverse Fourier transform of a tempered distribution $u \in \mathcal{S}'(\mathbb{R}^d)$. We use the normalization convention for which

$$\forall \phi \in L^1(\mathbb{R}^d), \quad \hat{\phi}(\zeta) := \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} \phi(t) e^{-it \cdot \zeta} dt \quad \text{and} \quad \check{\phi}(t) := \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} \phi(\zeta) e^{it \cdot \zeta} d\zeta.$$

With this normalization convention, the Fourier transform defines a unitary operator on $L^2(\mathbb{R}^d)$.

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Macroscopic properties of materials, such as the elasticity of perfect crystals, the resistivity of metals or the color of a chemical compound, can often be deduced from elementary processes which take place at the atomic scale (see e.g. [BdGDCG01, LBP03] and references therein). At the atomic scale, materials are described as systems composed of nuclei and electrons. The understanding of the electronic structures of materials remains an important topic in condensed matter physics and quantum chemistry (see e.g. [Mar04, KMW⁺18] and references therein). The properties of materials fall into two categories determined by the *electronic ground state* and by *electronic excited states*. For example, properties such as the phase transitions between structures, the charge density, elastic constants, nuclear vibrations and motion (in the adiabatic approximation) are related to the ground state, while properties as the optical absorption/emission, Pauli spin susceptibility are determined by excited states [Mar04]. Electronic structure calculation results allows to compute these properties for ideal perfect crystals with good accuracy. Real crystalline materials have defects, which have significant impact on properties of materials (see e.g. [FGH⁺14, Kax03, KN10, Pan78, Sto01] and references therein). In this thesis we focus on the mathematical modeling of various types of defected materials at the atomic scale. In particular, we are interested in the ground state electronic structures of materials.

In this introductory chapter we briefly present the scientific context for Chapters 2, 3 and 4, and summarize the main results of these chapters. We ignore the spin throughout this thesis. In Section 1.1

we start by presenting three models for finite systems: the N -body Schrödinger equation as well as two types of approximations of the N -body Schrödinger model, namely the Hartree–Fock (HF) approximation and Density Functional Theory (DFT). We also present the ground state problem for finite systems. We then explain in Section 1.2 how to describe an infinite system corresponding to a periodic crystal, as well as the associated ground state problem in the reduced Hartree–Fock (rHF) description. In Section 1.3 we present models of various defects: we first focus on a nonlinear model of local defects in insulating crystals, we then consider a linear model of defect in a paradigmatic metal, the free electron gas. We next present the model we consider to describe extended defects in a Fermi sea within a rHF framework. In Section 1.4 we consider the nonlinear junction of two perfect quasi one-dimensional materials, and study the ground state problem for the junction in the rHF model. Lastly, we briefly describe the on-going work of lattice dynamics in the Born–Oppenheimer approximation, and present a partial result in Section 1.5.

1.1 Mathematical models of electronic structure for finite systems

Finite quantum systems, for instance a finite crystal or a molecular system, can be described by the N -body non-relativistic spinless Schrödinger equation (see for example [LBP03]). In this section we first introduce the general N -body non-relativistic Schrödinger model and the ground state problem for finite systems. We shall see that the ground state problem is numerically unsolvable for N large, which calls for more tractable approximations. We next present the most widely used approximations of the N -body Schrödinger model: the Hartree–Fock approximation and Density Functional Theory.

1.1.1 The N -body Schrödinger model

Consider a spinless finite quantum system composed of M nuclei and N electrons in \mathbb{R}^3 , with $M, N \in \mathbb{N}^*$. Since nuclei are much heavier than electrons, their movement is often neglected for electronic structure calculations. That is, electrons are considered to experience the electronic potential generated by nuclei with fixed positions. This approximation is often called the *Born–Oppenheimer approximation* [BO27]. Under this approximation, the time-independent N -body non-relativistic Schrödinger operator for the system of N electrons in \mathbb{R}^3 is

$$H_N := \sum_{i=1}^N \left(-\frac{1}{2} \Delta_i \right) + \sum_{i=1}^N V(r_i) + \sum_{1 \leq i < j \leq N} \frac{1}{|r_i - r_j|}, \quad (1.1)$$

where Δ_i denotes the Laplace operator for the i -th coordinate (so that the first term of (1.1) stands for the kinetic energy), and

$$V(r) = \sum_{n=1}^M \frac{-z_n}{|r - R_n|} \quad (1.2)$$

denotes the classical Coulomb potential generated by the nuclei located at $\{R_n\}_{1 \leq n \leq M}$, with nuclear charges $\{z_n\}_{1 \leq n \leq M}$. The last term of (1.1) describes the Coulombic electron–electron interactions. As electrons are fermions, their wavefunctions are antisymmetric, hence it is convenient to introduce the following Hilbert space:

$$\bigwedge^N L^2(\mathbb{R}^3) = \left\{ \Psi \in L^2(\mathbb{R}^{3N}) \mid \forall \sigma \in \mathbb{S}_N, \Psi(r_{\sigma(1)}, \dots, r_{\sigma(N)}) = \epsilon(\sigma) \Psi(r_1, \dots, r_N) \right\},$$

where \mathbb{S}_N is the group of the permutations of $\{1, \dots, N\}$ and $\epsilon(\sigma)$ the parity of σ . Let us denote by

$$\mathfrak{H}_N := \left(\bigwedge^N L^2(\mathbb{R}^3) \right) \cap H^1(\mathbb{R}^{3N}).$$

A *pure state* of the N -electron system is described by a wavefunction Ψ belonging to \mathfrak{H}_N with $\|\Psi\|_{L^2(\mathbb{R}^{3N})} = 1$. The *electronic density* ρ_Ψ associated with Ψ is defined as the marginal density

$$\rho_\Psi(r) = N \int_{\mathbb{R}^{3(N-1)}} |\Psi(r, r_2, \dots, r_N)|^2 dr_2 \cdots dr_N. \quad (1.3)$$

Therefore

$$\rho_\Psi \geq 0, \quad \rho_\Psi \in L^1(\mathbb{R}^3), \quad \int_{\mathbb{R}^3} \rho_\Psi = N.$$

The N -body Hamiltonian H_N acts on the N -fermionic Hilbert space $\bigwedge^N L^2(\mathbb{R}^3)$ with its domain on the Hilbert space $\left(\bigwedge^N L^2(\mathbb{R}^3)\right) \cap H^2(\mathbb{R}^{3N})$. It is proved in [ZS65] that if $\sum_{n=1}^M z_n \geq N$, the essential spectrum of H_N is an interval of the form $[\Sigma_N, +\infty)$ with $\Sigma_N \leq 0$ and $\Sigma_N < 0$ if $N \geq 2$. The discrete spectrum of H_N is an infinite sequence of negative eigenvalues converging to Σ_N . The lowest eigenvalue (denoted by E_N^0) is called the *ground state energy* and the associated eigenfunctions are called *ground state(s)*. Higher eigenvalues describe *excited states*. Following the *HVZ Theorem* [ZS65, Hun66, RS78], it holds that $\Sigma_N = E_{N-1}^0$. The ground state energy of the finite system is also given by the following minimization problem

$$I_N = \inf \left\{ \langle \Psi | H_N | \Psi \rangle, \Psi \in \mathfrak{H}_N, \|\Psi\|_{L^2(\mathbb{R}^{3N})} = 1 \right\}. \quad (1.4)$$

The numerical computation of the problem (1.4) is very challenging, especially for large N (see for example [LBP03]). This is the reason why the N -body model is often approximated by nonlinear mean-field models. There are two major approximations (see for example [CLBM06]): *wavefunction methods*, which consist in restricting the minimization sets to smaller sets of wavefunctions, and *density functional theory (DFT)*, where the electronic states are described by the electronic density ρ_Ψ only, hence the physical observables are functionals of ρ_Ψ . We present in the next section the most widely used wavefunction method: the Hartree–Fock approximation, and in Section 1.1.3 the DFT approximation.

1.1.2 Hartree–Fock type models

The Hartree–Fock (HF) approximation consists in restricting the minimization set in (1.4) to states called *Slater determinants*:

$$\Psi(r_1, \dots, r_N) = \frac{1}{\sqrt{N!}} \begin{pmatrix} \phi_1(r_1) & \phi_1(r_2) & \cdots & \phi_1(r_N) \\ \phi_2(r_1) & \phi_2(r_2) & \cdots & \phi_2(r_N) \\ \cdots & \cdots & \cdots & \cdots \\ \phi_N(r_1) & \phi_N(r_2) & \cdots & \phi_N(r_N) \end{pmatrix}, \quad (1.5)$$

where the functions ϕ_i belonging to $H^1(\mathbb{R}^3)$ for all $1 \leq i \leq N$ and such that $\langle \phi_i | \phi_j \rangle_{L^2(\mathbb{R}^3)} = \delta_{i,j}$ are called *molecular orbitals*. It is convenient to introduce the *one-body density matrix* γ_Ψ associated with a wave Ψ , which is a self-adjoint trace-class operator acting on $L^2(\mathbb{R}^3; \mathbb{C})$ such that $0 \leq \gamma_\Psi \leq 1$ and $\text{Tr}(\gamma_\Psi) = N$. Its kernel is

$$\gamma_\Psi(r, r') = N \int_{\mathbb{R}^{3(N-1)}} \overline{\Psi(r, r_2, \dots, r_N)} \Psi(r', r_2, \dots, r_N) dr_2 \cdots dr_N. \quad (1.6)$$

The density matrix γ_Ψ obtained from (1.5) simply is the sum of the projectors onto the molecular orbitals:

$$\gamma_\Psi = \sum_{i=1}^N |\phi_i\rangle \langle \phi_i| = \sum_{i=1}^N (\phi_i, \cdot)_{L^2} \phi_i, \quad \gamma_\Psi(r, r) = \rho_\Psi(r) = \sum_{i=1}^N |\phi_i|^2(r),$$

with ρ_Ψ defined in (1.3). Remark that γ_Ψ is also an orthogonal projector onto an N -dimensional subspace of $L^2(\mathbb{R}^3)$, i.e., $\gamma_\Psi^2 = \gamma_\Psi$. With this notation, the HF energy of a Slater determinant Ψ is

$$\begin{aligned} \mathcal{E}^{\text{HF}}(\gamma_\Psi) &:= \langle \Psi | H_N | \Psi \rangle \\ &= \sum_{i=1}^N \frac{1}{2} \int_{\mathbb{R}^3} |\nabla \phi_i|^2 + \int_{\mathbb{R}^3} \rho_\Psi V + \frac{1}{2} \int_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{\rho_\Psi(r) \rho_\Psi(r')}{|r - r'|} dr dr' - \frac{1}{2} \int_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{|\gamma_\Psi(r, r')|^2}{|r - r'|} dr dr' \\ &= \text{Tr}_{L^2(\mathbb{R}^3)} \left(-\frac{1}{2} \Delta \gamma_\Psi \right) + \int_{\mathbb{R}^3} \rho_\Psi V + \frac{1}{2} D(\rho_\Psi, \rho_\Psi) - \frac{1}{2} \int_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{|\gamma_\Psi(r, r')|^2}{|r - r'|} dr dr', \end{aligned} \quad (1.7)$$

where

$$D(f, f) := \int_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{f(r)f(r')}{|r - r'|} dr dr' \quad (1.8)$$

describes the Coulomb electron-electron interactions through the electronic densities. In view of the N -body ground state problem (1.4), the *HF ground state* is given by

$$I_N^{\text{HF}} = \inf \{ \mathcal{E}^{\text{HF}}(\gamma_\Psi) \mid 0 \leq \gamma_\Psi^2 = \gamma_\Psi \leq 1, \text{Tr}(\gamma_\Psi) = N, \text{Tr}(-\Delta\gamma_\Psi) < +\infty \}. \quad (1.9)$$

As we have restricted the minimization set to the set of Slater determinants, the ground state energy I_N^{HF} is always greater or equal to the ground state I_N in the N -body Schrödinger model. The difference $I_N^{\text{HF}} - I_N$ is called the *correlation energy*, which means that in the HF approximation the electrons are "uncorrelated" one from another (they are still correlated through the Pauli exclusion principle, see for e.g. discussions in [LBP03, Chapter 1]). The HF approximation reduces the cost of computing the ground state problem by replacing the $L^2(\mathbb{R}^{3N})$ space to the N -dimensional subspace of $L^2(\mathbb{R}^3)$. However, as the HF energy functional is not convex, the existence and uniqueness of minimizers is not trivial. The existence of minimizers for $N < \sum_{n=1}^M z_n + 1$ was first proved by Lieb and Simon [LS77] and later by Lions [Lio84] by a different approach, in which the existence of infinitely many critical points of \mathcal{E}^{HF} is also proved. It was also shown by Solovej [Sol03] that there exists a positive constant C such that when $N > \sum_{n=1}^M z_n + C$ the problem (1.9) admits no minimizer. Another important result obtained by Lieb [Lie81] states that when relaxing the minimization set of (1.9) to its convex hull

$$\mathcal{P}_N := \{ \gamma \in \mathcal{S}(L^2(\mathbb{R}^3)) \mid 0 \leq \gamma \leq 1, \text{Tr}(\gamma) = N, \text{Tr}(-\Delta\gamma) < +\infty \}, \quad (1.10)$$

one still obtain the same minimizers. This result is important for numerical calculations [CLB00, Can01, CLB02]. Remark that any element of \mathcal{P}_N is not necessarily the density operator associated with some pure state. However any $\gamma \in \mathcal{P}_N$ is the one particle density operator associated with some *mixed state* (represented by a N -particle density operator) [Lie83, Theorem 2.2]. This is called the *N -representability* of density operators.

Euler–Lagrange equation of the HF energy functional. An easy computation shows that a critical point $\Psi = \frac{1}{\sqrt{N!}} \phi_1 \wedge \cdots \wedge \phi_N$ of \mathcal{E}^{HF} satisfies the following Euler–Lagrange equation:

$$\begin{cases} -\frac{1}{2}\Delta\phi_i + V\phi_i + \left(\sum_{j=1}^N |\phi_j|^2 \star \frac{1}{|\cdot|} \right) \phi_i - \sum_{j=1}^N \left(\phi_i \overline{\phi_j} \star \frac{1}{|\cdot|} \right) \phi_j = \sum_{j=1}^N \lambda_{ij} \phi_j, & i = 1, \dots, N, \\ \int_{\mathbb{R}^3} \overline{\phi_i} \phi_j = \delta_{i,j}, \end{cases}$$

where λ_{ij} are the Lagrange multipliers associated with the constraints $\int_{\mathbb{R}^3} \overline{\phi_i} \phi_j = \delta_{i,j}$. In view of the definition of the density matrix γ_Ψ , let us introduce the *Fock operator*:

$$\begin{aligned} H_{\gamma_\Psi}^{\text{HF}} &= -\frac{\Delta}{2} + V + \sum_{j=1}^N |\phi_j|^2 \star \frac{1}{|\cdot|} - \sum_{j=1}^N \left(\overline{\phi_j} \star \frac{1}{|\cdot|} \right) \phi_j \\ &= -\frac{\Delta}{2} + V + \rho_\Psi \star \frac{1}{|\cdot|} - \int_{\mathbb{R}^3} \frac{\gamma_\Psi(\cdot, r') \bullet(r')}{|\cdot - r'|} dr'. \end{aligned}$$

The operator $H_{\gamma_\Psi}^{\text{HF}}$ is also called the *mean-field Hamiltonian*. The last term of $H_{\gamma_\Psi}^{\text{HF}}$ is an integral operator acting through its kernel: for any $\psi \in L^2(\mathbb{R}^3)$

$$\left[\left(\int_{\mathbb{R}^3} \frac{\gamma_\Psi(\cdot, r') \bullet(r')}{|\cdot - r'|} dr' \right) \psi \right] (r) := \int \frac{\gamma_\Psi(r, r')}{|r - r'|} \psi(r') dr'.$$

For a Slater determinant Ψ , remark that any unitary transform $U(N)$ of the column vectors in (1.5) leaves the density matrix $\gamma_\Psi(r, r') = \sum_{i=1}^N \overline{\phi_i}(r) \phi_i(r')$ unchanged. There are two consequences of this observation: there are infinitely many critical points of the HF energy functional \mathcal{E}^{HF} , and one can use this

unitary-invariance to diagonalize the matrix of Lagrange multipliers λ_{ij} . By an abuse of notation we denote by $\lambda_1 \leq \dots \leq \lambda_N$ the diagonal elements of the matrix of Lagrange multipliers. The Euler–Lagrange equation can be written as:

$$\begin{cases} H_{\gamma\Psi}^{\text{HF}} \phi_i = \lambda_i \phi_i, & i = 1, \dots, N, \\ H_{\gamma\Psi}^{\text{HF}} = -\frac{\Delta}{2} + V + \rho\Psi \star \frac{1}{|\cdot|} - \int_{\mathbb{R}^3} \frac{\gamma\Psi(\cdot, r') \bullet (r')}{|\cdot - r'|} dr', \\ \gamma\Psi = \sum_{i=1}^N |\phi_i\rangle\langle\phi_i|, & \rho\Psi = \sum_{i=1}^N |\phi_i|^2. \end{cases} \quad (1.11)$$

Note that the elements $\lambda_1 \leq \dots \leq \lambda_N$ are also eigenvalues (counting multiplicities) of $H_{\gamma\Psi}^{\text{HF}}$. Remark also that the system of equations (1.11) is self-consistent in the sense that the operator $H_{\gamma\Psi}^{\text{HF}}$ itself is constructed from its eigenfunctions $(\phi_i)_{1 \leq i \leq N}$ through $\gamma\Psi$ and $\rho\Psi$. It is proved in [BLLS94, BLS94] that $\lambda_{N+1} > \lambda_N$, which is called the *no unfilled shells* property of the HF theory. This implies that the solution of the self-consistent equation (1.11) can be written in the following compact form, which is important when extending the HF formalism to infinite systems:

$$\gamma\Psi = \mathbb{1}_{(-\infty, \epsilon_F]} (H_{\gamma\Psi}^{\text{HF}}), \quad (1.12)$$

where $\epsilon_F \in [\lambda_N, \lambda_{N+1})$.

Reduced Hartree–Fock energy functional. The HF functional (1.7) is not a convex functional of the density $\rho\Psi$ because of the last term called the *exchange term*. By discarding this term one obtains the *Hartree functional*, also called *reduced Hartree–Fock* (rHF) energy functional:

$$\mathcal{E}^{\text{rHF}}(\gamma\Psi) := \text{Tr}_{L^2(\mathbb{R}^3)} \left(\left(-\frac{1}{2}\Delta + V \right) \gamma\Psi \right) + \frac{1}{2}D(\rho\Psi, \rho\Psi). \quad (1.13)$$

The corresponding ground state is given by the solution of the following minimization problem:

$$I_N^{\text{rHF}} = \inf \{ \mathcal{E}^{\text{rHF}}(\gamma) \mid \gamma \in \mathcal{P}_N \}, \quad (1.14)$$

with \mathcal{P}_N defined in (1.10). The rHF energy functional is a convex functional of the density matrix γ . The existence of minimizers of (1.14) is thoroughly studied in [Sol91] in the context of the *ionization conjecture*. Solovej has shown that there exists a critical value $\sum_{n=1}^M z_n \leq N_{\text{rHF}} \leq 2 \sum_{n=1}^M z_n$ such that for all $0 < N \leq N_{\text{rHF}}$ minimizers of (1.14) exist; and for $N \geq N_{\text{rHF}}$, the energy I_N^{rHF} is constant, meaning that there is no more binding of electrons. These minimizers share the same density thanks to the strict convexity of $\rho \mapsto D(\rho, \rho)$.

The rHF model is a one-electron description of the quantum system (the ground state can be described by a mean–field Hamiltonian), but electrons "interact" with each other through the common electronic density ρ in the term $D(\cdot, \cdot)$. The rHF description is therefore a simple framework which allows one to conduct rigorous mathematical analysis, while still being realistic enough to describe the physics of quantum systems. Furthermore, it can be seen as a good approximation of Kohn–Sham models [KS65, DG90, LLS19] presented the next section, which are commonly used in solid-state physics. Besides, most results obtained on the rHF model can be extended to the Kohn–Sham LDA model [AC09], up to possibly some assumptions on the uniqueness of the ground-state density matrix or on the coercivity of the second-order derivative of the Kohn–Sham energy functional at the ground-state under consideration. Due to these reasons, in the sequel we shall extend the rHF description to infinite systems and use this framework to treat extended defects, the junction of quasi 1D materials as well as lattice dynamics respectively in Sections 1.3.2, 1.4 and 1.5. Before this we present another important approximation of the N -body Schrödinger equation.

1.1.3 Density functional theory

The key idea of density functional theory (DFT) is that the properties of many body quantum system can be described as functionals of the electronic density *only*. More precisely, one transforms the ground state problem (1.4) to a minimization problem of the following form:

$$\inf \left\{ \mathcal{E}(\rho) + \int_{\mathbb{R}^3} \rho V, \rho \in L^1(\mathbb{R}^3), \rho \geq 0, \int_{\mathbb{R}^3} \rho = N \right\}, \quad (1.15)$$

where $\mathcal{E}(\cdot)$ depends only on the electronic density ρ and does not depend on the external potential V . It is not obvious to relate the ground state problem (1.4) to (1.15). The first theoretical justification is given by the cornerstone paper of Hohenberg and Kohn [HK64], where the authors prove that the ground state energy of an inhomogeneous electron gas can be described by a universal density functional independent of the external potential. We present here the approach of Levy [Lev79] and Lieb [Lie83]. In [Lie83, Theorem 1.2] Lieb proves the following *N-representability* of densities:

$$\begin{aligned} & \left\{ \rho \mid \exists \Psi \in \mathfrak{H}_N, \|\Psi\|_{L^2(\mathbb{R}^{3N})} = 1, \rho_\Psi = \rho \right\} \\ & = \left\{ \rho \mid \rho \in L^1(\mathbb{R}^3), \rho \geq 0, \int_{\mathbb{R}^3} \rho = N, \sqrt{\rho} \in H^1(\mathbb{R}^3), \right\} := \mathcal{I}_N. \end{aligned}$$

The *N-representability* implies that given any density ρ in \mathcal{I}_N there exists a wavefunction Ψ such that its density ρ_Ψ matches ρ . The *Levy–Lieb functional* writes

$$\mathcal{E}^{\text{LL}}(\rho) := \inf \left\{ \langle \Psi | H_N^0 | \Psi \rangle, \Psi \in \mathfrak{H}_N, \|\Psi\|_{L^2(\mathbb{R}^{3N})} = 1, \rho_\Psi = \rho \right\},$$

where H_N^0 is the Hamiltonian operator H_N in the absence of potential V :

$$H_N^0 := \sum_{i=1}^N \left(-\frac{1}{2} \Delta_i \right) + \sum_{1 \leq i < j \leq N} \frac{1}{|r_i - r_j|}. \quad (1.16)$$

The minimization problem (1.4) is then equivalent to

$$\inf \left\{ \mathcal{E}^{\text{LL}}(\rho) + \int_{\mathbb{R}^3} \rho V, \rho \in \mathcal{I}_N \right\}. \quad (1.17)$$

This transforms the *N*-body minimization problem (1.4) to a minimization of the Levy–Lieb functional over the set \mathcal{I}_N . However the functional $\mathcal{E}^{\text{LL}}(\cdot)$ is unknown. We present here several common approximations.

Thomas–Fermi type models. Before the rigorous formalization of [HK64], Thomas–Fermi type models were already used. We briefly review some of them here, more details can be found in [LIE, Lie81, CBL98]. The *Thomas–Fermi* (TF), the *Thomas–Fermi–von Weizsäcker* (TFW) and *Thomas–Fermi–Dirac–von Weizsäcker* (TFDW) are DFT models where the energy functionals are explicit functionals of the electronic density. Introducing the physical constants $C_{\text{TF}} = \left(\frac{6^{5/3} \pi^{4/3}}{10} \right)$, $C_{\text{W}} = 0.093$, $C_{\text{D}} = \frac{3}{4} \left(\frac{3}{\pi} \right)^{1/3}$ (see for example [CLBM06] for reference), the *TF energy functional* writes

$$\mathcal{E}^{\text{TF}}(\rho) = C_{\text{TF}} \int_{\mathbb{R}^3} \rho^{5/3} + \frac{1}{2} \int_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{\rho(r)\rho(r')}{|r - r'|} dr dr'. \quad (1.18)$$

In the TF approximation, the kinetic energy term is replaced by $C_{\text{TF}} \int_{\mathbb{R}^3} \rho^{5/3}$, which compounds the semi-classical approximation of the kinetic energy of a homogeneous non-interacting electrons gas: given a Fermi energy $\mu > 0$, the electron gas has a constant density (see, for e.g. [FLLS13])

$$\rho_0 = \frac{1}{(2\pi)^3} \int_{|p|^2 < \mu} dp = \frac{1}{6\pi^2} \mu^{3/2}.$$

The semi-classical kinetic energy of the homogeneous gas is therefore given by

$$\frac{1}{(2\pi)^3} \int_{|p|^2 < \mu} |p|^2 dp = \frac{1}{10\pi^2} \mu^{\frac{5}{2}} = \frac{6^{5/3} \pi^{4/3}}{10} \rho_0^{5/3} = C_{\text{TF}} \rho_0^{5/3}.$$

The above equation provides an exact relationship between the semi-classical kinetic energy of a homogeneous gas and its constant density. For a normalised N -body wavefunction Ψ , the lower bound of its kinetic energy $\int |\nabla \Psi|^2$ by $\int_{\mathbb{R}^3} \rho_{\Psi}^{5/3}$ is given by the *Lieb–Thirring inequality* [LT75, LT91]. It can be formulated as follows [FLLS13]: for all $\Psi \in \mathfrak{H}_N$, there exists a constant $0 < r_3 \leq 1$ such that

$$\text{Tr}(-\Delta \gamma_{\Psi}) \geq r_3 C_{\text{TF}} \int_{\mathbb{R}^3} \rho_{\Psi}^{5/3}. \quad (1.19)$$

There are generalizations of Lieb–Thirring inequalities for other dimensions than 3, see for example [HLW00] and references therein. This inequality is also the foundation of some useful estimates in Chapter 2.

Adding the von Weizsäcker kinetic correction term to the TF energy functional, one obtains the *Thomas–Fermi–von Weizsäcker energy functional*

$$\mathcal{E}^{\text{TFW}}(\rho) = C_{\text{W}} \int_{\mathbb{R}^3} |\nabla \sqrt{\rho}|^2 + C_{\text{TF}} \int_{\mathbb{R}^3} \rho^{5/3} + \frac{1}{2} \int_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{\rho(r)\rho(r')}{|r-r'|} dr dr'. \quad (1.20)$$

The von Weizsäcker kinetic correction term is obtained by studying perturbations of the density matrix of the non-interacting electron gas [LBP03]. Remark that for any density matrix $0 \leq \gamma_{\Psi} \leq 1$ associated to a wavefunction Ψ with a finite kinetic energy, the von Weizsäcker correction term is controlled by the *Hoffman–Ostenhoff inequality* [HOHO77]:

$$\text{Tr}(-\Delta \gamma_{\Psi}) \geq \int_{\mathbb{R}^3} |\nabla \sqrt{\rho_{\Psi}}|^2. \quad (1.21)$$

Inequalities similar to (1.21) will be used in the proofs of results in the following chapters. The advantage of the TF and TFW energy functional is that they are strictly convex functionals of the density. The last model consists in taking into account the exchange term. By using again the homogeneous non-interacting electron gas as a reference, the exchange terms can be approximated as

$$-\frac{1}{2} \int_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{|\gamma(r, r')|^2}{|r-r'|} dr dr' \approx -C_{\text{D}} \int_{\mathbb{R}^3} \rho_{\gamma}^{4/3}.$$

Adding this correction term to the TFW energy functional, one obtains the *Thomas–Fermi–Dirac–von Weizsäcker energy functional*

$$\mathcal{E}^{\text{TFDW}}(\rho) = C_{\text{W}} \int_{\mathbb{R}^3} |\nabla \sqrt{\rho}|^2 + C_{\text{TF}} \int_{\mathbb{R}^3} \rho^{5/3} - C_{\text{D}} \int_{\mathbb{R}^3} \rho^{4/3} + \frac{1}{2} \int_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{\rho(r)\rho(r')}{|r-r'|} dr dr'. \quad (1.22)$$

Note that the TFDW energy functional is no longer convex in the density. Thomas–Fermi type models are good toy models which have nice mathematical properties. However they are currently not often used for quantitative prediction, for which Kohn–Sham models are preferred.

Kohn–Sham models. When restricting the Levy–Lieb functional to non-interacting electrons, that is by retaining in H_N^0 defined in (1.16) only the kinetic part,

$$T^0 := -\frac{1}{2} \sum_{i=1}^N \Delta_{r_i},$$

the Levy–Lieb functional becomes the *Kohn–Sham kinetic energy functional*

$$\mathcal{T}^{\text{KS}}(\rho) = \inf \left\{ \langle \Psi | T^0 | \Psi \rangle, \Psi \in \mathfrak{H}_N, \|\Psi\|_{L^2(\mathbb{R}^{3N})} = 1, \rho_{\Psi} = \rho \right\}. \quad (1.23)$$

When (1.23) admits a minimizer in the form of a Slater determinant (which is not always true [LBP03]), the Kohn–Sham kinetic energy $\mathcal{T}^{\text{KS}}(\rho)$ can be simplified as

$$\mathcal{T}^{\text{KS}}(\rho) := \inf \left\{ \frac{1}{2} \sum_{i=1}^N \int_{\mathbb{R}^3} |\nabla \phi_i|^2, \phi_i \in H^1(\mathbb{R}^3), \int_{\mathbb{R}^3} \overline{\phi_i} \phi_j = \delta_{i,j}, \sum_{i=1}^N |\phi_i|^2 = \rho \right\}. \quad (1.24)$$

The *exchange–correlation energy* is defined as the error between the Lieb–Levy functional energy and the sum of the Kohn–Sham kinetic energy and the self-interacting Coulomb energy:

$$\mathcal{E}^{\text{xc}}(\rho) := \mathcal{E}^{\text{LL}}(\rho) - \mathcal{T}^{\text{KS}}(\rho) - \frac{1}{2}D(\rho, \rho).$$

By definition, the *Kohn–Sham* [KS65] energy functional is a rewriting of the Lieb–Levy energy functional:

$$\mathcal{E}^{\text{KS}}(\rho) := \mathcal{T}^{\text{KS}}(\rho) + \frac{1}{2}D(\rho, \rho) + \mathcal{E}^{\text{xc}}(\rho).$$

However, the exchange–correlation energy is unknown. In practice, various approximations of $\mathcal{E}^{\text{xc}}(\rho)$ were proposed (see for example [LBP03, AC09] and references therein). The most widely used methods in condensed matter physics are the *Local Density Approximations (LDA)* [PZ81, Bec88], which assumes that the exchange–correlation energy of the system behaves locally as that of a uniform electron gas, and the *Generalized gradient approximation (GGA)* [PY86, PBE96], which improves LDA by adding local density gradients.

When the minimization problem (1.23) admits a minimizer in the form of a Slater determinant, the Kohn–Sham energy functional can also be written similarly to (1.13) as

$$\mathcal{E}^{\text{KS}}(\gamma) = \text{Tr}_{L^2(\mathbb{R}^3)} \left(\left(-\frac{1}{2}\Delta + V \right) \gamma \right) + \frac{1}{2}D(\rho_\gamma, \rho_\gamma) + \mathcal{E}^{\text{xc}}(\rho_\gamma).$$

However from the point of view of theoretical chemistry, unlike the HF theory which aims at approximating the original problem [LBP03], the Kohn–Sham approach is exact, provided of course one knows exactly the exchange–correlation energy. The existence of Kohn–Sham minimizers for commonly used exchange–correlation energy \mathcal{E}^{xc} is provided in [LB93].

1.2 Infinite periodic crystals

In the previous section, models for quantum system with a finite number of electrons were presented. At the mesoscopic scale, one encounters a large number of atoms or molecules so that the system still obeys the laws of quantum mechanics. In the N -body Schrödinger model, even the definition of the ground state energy is not clear in general when N tends to infinity, not to mention that its numerical computation is out of reach. One needs to reduce the dimensionality of the problem by exploring the symmetries of the system. This is the case when one studies perfect materials, which are often described by infinitely many atoms arranged periodically, together with their electrons. Mathematically, a perfect crystal is characterized by a \mathcal{R} -periodic nuclear charge distribution, where \mathcal{R} is the Bravais lattice: for linearly independent vectors $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ belonging to \mathbb{R}^3 ,

$$\mathcal{R} := \{n_1 \mathbf{a}_1 + n_2 \mathbf{a}_2 + n_3 \mathbf{a}_3, (n_1, n_2, n_3) \in \mathbb{Z}^3\}.$$

Let \mathcal{R}^* be the reciprocal lattice of \mathcal{R} generated by the dual vectors \mathbf{a}_i^* such that $\mathbf{a}_i \cdot \mathbf{a}_j^* = 2\pi \delta_{ij}$,

$$\mathcal{R}^* := \{n_1^* \mathbf{a}_1^* + n_2^* \mathbf{a}_2^* + n_3^* \mathbf{a}_3^*, (n_1^*, n_2^*, n_3^*) \in \mathbb{Z}^3\}.$$

Denote by Γ the Wigner–Seitz cell, *i.e.*, the unique primitive cell of \mathcal{R} constructed by a Voronoi decomposition; and by Γ^* the first Brillouin zone, which is the Wigner–Seitz cell of \mathcal{R}^* . As an example, for a cubic

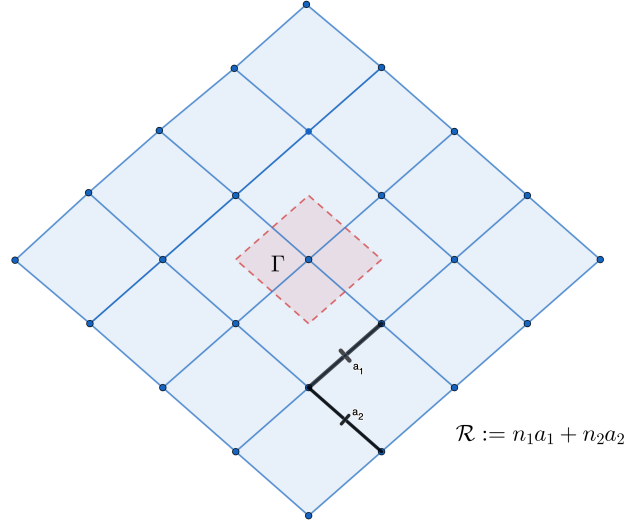


Figure 1.1: An example of a Bravais lattice with its Wigner-Seitz cell Γ .

lattice of parameter $a > 0$, the Bravais lattice is $\mathcal{R} = a\mathbb{Z}^3$, the dual lattice is $\mathcal{R}^* = \frac{2\pi}{a}\mathbb{Z}^3$, the Wigner-Seitz cell is $\Gamma = [-a/2, a/2]^3$ and the first Brillouin zone is $\Gamma^* = [-\pi/a, \pi/a]^3$.

By taking advantage of the \mathcal{R} -periodicity of the crystal, the original problem on the whole space can be reduced to a family of problems on the unit cell Γ . Such reduction technique in mathematics and in condensed matter physics is called the *Bloch decomposition* [RS78]. In this section, we first introduce the Bloch decomposition in Section 1.2.1 as it is a fundamental ingredient to describe systems with partial translation invariance treated in Section 1.3, Section 1.4, Chapter 2 and Chapter 3. We next introduce in Section 1.2.2 the formulation of the electronic ground state problem under the rHF description (1.13) for infinite periodic crystals.

1.2.1 Bloch decomposition

Given a Bravais lattice \mathcal{R} , denote by τ_R the translation operator acting on $L^2_{\text{loc}}(\mathbb{R}^3)$ for $R \in \mathcal{R}$:

$$\forall u \in L^2_{\text{loc}}(\mathbb{R}^3), \quad (\tau_R u)(\cdot) = u(\cdot - R).$$

An operator A on $L^2(\mathbb{R}^3)$ is called \mathcal{R} -translation invariant if it commutes with τ_R for all $R \in \mathcal{R}$. Introduce the L^p spaces (resp. H^1 space) of functions which are \mathcal{R} -periodic: for $1 \leq p \leq +\infty$,

$$\begin{aligned} L^p_{\text{per}}(\Gamma) &:= \left\{ u \in L^p_{\text{loc}}(\mathbb{R}^3) \mid \|u\|_{L^p(\Gamma)} < +\infty, \tau_R u = u, \forall R \in \mathcal{R} \right\}, \\ H^1_{\text{per}}(\Gamma) &:= \left\{ u \in L^2_{\text{per}}(\Gamma) \mid \nabla u \in L^2_{\text{per}}(\Gamma) \right\}. \end{aligned}$$

Let us also introduce the following *constant fiber direct integral* of Hilbert spaces [RS78, Theorem XIII.84]:

$$L^2(\Gamma^*; L^2_{\text{per}}(\Gamma)) := \int_{\Gamma^*}^{\oplus} L^2_{\text{per}}(\Gamma) d\xi,$$

where $\int_{\Gamma^*}^{\oplus} = |\Gamma^*|^{-1} \int_{\Gamma^*}$. The constant fiber direct integral is a generalization of the direct sum of Hilbert spaces. The *Bloch transform* \mathcal{B} is a unitary operator from $L^2(\mathbb{R}^3)$ to $L^2(\Gamma^*; L^2_{\text{per}}(\Gamma))$, defined on the dense subspace of $\mathcal{S}(\mathbb{R}^3)$ of $L^2(\mathbb{R}^3)$:

$$\forall x \in \Gamma, \xi \in \Gamma^*, \quad (\mathcal{B}\phi)_{\xi}(x) := \sum_{R \in \mathcal{R}} e^{-i(x+R)\cdot\xi} \phi(x+R) = \frac{(2\pi)^{\frac{3}{2}}}{|\Gamma|} \sum_{K \in \mathcal{R}^*} e^{iK\cdot x} \hat{\phi}(\xi+K). \quad (1.25)$$

The second equality can be obtained by the Poisson summation formula (see for example [Pin02])

$$\forall \phi \in \mathcal{S}(\mathbb{R}^3), \quad \sum_{R \in \mathcal{R}} \phi(x + R) = \frac{(2\pi)^{\frac{3}{2}}}{|\Gamma|} \sum_{K \in \mathcal{R}^*} \hat{\phi}(K) e^{iK \cdot x}.$$

The *inverse Bloch transform* is given by

$$\forall R \in \mathcal{R}, \text{ for a.a. } x \in \Gamma, \quad (\mathcal{B}^{-1} f_{\bullet})(x + R) := \int_{\Gamma^*} e^{i(R+x)\xi} f_{\xi}(x) d\xi.$$

For almost all $\xi \in \mathbb{R}^3$, we have $(\mathcal{B}\phi)_{\xi+K}(x) = (\mathcal{B}\phi)_{\xi}(x) e^{-iK \cdot x}$ for all $K \in \mathcal{R}^*$. For any $A \in \mathcal{L}(L^2(\mathbb{R}^3))$ such that $\tau_R A = A \tau_R$, there exists (see for e.g. [RS78, Theorem XIII.85]) $A_{\bullet} \in L^\infty(\Gamma^*; \mathcal{L}(L^2_{\text{per}}(\Gamma)))$ such that for all $u \in L^2(\mathbb{R}^3)$,

$$(\mathcal{B}(Au))_{\xi} = A_{\xi}(\mathcal{B}u)_{\xi} \quad \text{for a.a. } \xi \in \Gamma^*. \quad (1.26)$$

We denote by

$$A = \mathcal{B}^{-1} \left(\int_{\Gamma^*}^{\oplus} A_{\xi} d\xi \right) \mathcal{B} \quad (1.27)$$

the decomposition of an operator A which is \mathcal{R} -translation invariant. In addition,

$$\|A\|_{\mathcal{L}(L^2(\mathbb{R}^3))} = \left\| \|A_{\bullet}\|_{\mathcal{L}(L^2_{\text{per}}(\Gamma))} \right\|_{L^\infty(\Gamma^*)}.$$

Moreover, the following spectral decomposition holds:

$$\sigma(A) = \overline{\bigcup_{\xi \in \Gamma^*} \sigma(A_{\xi})}. \quad (1.28)$$

The decomposition (1.27) is useful for instance when we study the band theory of periodic systems in Section 1.2.2. Furthermore, if A is positive and locally trace-class, then for almost all $\xi \in \Gamma^*$, A_{ξ} is locally trace-class. The densities of these operators are related by the formula

$$\rho_A = \int_{\Gamma^*} \rho_{A_{\xi}} d\xi.$$

If for almost all $\xi \in \Gamma^*$, A_{ξ} is positive and trace-class, we can define the *trace per unit volume* for the operator A as

$$\underline{\text{Tr}}(A) := \int_{\Gamma^*} \text{Tr}_{L^2_{\text{per}}(\Gamma)}(A_{\xi}) d\xi.$$

The trace per unit volume provides a measurement of the trace of A in each unit-cell, which is crucial when treating periodic systems, since the operators considered in periodic systems (for example, the total energy operator) are in general not trace class when considered on $L^2(\mathbb{R}^3)$.

1.2.2 Ground state of infinite periodic systems

We describe in this section the periodic rHF formalism to model infinite periodic systems, which is the analogue of (1.14) for finite systems, relying on the results of [CLBL01, CDL08a, Lew09, CL10, CLS12, CS12]. Infinite periodic systems in the HF and rHF descriptions have been rigorously studied by a thermodynamic limit argument in [CLBL01, CLBL02], where the existence of the ground state and the uniqueness of the ground state density have been proven. The periodic rHF ground state has also been studied in [CDL08a], where the uniqueness and the characterization of the minimizer through a self-consistent Euler–Lagrange equation are given. Let us also mention that the periodic TF model has been thoroughly studied in [LIE] and a thermodynamic limit argument has been provided to justify it. Similar results have been obtained in [CBL98] for the TFW model. To our knowledge, there are no rigorous mathematical results on other mean–field models such as HF or Kohn–Sham. These models are much more difficult to study because of

their non-convexity, leading to possible symmetry breakings and the existence of multiple ground-state densities for a given nuclear configuration.

Consider a periodic system with a \mathcal{R} -periodic nuclear charge distribution μ_{per}^0 such that the charge per unit cell $\int_{\Gamma} \mu_{\text{per}}^0 = Z$ with $Z \in \mathbb{N}^+$. By employing the notion of trace per unit cell, the convex set describing finite kinetic energy per unit volume for the infinite periodic system is given by

$$\mathcal{P}_{\text{per}} := \left\{ \gamma \in \mathcal{S}(L^2(\mathbb{R}^3)) \mid 0 \leq \gamma \leq 1, \forall k \in \mathcal{R}, \tau_k \gamma = \gamma \tau_k, \int_{\Gamma^*} \text{Tr}_{L^2_{\text{per}}(\Gamma)} \left((1 - \Delta_{\xi})^{1/2} \gamma_{\xi} (1 - \Delta_{\xi})^{1/2} \right) d\xi < +\infty \right\}, \quad (1.29)$$

where recall that $\mathcal{S}(\mathfrak{H})$ is the space of bounded self-adjoint operators on \mathfrak{H} , and the density matrix is Bloch-decomposed as

$$\gamma = \mathcal{B}^{-1} \left(\int_{\Gamma^*}^{\oplus} \gamma_{\xi} d\xi \right) \mathcal{B}, \quad \text{with } \gamma_{\xi} \in \mathcal{S}(L^2_{\text{per}}(\Gamma)) \text{ and } 0 \leq \gamma_{\xi}^2 \leq \gamma_{\xi} \leq 1,$$

and the Laplace operator Δ on $L^2(\mathbb{R}^3)$ can be written as

$$-\Delta = \mathcal{B}^{-1} \left(\int_{\Gamma^*}^{\oplus} -\Delta_{\xi} d\xi \right) \mathcal{B}, \quad -\Delta_{\xi} = (-i\nabla_{\xi})^2, \quad \nabla_{\xi} := \nabla + i\xi.$$

Remark that the convex set (1.29) is a periodic analogue of the convex set (1.10) for systems with a finite number of electrons. The whole space Coulomb interaction energy (1.8) is also replaced by its periodic analog

$$D_{G_{\Gamma}}(f, f) := \int_{\Gamma} \int_{\Gamma} f(x) G_{\Gamma}(x - y) f(y) dx dy,$$

so that it corresponds to the Coulomb interaction energy per unit volume, and where G_{Γ} is the unique \mathcal{R} -periodic solution of the following Poisson equation:

$$-\Delta G = 4\pi \left(\sum_{y \in \mathcal{R}} \delta(\cdot - y) - 1 \right), \quad \int_{\Gamma} G = 0,$$

with δ the Dirac measure. Therefore one can define the *periodic rHF energy functional*, in analogy with the rHF energy functional of the N -body system defined in (1.13):

$$\mathcal{E}_{\text{per}}^{\text{rHF}}(\gamma) := \int_{\Gamma^*} \text{Tr}_{L^2_{\text{per}}(\Gamma)} \left(-\frac{1}{2} \Delta_{\xi} \gamma_{\xi} \right) d\xi + \frac{1}{2} D_{G_{\Gamma}}(\rho_{\gamma} - \mu_{\text{per}}^0, \rho_{\gamma} - \mu_{\text{per}}^0), \quad (1.30)$$

where the following notation is used

$$\forall \xi \in \Gamma^*, \quad \text{Tr}_{L^2_{\text{per}}(\Gamma)} \left(-\frac{1}{2} \Delta_{\xi} \gamma_{\xi} \right) := \frac{1}{2} \text{Tr}_{L^2_{\text{per}}(\Gamma)} (|\nabla_{\xi}| \gamma_{\xi} |\nabla_{\xi}|).$$

The ground state problem (1.14) for the periodic system is

$$I_{\text{per}}^{\text{rHF}} = \inf \left\{ \mathcal{E}_{\text{per}}^{\text{rHF}}(\gamma) \mid \gamma \in \mathcal{P}_{\text{per}}, \text{Tr}_{L^2_{\text{per}}(\Gamma)}(\gamma) = Z \right\}. \quad (1.31)$$

The definition of the periodic ground state problem (1.31) suggests that the periodic system at its ground state is translation invariant by elements of \mathcal{R} (no spontaneous symmetry breaking). The Euler–Lagrange equation associated with the periodic rHF energy functional (1.30) can be written as [CDL08a]

$$\begin{cases} \gamma_{\text{per}}^0 = \mathbb{1}_{(-\infty, \epsilon_F]}(H_{\text{per}}^0), \\ H_{\text{per}}^0 := -\frac{\Delta}{2} + V_{\text{per}}^0, \\ -\Delta V_{\text{per}}^0 = 4\pi (\rho_{\gamma_{\text{per}}^0} - \mu_{\text{per}}^0), \end{cases} \quad (1.32)$$

where ϵ_F is called the *Fermi level*. This number indicates the highest energy attainable for electrons, and can be considered as the Lagrange multiplier of the charge constraint $\text{Tr}_{L^2_{\text{per}}(\Gamma)}(\gamma_{\text{per}}^0) = Z$. Remark that the system of equations (1.32) is self-consistent, and is the periodic analog of (1.12) for the N -body system.

The mean-field Hamiltonian H_{per}^0 and the spectral projector γ_{per}^0 are τ_R -translation invariant for any element $R \in \mathcal{R}$. In particular, by the Bloch decomposition (1.25) the mean-field Hamiltonian is decomposed as

$$H_{\text{per}}^0 = \mathcal{B}^{-1} \left(\int_{\Gamma^*}^{\oplus} H_{\text{per},\xi}^0 d\xi \right) \mathcal{B}, \quad H_{\text{per},\xi}^0 = -\frac{1}{2}\Delta_{\xi} + V_{\text{per}}^0,$$

and the periodic ground state is decomposed as

$$\gamma_{\text{per}}^0 = \mathcal{B}^{-1} \left(\int_{\Gamma^*}^{\oplus} \gamma_{\text{per},\xi}^0 d\xi \right) \mathcal{B}, \quad \gamma_{\text{per},\xi}^0 = \mathbf{1}_{(-\infty, \epsilon_F]}(H_{\text{per},\xi}^0).$$

In the full periodic case Γ is bounded (when there is a partial periodicity it is no more the case; the reduction theory and the integral decomposition will be adapted), the operator $H_{\text{per},\xi}^0$ is bounded from below and has a compact resolvent for any $\xi \in \Gamma^*$. As a consequence, there exist a non-decreasing sequence $(\epsilon_{n,\xi})_{n \geq 1}$ of real numbers going to $+\infty$ and an orthonormal basis $(e_{n,\xi})_{n \geq 1}$ of $L^2_{\text{per}}(\Gamma)$ such that

$$H_{\text{per},\xi}^0 = \sum_{n=1}^{+\infty} \epsilon_{n,\xi} |e_{n,\xi}\rangle \langle e_{n,\xi}|,$$

and the decomposed ground state of the periodic system reads

$$\gamma_{\text{per},\xi}^0 = \sum_{n=1}^{+\infty} \mathbf{1}_{\epsilon_{n,\xi} \leq \epsilon_F} |e_{n,\xi}\rangle \langle e_{n,\xi}|.$$

The density associated with γ_{per}^0 simply writes

$$\rho_{\gamma_{\text{per}}^0}(x) = \int_{\Gamma^*} \sum_{n=1}^{+\infty} \mathbf{1}_{\epsilon_{n,\xi} \leq \epsilon_F} |e_{n,\xi}(x)|^2 d\xi.$$

The physical interpretation of the above decomposition is that, for a given $\xi \in \Gamma^*$, the non-decreasing sequence $(\epsilon_{n,\xi})_{n \geq 1}$ represents the energy levels of the periodic system, and the Fermi level ϵ_F represents the highest occupied energy level. The ground state γ_{per}^0 implies that all energy levels up to ϵ_F have been filled.

The mapping $\xi \mapsto \epsilon_{n,\xi}$ is \mathcal{R}^* -periodic Lipschitz continuous, and analytic away from crossings [Tho73, RS78]. Hence in view of (1.28) we obtain the spectral decomposition of $H_{\text{per},\xi}^0$:

$$\sigma(H_{\text{per}}^0) = \overline{\bigcup_{\xi \in \Gamma^*} \sigma(H_{\text{per},\xi}^0)} = \bigcup_{n \geq 1} [\Sigma_n^-, \Sigma_n^+], \quad \Sigma_n^- = \min_{\xi \in \Gamma^*} \epsilon_{n,\xi}, \quad \Sigma_n^+ = \max_{\xi \in \Gamma^*} \epsilon_{n,\xi}. \quad (1.33)$$

The spectrum of H_{per}^0 therefore consists of bands which represent the energy levels of the system (see Fig. 1.2 for an illustration), and gives information about the physical properties of the system such as its electrical and optical properties [AM11]. In our context, the band structure is key to distinguish insulators from metals. This separation is important for the rest of this manuscript when studying defects in materials as well as lattice dynamics. More precisely, assume that a periodic system is described by a one-particle Hamiltonian H_{per}^0 and its ground state is given by a spectral projector $\mathbf{1}_{(-\infty, \epsilon_F]}(H_{\text{per}}^0)$. Recall that the Fermi level ϵ_F is the highest occupied energy level. We say that the system is

- an *insulator* if the Fermi level ϵ_F is in a gap of the spectrum of H_{per}^0 ;
- a *metal* if ϵ_F lays inside a band of $\sigma(H_{\text{per}}^0)$.

See Fig. 1.3 for an illustration. In other words, the system is insulating if and only if there exists $N \in \mathbb{N}^*$ such that $\Sigma_N^+ < \epsilon_F < \Sigma_{N+1}^-$; the system is a metal if ϵ_F lays in the interior of $\sigma(H_{\text{per}}^0)$ in \mathbb{R} . In the sequel we shall see that the existence of a gap around the Fermi level ϵ_F is crucial for some mathematical arguments to work.

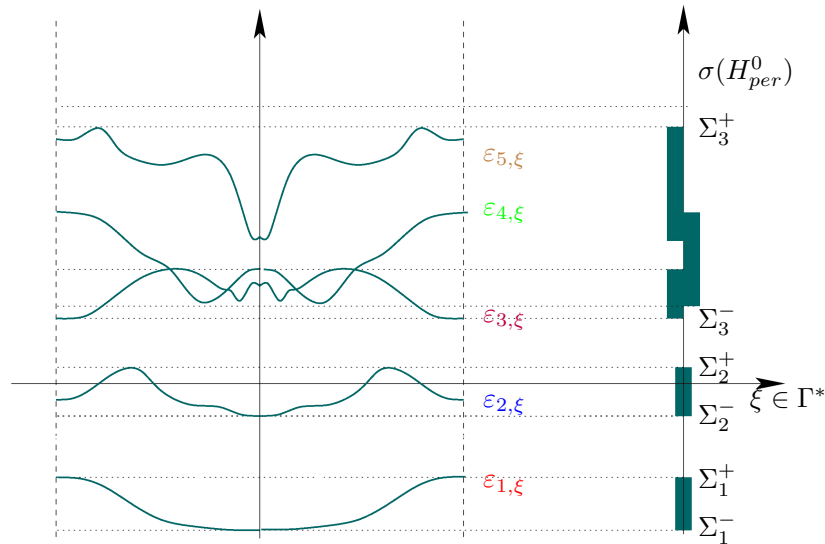


Figure 1.2: The band structure of the spectrum of H_{per}^0 .

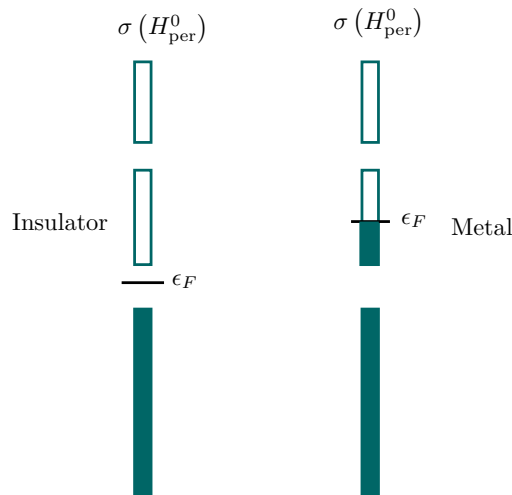


Figure 1.3: Insulators and metals from the point of view of spectral theory.

1.3 Mean-field models for defects in materials

Perfect materials are idealizations, and do not exist in the real world. Various defects exist everywhere, sometimes in a desired way, like doping semiconductors to change their conductivity or adding tin to copper to lower the melting temperature of the resulting material. Most of the time they are present in an uncontrolled manner in materials. For example there may be vacancies at lattice sites or atoms of different types exchanging their positions (antisite defects). There may also be misaligned crystal lattices (dislocation defects). These defects have a significant impact on properties of materials. We refer to [Sto01, DE07] and references therein for more details from a physical point a view.

The first-principle modeling of defects remains an important subject in condensed matter physics (see e.g. [FGH⁺14, Kax03, KN10, Pan78] and references therein). Several correlated-electron models for crystals with defects have recently been proposed in the physics literature among which Hubbard models, Dynamical Mean-Field Theory (DMFT), Green's function methods (GW, Bethe-Salpeter), or Monte Carlo methods, see e.g. the recent monograph [MRC16] and references therein. In the mathematical literature, the case of effective linear one-body Hamiltonians describing independent electrons in solids has been thoroughly

investigated, in particular to study the effect of disorder on transport properties (see e.g. [BvESB94, Hun08] and references therein). Nonlinear mean–field models are much more difficult to handle: local defects are considered as perturbations of an infinitely extended reference system [CDL08a], so that the energy of the system with defect is also infinite. Moreover, one also has to encode nonlinear effects such as the electrostatic potential caused by the defect or the change in the lattice configuration. Let us mention that when considering the rHF model with a positive temperature, also called Schrödinger–Poisson model in [Nie90], Nier has treated local defects with Dirichlet boundary condition and in the whole space, as well as periodic defects within a periodic background in [Nie93b, Nie93a]. There are also extensions on the dynamical properties of the Schrödinger–Poisson model, see [BAM05, BACDFM09] and reference therein.

We summarize in Section 1.3.1 various results on local defects for insulators described by mean–field models, and for a model metallic system (a free Fermi sea) described by an effective linear model. We then discuss our contribution to the modeling of some extended defects in a Fermi sea in Section 1.3.2.

1.3.1 Mean–field models for local defects

In this section we first review the approach presented in [CDL08a] to describe local defects in insulators in a rHF model. We next present a linear defect model in metals [FLLS11, FLLS13], where metals are modeled as a Fermi sea. The latter series of works lays the foundation for the modeling extended defects in a Fermi sea within the rHF description that we consider in Section 1.3.2.

Local defects in insulators: a rHF model. For insulators, a rHF model with Coulomb interactions has been proposed in [CDL08a, CL10] to study a local defect in an insulating (or semiconducting) crystal, based on ideas and techniques from [HLS05a, HLS05b, HLS07, HLSS07, HLS09a]. We summarize here several definitions and ideas for treating defects as perturbations in infinite systems, as these ideas will be used throughout this manuscript.

Consider a perfect 3D crystal described by the periodic rHF energy functional (1.30) with a \mathcal{R} -periodic nuclear density μ_{per}^0 . In this section we restrict ourselves to insulators or semi-conductors. More precisely, in view of the spectral decomposition (1.33), we assume that the following assumption holds (See Fig.1.2 for an illustration).

Assumption 1. Assume that $\Sigma_Z^+ < \Sigma_{Z+1}^-$, and that the Fermi level ϵ_F is in the spectral gap $(\Sigma_Z^+, \Sigma_{Z+1}^-)$ of H_{per}^0 .

The local defect is modeled by a function $\nu \in L^1(\mathbb{R}^3) \cap L^2(\mathbb{R}^3)$ added to the periodic background, so that the nuclear density of a crystal with local defect is described by

$$\mu = \mu_{\text{per}}^0 + \nu.$$

The infinite rHF energy functional (1.13) associated with μ for a trial density matrix γ formally writes

$$\mathcal{E}_{\nu}^{\text{rHF}}(\gamma) \text{ “ = ” } \text{Tr} \left(-\frac{1}{2} \Delta \gamma \right) + \frac{1}{2} D(\rho_{\gamma} - \mu, \rho_{\gamma} - \mu). \quad (1.34)$$

We consider the formal decomposition

$$\gamma = \gamma_{\text{per}}^0 + Q,$$

where Q is a self-adjoint operator acting on $L^2(\mathbb{R}^3)$ and γ_{per}^0 is the density matrix of the perfect crystal obtained in (1.32). One expects to be able to give a meaning to the difference of the two infinite free energies

$$\begin{aligned} & \text{“ } (\mathcal{E}_{\nu}^{\text{rHF}}(\gamma_{\text{per}}^0 + Q) - \epsilon_F \text{Tr}(\gamma_{\text{per}}^0 + Q)) - (\mathcal{E}_{\nu}^{\text{rHF}}(\gamma_{\text{per}}^0) - \epsilon_F \text{Tr}(\gamma_{\text{per}}^0)) \text{”} \\ & = \text{“ } \text{Tr}((H_{\text{per}} - \epsilon_F)Q) - D(\rho_Q, \nu) + \frac{1}{2} D(\rho_Q, \rho_Q) \text{”}. \end{aligned} \quad (1.35)$$

For Q to be an admissible perturbation of the reference state γ_{per}^0 , Pauli's principle requires that $0 \leq \gamma_{\text{per}}^0 + Q \leq 1$. The operator Q also appears to be Hilbert-Schmidt. Nevertheless Q is in general not trace-class [CL10] and the right hand side of the above equation may have no mathematical meaning. Instead, one can give sense to a generalized γ_{per}^0 -trace

$$\text{Tr}_{\gamma_{\text{per}}^0}(Q) := \text{Tr}_{L^2(\mathbb{R}^3)}(Q^{++} + Q^{--}), \quad (1.36)$$

where

$$Q^{++} := (1 - \gamma_{\text{per}}^0) Q (1 - \gamma_{\text{per}}^0), \quad Q^{--} := \gamma_{\text{per}}^0 Q \gamma_{\text{per}}^0.$$

Denote by $\mathfrak{S}_1^{\gamma_{\text{per}}^0}$ the space of operators having a finite γ_{per}^0 -trace. Remark that when an operator A is trace-class $\text{Tr}_{\gamma_{\text{per}}^0}(A) = \text{Tr}_{L^2(\mathbb{R}^3)}(A)$. We also refer the reader to [Lew09, Appendix A] for a pedagogic summary of properties of density matrices describing perturbations of a quantum system around a reference state (in our case, Q is seen as a perturbation and γ_{per}^0 as the reference state).

The admissible perturbative states are the following convex set:

$$\mathcal{K}_{\gamma_{\text{per}}^0} := \left\{ Q \in \mathcal{Q}_{\gamma_{\text{per}}^0} \mid -\gamma_{\text{per}}^0 \leq Q \leq 1 - \gamma_{\text{per}}^0 \right\}, \quad (1.37)$$

where $\mathcal{Q}_{\gamma_{\text{per}}^0}$ is the Banach space of operators having finite γ_{per}^0 -trace and finite kinetic energy:

$$\mathcal{Q}_{\gamma_{\text{per}}^0} := \left\{ Q \in \mathfrak{S}_1^{\gamma_{\text{per}}^0}(L^2(\mathbb{R}^3)) \mid Q^* = Q, \|\nabla|Q\| \in \mathfrak{S}_2(L^2(\mathbb{R}^3)), \right. \\ \left. \|\nabla|Q^{++}\| \in \mathfrak{S}_1(L^2(\mathbb{R}^3)), \|\nabla|Q^{--}\| \in \mathfrak{S}_1(L^2(\mathbb{R}^3)) \right\},$$

equipped with its natural norm

$$\|Q\|_{\mathcal{Q}_{\gamma_{\text{per}}^0}} := \|Q\|_{\mathfrak{S}_2} + \|Q^{++}\|_{\mathfrak{S}_1} + \|Q^{--}\|_{\mathfrak{S}_1} + \|\nabla|Q\|_{\mathfrak{S}_2} + \|\nabla|Q^{++}\|_{\mathfrak{S}_1} + \|\nabla|Q^{--}\|_{\mathfrak{S}_1}.$$

Furthermore, for any $Q \in \mathcal{K}_{\gamma_{\text{per}}^0}$ a simple algebraic calculation shows that

$$Q^{++} \geq 0, \quad Q^{--} \leq 0, \quad 0 \leq Q^2 \leq Q^{++} - Q^{--}.$$

Remark that $\mathcal{K}_{\gamma_{\text{per}}^0}$ is not empty since it contains at least 0. Note also that $\mathcal{K}_{\gamma_{\text{per}}^0}$ is the convex hull of states in $\mathcal{Q}_{\gamma_{\text{per}}^0}$ of the special form $\gamma - \gamma_{\text{per}}^0$, where γ is an orthogonal projector [CDL08a]. In view of the formal difference (1.35), one can define a *renormalized rHF energy functional* associated with ν :

$$\forall Q \in \mathcal{K}_{\gamma_{\text{per}}^0}, \quad \mathcal{E}_{\nu}^{\text{rHF}}(Q) := \text{Tr}_{\gamma_{\text{per}}^0}(H_{\text{per}}^0 Q) - D(\rho_Q, \nu) + \frac{1}{2}D(\rho_Q, \rho_Q), \quad (1.38)$$

where for any κ in the gap $(\Sigma_Z^+, \Sigma_{Z+1}^-)$ of H_{per}^0 ,

$$\text{Tr}_{\gamma_{\text{per}}^0}(H_{\text{per}}^0 Q) := \text{Tr}_{L^2(\mathbb{R}^3)}\left(|H_{\text{per}}^0 - \kappa|^{1/2} (Q^{++} - Q^{--}) |H_{\text{per}}^0 - \kappa|^{1/2}\right) + \kappa \text{Tr}_{\gamma_{\text{per}}^0}(Q). \quad (1.39)$$

It can be shown that the expression (1.39) is independent of $\kappa \in (\Sigma_Z^+, \Sigma_{Z+1}^-)$. The relative ground state energy of a crystal with a defect ν is obtained by solving the following minimization problem

$$I_{\nu}^{\text{rHF}} = \inf \left\{ \mathcal{E}_{\nu}^{\text{rHF}}(Q) \mid Q \in \mathcal{K}_{\gamma_{\text{per}}^0} \right\}.$$

If $\nu \in L^1(\mathbb{R}^3) \cap L^2(\mathbb{R}^3)$ and Assumption 1 holds, it has been shown in [CDL08a, Theorem 2] that the above minimization problem admits minimizers which share the same density, and that any minimizer \bar{Q} satisfies the following self-consistent equation:

$$\begin{cases} \bar{Q} = \mathbf{1}_{(-\infty, \epsilon_F)}(H_{\bar{Q}}) - \gamma_{\text{per}}^0 + \delta, \\ H_{\bar{Q}} := H_{\text{per}}^0 + (\rho_{\bar{Q}} - \nu) \star |\cdot|^{-1}, \end{cases} \quad (1.40)$$

where δ is a finite-rank self-adjoint operator satisfying $0 \leq \delta \leq 1$ and $\text{Ran}(\delta) \subseteq \text{Ker}(H_{\bar{Q}} - \epsilon_F)$.

Other works around local defects in insulators. Various extensions of the model in [CDL08a] were considered: the zero-frequency dielectric polarizability of insulating crystals can be inferred from the rHF model by a homogenization procedure [CL10]. Extensions to the time-dependent setting are discussed in [CS12], where authors considered a time-dependent defect $\nu(t)$ and studied the well-posedness of the associated nonlinear Hartree dynamics. The numerical analysis of the rHF model of defects is dealt with in [GL16] by a super-cell algorithm (see also [CDL08b]). Ideas similar to [CDL08a] have been applied to Thomas–Fermi–Dirac–von Weizsäcker model [CE11] and their approaches are mathematically justified by a thermodynamic limit argument. Let us also mention the works [LR13a, LR13b] for the study of polarons in crystals, and the works [CLL13, Lah14] in which crystals with stationary random distributions of local defects are considered. Let us also mention that the well-posedness of the Hartree dynamics for infinitely many electrons in a Fermi sea is proved in [LS15].

Local defects in the Fermi sea: a linear model. The above mentioned works are valid only for insulators and semiconductors, and crucially rely on the existence of a spectral gap in the spectrum of the mean-field Hamiltonian H_{per}^0 (Assumption 1) of the corresponding perfect crystal. Mean-field model for defects in metals are much more difficult to analyze since small perturbations can cause electrons to escape at infinity. On the other hand, many interesting physical problems, such as electronic transport, occur in metals. In [FLLS11, FLLS13], the authors have considered local perturbations of the Fermi sea of the free-electron gas in a linear model with external potentials. In their work, the ground state of a free Fermi gas is given by $\Pi^- := \mathbb{1}_{(-\infty, \epsilon_F]}(-\Delta)$ for a chemical potential $\epsilon_F > 0$. This electron gas has a constant density¹

As ϵ_F belongs to $\sigma_{\text{ess}}(-\Delta) = [0, +\infty)$, the techniques required to study ground state properties of a free Fermi sea are different from the techniques used in (1.32) for insulators, since in the latter case the gap condition in the spectrum of H_{per}^0 (Assumption 1) is crucial. However, the perturbative approach can still be applied. Following ideas similar to those used to define defects in insulating systems, the perturbation of the reference state Π^- can also be described by a one-body density matrix satisfying

$$-\Pi^- \leq Q \leq 1 - \Pi^-.$$

The relative kinetic energy of the perturbation is defined as

$$\text{Tr}_{\Pi}((-\Delta - \epsilon_F)Q) := \text{Tr} \left(|-\Delta - \epsilon_F|^{1/2} (Q^{\Pi,++} - Q^{\Pi,--}) |-\Delta - \epsilon_F|^{1/2} \right), \quad (1.42)$$

with $Q^{\Pi,++} := (1 - \Pi^-) Q (1 - \Pi^-)$ and $Q^{\Pi,--} := \Pi^- Q \Pi^-$. The above definition looks like the definition (1.39), however as ϵ_F belongs to $\sigma_{\text{ess}}(-\Delta) = [0, +\infty)$, a defect state Q with a finite relative kinetic energy may not even be a compact operator [FLLS13, Remark 2.4]. In particular, it does not belong to the set $\mathcal{K}_{\gamma_{\text{per}}^0}$ defined in (1.37). Since the reference system is a metal (see Fig. 1.3), perturbations are much more delicate to handle, as even a small perturbation is not stable. However one still hope to control the perturbation in some sense, for example by requiring that the perturbation has a finite kinetic energy. A new Banach space of defects is introduced to this end:

$$\mathcal{X}_{\Pi} := \left\{ Q \in \mathcal{S}(L^2(\mathbb{R}^d)) \mid \begin{aligned} &|-\Delta - \epsilon_F|^{1/2} Q \in \mathfrak{S}_2(L^2(\mathbb{R}^d)), \\ &|-\Delta - \epsilon_F|^{1/2} Q^{\Pi, \pm\pm} |-\Delta - \epsilon_F|^{1/2} \in \mathfrak{S}_1(L^2(\mathbb{R}^d)) \end{aligned} \right\},$$

equipped with the norm

$$\begin{aligned} \|Q\|_{\mathcal{X}_{\Pi}} := & \|Q\|_{\mathcal{L}(L^2(\mathbb{R}^d))} + \left\| |-\Delta - \epsilon_F|^{1/2} Q \right\|_{\mathfrak{S}_2(L^2(\mathbb{R}^d))} \\ & + \sum_{\alpha \in \{+, -\}} \left\| |-\Delta - \epsilon_F|^{1/2} Q^{\alpha\alpha} |-\Delta - \epsilon_F|^{1/2} \right\|_{\mathfrak{S}_1(L^2(\mathbb{R}^d))}. \end{aligned}$$

¹The constant density is

$$\rho_0 = |S^{d-1}| d^{-1} (2\pi)^{-d} \epsilon_F^{d/2}, \quad (1.41)$$

where d is the dimension and S^n the n -dimensional sphere.

Admissible states belong to the convex set of states compatible with Pauli's principle:

$$\mathcal{K}_\Pi := \left\{ Q \in \mathcal{X}_\Pi \mid -\Pi^- \leq Q \leq 1 - \Pi^- \right\}. \quad (1.43)$$

As mentioned in Section 1.1.3, the Lieb–Thirring inequality (1.19) provides a lower bound on the kinetic energy of a density matrix in terms of its density. For states in \mathcal{K}_Π , the authors of [FLLS13, FLLS11] have proved a Lieb–Thirring type inequality: for $d \geq 2$, there exists $K(d) \in \mathbb{R}^+$ such that

$$\mathrm{Tr}_\Pi ((-\Delta - \epsilon_F) Q) \geq K(d) \int_{\mathbb{R}^d} \left((\rho_0 + \rho_Q)^{1+\frac{2}{d}} - \rho_0^{1+\frac{2}{d}} - \frac{2+d}{d} \rho_0^{\frac{2}{d}} \rho_Q \right). \quad (1.44)$$

This inequality provides a lower bound of the relative kinetic energy of defect state Q by its density ρ_Q . However for $d = 1$ there is no such inequality as (1.44) since the off-diagonal terms $Q^{\pm\mp}$ diverge [FLLS13, Theorem 2.5], due to 1D Peierls oscillations [Pei55]. Nevertheless, one can prove the following result, which is one of the key estimate that will be used for the extended defects in a Fermi sea considered in Section 1.3.2 and Chapter 2.

Theorem 1.1 (Lieb–Thirring inequality, $d = 1$ [FLLS13, Theorem 2.2]). *Assume that $d = 1$ and $\epsilon_F > 0$. Let $Q \in \mathcal{K}_\Pi$. Then Q is locally trace-class and the corresponding densities satisfy*

$$\rho_{Q^{\pm\pm}} \in L^3(\mathbb{R}) \cap L^2(\mathbb{R}), \quad \int_{\mathbb{R}} \frac{\sqrt{\epsilon_F}|k|}{(\sqrt{\epsilon_F} + |k|) \log \left(\frac{2\sqrt{\epsilon_F} + |k|}{|2\sqrt{\epsilon_F} - |k||} \right)} \left| \widehat{\rho_{Q^{\pm\mp}}}(k) \right|^2 dk < +\infty. \quad (1.45)$$

Moreover, there exist two positive constants K_1 and K_2 such that

$$\begin{aligned} \mathrm{Tr}_\Pi ((-\Delta - \epsilon_F) Q) \geq & K_1 \int_{\mathbb{R}} \left((\rho_0 + \rho_Q^{++}(x) + \rho_Q^{--}(x))^3 - \rho_0^3 - 3\rho_0^2 (\rho_Q^{++}(x) + \rho_Q^{--}(x)) \right) dx \\ & + K_2 \int_{\mathbb{R}} \frac{\sqrt{\epsilon_F}|k|}{(\sqrt{\epsilon_F} + |k|) \log \left(\frac{2\sqrt{\epsilon_F} + |k|}{|2\sqrt{\epsilon_F} - |k||} \right)} \left| \widehat{\rho_Q^{+-}}(k) + \widehat{\rho_Q^{-+}}(k) \right|^2 dk. \end{aligned} \quad (1.46)$$

Remark that due to the logarithmic divergence of $|k|$ at $2\sqrt{\epsilon_F}$, the last term in (1.46) is not bounded from below by $\rho_Q^{+-}(x) + \rho_Q^{-+}(x)$.

It is worth noting that a dual formulation of (1.44), which involves an external potential V , can be obtained by a Legendre–Fenchel transform [FLLS11]. For $d \geq 2$ and $V \in L^2(\mathbb{R}^d) \cap L^{1+d/2}(\mathbb{R}^d)$, denote by

$$\Pi_V^- := \mathbb{1}_{(-\infty, 0]}(-\Delta + V - \epsilon_F), \quad Q_V := \Pi_V^- - \Pi^-.$$

It is shown in [FLLS13, Theorem 2.3] that

$$\begin{aligned} & \mathrm{Tr}_{L^2(\mathbb{R}^3)} \left(|-\Delta + V - \epsilon_F|^{\frac{1}{2}} (\Pi_V^+ Q_V \Pi_V^+ - \Pi_V^- Q_V \Pi_V^-) |-\Delta + V - \epsilon_F|^{\frac{1}{2}} \right) \\ & = \min_{-\Pi^- \leq Q \leq \Pi^+, |-\Delta - \epsilon_F|^{1/2} Q^{\pm\pm} |-\Delta - \epsilon_F|^{1/2} \in \mathfrak{S}_1} \left(\mathrm{Tr}_\Pi ((-\Delta - \epsilon_F) Q) + \int_{\mathbb{R}^d} V \rho_Q \right). \end{aligned}$$

The 1D analog of this equality is given in [FLLS13, Theorem 2.4]. This requires more assumptions on V in order to cancel the singularity in $|k|$ at $2\sqrt{\epsilon_F}$. The above expression means that the minimum relative kinetic energy of a V -perturbed Fermi sea is attained by Q_V , provided that the perturbation has a small kinetic energy (in the sense that $|-\Delta - \epsilon_F|^{1/2} Q^{\pm\pm} |-\Delta - \epsilon_F|^{1/2} \in \mathfrak{S}_1$). This idea is generalized in [CCS18] when treating nonlinear perturbations in a Fermi sea, as discussed in the next section.

1.3.2 Extended defects in a Fermi sea

We summarize in this section the main results obtained in [CCS18]. The aim is to establish a rHF model for a particular instance of infinitely extended defects in a 3D Fermi sea with Coulomb or Yukawa interactions. As mentioned above, the rHF model is of particular interest from a mathematical viewpoint since it is strictly convex in the density; while on the physical side, it can be seen as a good approximation of the (extended) Kohn-Sham LDA model [KS65, DG90, LLS19].

More precisely, we consider 2D-translation invariant defects in a 3D homogeneous electron gas. A typical situation is the case when a slice of finite width of the jellium modeling the uniform nuclear distribution is taken out, see Fig. 1.4. This gives rise to a model describing the uncharged state of a capacitor

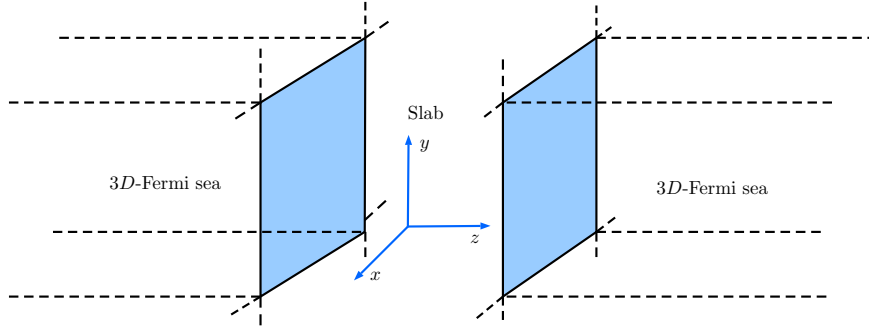


Figure 1.4: An example of an extended defect in a Fermi sea: in a 3D space, a $2D \times d$ slab of uniformly distributed nuclei is removed, where $d \in \mathbb{R}^+$ represents the width of the slab.

composed of two semi-infinite leads separated by some dielectric medium or vacuum. This could be a first step towards the construction of a mean-field model for electronic transport. The mathematical analysis heavily relies on the translation invariance in the directions parallel to the slice. Technically, this allows us to reduce the study of a 3D model to the one of a family of 1D problems labeled by a 2D quasi-momentum. The situation we consider here is the one for which the technical issues are more acute since the family of effective problems are set in dimension 1, which raises integrability issues due to the Peierls oscillations discussed in Theorem 1.1.

Summary of the main results of Chapter 2.

Elements of \mathbb{R}^3 are denoted by $\mathbf{r} = (r, z)$, where $r = (x, y) \in \mathbb{R}^2$ and $z \in \mathbb{R}$. The extended defect is assumed to be (x, y) -translation invariant. The main difficulties with respect to the study of local defects mentioned in the previous sections are: (i) infinitely extended defects are not local since they are (x, y) -translation invariant, hence they cannot be considered *a priori* as a small perturbation, (ii) there are infinitely many interacting electrons in the Fermi sea as we consider Coulomb (resp. Yukawa) interactions, which differs from the linear model considered in [FLLS11, FLLS13] presented in Section 1.3.1. (iii) the system is metallic so that Assumption 1 fails.

The main idea is to fully explore the 2D-translation invariance of the extended defect to transform the original problem into a family of 1D problems indexed by a momentum variable: following the same spirit of the Bloch decomposition introduced in Section 1.2.2 for \mathcal{R} -periodic operators, we introduce a decomposition of (x, y) -translation invariant operators by the following unitary transform \mathcal{U} (which corresponds to a partial Fourier transform) from $L^2(\mathbb{R}^3)$ to $L^2(\mathbb{R}^2, L^2(\mathbb{R}))$ for $q \in \mathbb{R}^2$ and $z \in \mathbb{R}$:

$$\Phi \mapsto (\mathcal{U}\Phi)_q(z) := \frac{1}{2\pi} \int_{\mathbb{R}^2} e^{-iq \cdot r} \Phi(r, z) dr.$$

Since the (rHF) kinetic energy operator for a perfect 3D Fermi sea is (x, y) -translation invariant, hence it

is decomposed by \mathcal{U} :

$$T := -\frac{1}{2}\Delta = \mathcal{U}^{-1} \left(\int_{\mathbb{R}^2}^{\oplus} T_q dq \right) \mathcal{U}, \quad T_q := -\frac{1}{2} \frac{d^2}{dz^2} + \frac{|q|^2}{2}.$$

Remark that T_q acts on $L^2(\mathbb{R})$ for all $q \in \mathbb{R}^2$. This kind of momentum representation is very widely used among physicists when treating systems with partial symmetries. In view of (1.41), the reference state of a perfect Fermi sea is determined either by fixing the Fermi level ϵ_F or by given a uniform density ρ_0 . We choose to fix the Fermi level $\epsilon_F > 0$. Therefore the reference state of a perfect 3D Fermi sea at its "ground state" is described by the following one-body density matrix

$$\gamma_0 := \mathbb{1}_{(-\infty, \epsilon_F]}(T).$$

This operator is also (x, y) -translation invariant, so that it can be decomposed by \mathcal{U} as:

$$\gamma_0 = \mathcal{U}^{-1} \left(\int_{\mathbb{R}^2}^{\oplus} \gamma_{0,q} dq \right) \mathcal{U}, \quad \gamma_{0,q} := \begin{cases} \mathbb{1}_{(-\infty, \epsilon_F]}(T_q) & \text{if } q \in \overline{\mathfrak{B}}_{\epsilon_F}, \\ 0 & \text{if } q \in \mathbb{R}^2 \setminus \overline{\mathfrak{B}}_{\epsilon_F}, \end{cases}$$

where $\overline{\mathfrak{B}}_R := \{q \in \mathbb{R}^2 \mid |q|^2/2 \leq R\}$ for $R \in \mathbb{R}^+$. It can be shown that the unperturbed Fermi has a constant density ρ_0 such that $\epsilon_F = (6\pi^2\rho_0)^{2/3}/2$, see Section 2.5.2 for a detailed calculation.

The state γ_0 can be seen as the rHF ground-state density matrix of an infinite, locally neutral system, whose nuclear distribution is a jellium of uniform density ρ_0 . This suggests that the perfect Fermi sea at its ground state can be seen as a neutral metallic system with uniform nuclear and electronic density.

Similarly to local defects, the state of the 3D Fermi sea with a slice-like defect can be written as

$$\gamma = \gamma_0 + Q,$$

except that the operator Q is not-local in the sense that it is also (x, y) -translation invariant. Recall that for a \mathcal{R} -periodic systems we have employed the Bloch decomposition \mathcal{B} to define a relative kinetic energy per unit cell in (1.30). In (x, y) -translation invariant systems, we can define the following *renormalized kinetic energy per unit area* through the partial Fourier transform \mathcal{U} :

$$\underline{\text{Tr}}((T - \epsilon_F)Q) := \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} \text{Tr}_{L^2(\mathbb{R})} \left(|T_q - \epsilon_F|^{1/2} (Q_q^{++} - Q_q^{--}) |T_q - \epsilon_F|^{1/2} \right) dq,$$

where

$$Q_q^{++} := (1 - \gamma_{0,q})Q_q(1 - \gamma_{0,q}), \quad Q_q^{--} := \gamma_{0,q}Q_q\gamma_{0,q}.$$

In analogy to (1.37), we introduce the following convex set of admissible perturbative states Q :

$$\mathcal{K} := \left\{ Q := \mathcal{U}^{-1} \left(\int_{\mathbb{R}^2}^{\oplus} Q_q dq \right) \mathcal{U} \mid q \mapsto Q_q \in L^\infty(\mathbb{R}^2; \mathcal{S}(L^2(\mathbb{R}))), Q_q \in \mathcal{K}_q, \underline{\text{Tr}}((T - \epsilon_F)Q) < \infty \right\},$$

where the convex set $\mathcal{K}_q := \{Q_q \in \mathcal{X}_q \mid -\gamma_{0,q} \leq Q_q \leq 1 - \gamma_{0,q}\}$ is the space of operators with finite kinetic energies similar to the Banach space defined in (1.43), and where

$$\mathcal{X}_q := \left\{ Q_q \in \mathcal{S}(L^2(\mathbb{R})) \mid |T_q - \epsilon_F|^{1/2} Q_q \in \mathfrak{S}_2(L^2(\mathbb{R})), |T_q - \epsilon_F|^{1/2} Q_q^{\pm\pm} |T_q - \epsilon_F|^{1/2} \in \mathfrak{S}_1(L^2(\mathbb{R})) \right\},$$

equipped with the norm

$$\begin{aligned} \|Q_q\|_{\mathcal{X}_q} &:= \|Q_q\|_{\mathcal{L}(L^2(\mathbb{R}))} + \left\| |T_q - \epsilon_F|^{1/2} Q_q \right\|_{\mathfrak{S}_2(L^2(\mathbb{R}))} \\ &\quad + \sum_{\alpha \in \{+, -\}} \left\| |T_q - \epsilon_F|^{1/2} Q_q^{\alpha\alpha} |T_q - \epsilon_F|^{1/2} \right\|_{\mathfrak{S}_1(L^2(\mathbb{R}))}. \end{aligned}$$

The following proposition gives a meaning to densities of operators in \mathcal{K} . In particular, we obtain a Lieb-Thirring like inequality analogous to (1.44).

Theorem 1.2. (*Lieb–Thirring inequality for operators in \mathcal{K} [Chapter 2, Proposition 2.2]*) Any $Q \in \mathcal{K}$ is locally trace-class, its density ρ_Q is a function of the variable z only, and

$$\rho_Q \in L^p(\mathbb{R}) + L^2(\mathbb{R})$$

for any $1 < p < 5/3$. In addition, for all $1 < p < 5/3$ and all $c > 0$, there exist two positive constants $\eta_{c,-}, \eta_{p,c,+}$ such that

$$\forall Q \in \mathcal{K}, \quad \underline{\text{Tr}}((T - \epsilon_F)Q) \geq \eta_{c,-} \|\rho_Q^{c,-}\|_{L^2(\mathbb{R})}^2 + \eta_{p,c,+} \|\rho_Q^{c,+}\|_{L^p(\mathbb{R})}^p,$$

where $\rho_Q = \rho_Q^{c,-} + \rho_Q^{c,+}$ with

$$\rho_Q^{c,-} := \frac{1}{(2\pi)^2} \int_{\overline{\mathfrak{B}}_{\epsilon_F+c}} \rho_{Q_q} dq \in L^2(\mathbb{R}), \quad \text{and} \quad \rho_Q^{c,+} := \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2 \setminus \overline{\mathfrak{B}}_{\epsilon_F+c}} \rho_{Q_q} dq \in L^p(\mathbb{R}).$$

Since operators in \mathcal{K} are (x, y) -translation invariant, their densities depend only on the variable z . In Theorem 1.1 we have discussed that a 1D Lieb–Thirring inequality analogous to (1.44) is not available. However the above proposition suggests that a quasi 1D Lieb–Thirring like inequality is possible. As a matter of fact, in this case, the logarithmic divergence at $2\sqrt{\epsilon_F}$ is averaged by the momentum representation $q \in \mathbb{R}^2$, so that the 1D Peierls oscillations disappear. In this sense, (x, y) -translation invariant systems are quasi 1D, but they are very different from actual 1D systems. However, recall that in the rHF approximation electrons interact with each other through the electronic density. As the electronic densities are (x, y) -translation invariant, the Coulomb electron-electron interactions are actually one dimensional. One can define the 1D Coulomb space

$$\underline{\mathcal{C}} := \left\{ f \in \mathcal{S}'(\mathbb{R}) \mid \hat{f} \in L^1_{\text{loc}}(\mathbb{R}), \frac{\hat{f}(k)}{|k|} \in L^2(\mathbb{R}) \right\}.$$

The above definition implies that densities in $\underline{\mathcal{C}}$ are neutral in a weak sense: if $\rho \in \underline{\mathcal{C}} \cap L^1(\mathbb{R})$, then $\int_{\mathbb{R}} \rho = (2\pi)^{1/2} \hat{\rho}(0) = 0$ since the function $k \mapsto \frac{|\hat{\rho}(k)|^2}{|k|^2}$ has to be integrable in the vicinity of 0. This implies that the defect state Q is also charge neutral in our context. Due to this constraint, it is convenient to introduce the renormalized Yukawa space for a parameter $m \geq 0$:

$$\underline{\mathcal{C}}_m := \left\{ f \in \mathcal{S}'(\mathbb{R}) \mid \hat{f} \in L^1_{\text{loc}}(\mathbb{R}), \frac{\hat{f}(k)}{\sqrt{|k|^2 + m^2}} \in L^2(\mathbb{R}) \right\}.$$

Densities in Yukawa space are no longer necessarily neutral. We shall see in the sequel and in Chapter 2 that one can define a meaningful mean-field potential through the 1D Yukawa kernel $m^{-1}e^{-m|\cdot|}$, while we were not able to do the same with the 1D Coulomb kernel $-|\cdot|$, as it requires some extra decay properties on the densities.

Let us introduce the Yukawa interactions:

$$\forall f, g \in \underline{\mathcal{C}}_m, \quad \underline{D}_m(f, g) := 2 \int_{\mathbb{R}} \frac{\overline{\hat{f}(k)} \hat{g}(k)}{|k|^2 + m^2} dk.$$

Yukawa interactions are short-ranged when m is large. When $m = 0$ one recovers the long-ranged Coulomb interaction. We therefore denote the Coulomb space $\underline{\mathcal{C}}$ by $\underline{\mathcal{C}}_0$ in the sequel.

Consider an (x, y) -translation invariant slice-like defect ν , typically a sharp trench

$$\nu = -\rho_0 \mathbb{1}_{[-w/2, w/2]}(z).$$

The associated *renormalized free energy per unit area* is defined as, similarly to (1.38):

$$\mathcal{E}_{\nu, m}(Q) := \underline{\text{Tr}}((T - \epsilon_F)Q) + \frac{1}{2} \underline{D}_m(\rho_Q - \nu, \rho_Q - \nu).$$

Introduce also the (possibly empty) space $\mathcal{F}_\nu := \{Q \in \mathcal{K} \mid \rho_Q - \nu \in \underline{\mathcal{C}}_0\}$ for Coulomb interactions. We first prove that a 3D Fermi sea with extended defects with the Yukawa (resp.) Coulomb interactions admits minimizers, and that all the minimizers share the same density.

Theorem 1.3 (Existence of minimizers for Yukawa and Coulomb interactions [Chapter 2, Theorem 2.6]).

(1) *Yukawa interaction: for any $\nu \in H^{-1}(\mathbb{R})$, the minimization problem*

$$\boxed{I_{\nu,m} = \inf\{\mathcal{E}_{\nu,m}(Q), Q \in \mathcal{K}\}} \quad (1.47)$$

has a minimizer $Q_{\nu,m}$ and all the minimizers share the same density $\rho_{\nu,m}$.

(2) *Coulomb interaction: for any $\nu \in L^1(\mathbb{R})$ such that $|\cdot|\nu(\cdot) \in L^1(\mathbb{R})$, the set \mathcal{F}_ν is non-empty, the minimization problem*

$$\boxed{I_{\nu,0} = \inf\{\mathcal{E}_{\nu,0}(Q), Q \in \mathcal{F}_\nu\}} \quad (1.48)$$

has a minimizer $Q_{\nu,0}$, and all the minimizers share the same density $\rho_{\nu,0}$.

From theoretical and numerical points of view, it is natural to investigate whether one recovers the ground state with Coulomb interactions when the Yukawa parameter m tends to 0, and whether the Yukawa minimizers converge to the Coulomb minimizers in some sense. The following theorem provides an answer to these questions.

Theorem 1.4 (Convergence of Yukawa minimizers to Coulomb minimizers [Chapter 2, Theorem 2.6]). *For any $\nu \in H^{-1}(\mathbb{R})$, the function $(0, +\infty) \ni m \mapsto I_{\nu,m} \in \mathbb{R}_+$ is continuous, non-increasing, and*

$$\lim_{m \rightarrow 0} I_{\nu,m} \leq I_{\nu,0} \quad \text{and} \quad \lim_{m \rightarrow +\infty} I_{\nu,m} = 0,$$

with the convention that $I_{\nu,0} = +\infty$ if \mathcal{F}_ν is empty. When $\nu \in L^1(\mathbb{R})$ and $|\cdot|\nu(\cdot) \in L^1(\mathbb{R})$,

$$\lim_{m \rightarrow 0} I_{\nu,m} = I_{\nu,0}.$$

Moreover, if $\nu \in L^1(\mathbb{R})$ and $|\cdot|\nu(\cdot) \in L^1(\mathbb{R})$, there exists a sequence $(m_k)_{k \in \mathbb{N}}$ of positive real numbers decreasing to zero, and a sequence $(Q_{\nu,m_k})_{k \in \mathbb{N}}$ of elements of \mathcal{K} such that, for each $k \in \mathbb{N}$, Q_{ν,m_k} is a minimizer of (1.47) for $m = m_k$, converging to a minimizer $Q_{\nu,0}$ of (1.48) in the following sense:

$$\mathcal{U} Q_{\nu,m_k} \mathcal{U}^{-1} \xrightarrow{k \rightarrow \infty} \mathcal{U} Q_{\nu,0} \mathcal{U}^{-1} \quad \text{for the weak-* topology of } L^\infty(\mathbb{R}^2; \mathcal{S}(L^2(\mathbb{R}))); \quad (1.49)$$

$$\mathcal{U} |T - \epsilon_F|^{1/2} Q_{\nu,m_k} \mathcal{U}^{-1} \xrightarrow{k \rightarrow \infty} \mathcal{U} |T - \epsilon_F|^{1/2} Q_{\nu,0} \mathcal{U}^{-1} \quad \text{weakly in } L^2(\mathbb{R}^2; \mathfrak{S}_2(L^2(\mathbb{R}))). \quad (1.50)$$

In the Yukawa case ($m > 0$), we are able to characterize the minimizers of (1.47) analogously to (1.40).

Theorem 1.5 (Characterization of the minimizer for Yukawa interaction [Chapter 2, Theorem 2.8]). *Let $\nu \in H^{-1}(\mathbb{R})$ and $m > 0$. The minimizer $Q_{\nu,m}$ of problem (1.47) is unique and is the unique solution in \mathcal{K} to the self-consistent equations:*

$$\begin{cases} \gamma_{\nu,m} := \mathbf{1}_{(-\infty, \epsilon_F]}(T + V_{\nu,m}), \\ V_{\nu,m} := \frac{e^{-m|\cdot|}}{m} \star (\rho_{Q_{\nu,m}} - \nu), \\ Q_{\nu,m} := \gamma_{\nu,m} - \gamma_0. \end{cases} \quad (1.51)$$

The proof of the above theorem is rather technical because of the metallic nature of the system, and we were not able to provide similar results in the Coulomb case, mainly due to the 1D Coulomb interactions giving rise to the mean-field potential $V_{0,m} = |\cdot| \star (\rho_{Q_{\nu,0}} - \nu)$ that may diverge. This leads to some technical issues which prevent to defining a suitable mean-field Hamiltonian. Moreover, although Yukawa minimizers can be completely characterized by Theorem 1.5, we were not able to show that Coulomb minimizers a self-consistent equation similar to (1.51).

1.4 Junction of quasi 1D systems with Coulomb interactions

Atomic junctions of quasi 1D systems appear for instance when studying the surface states of one-dimensional (1D) crystals [Aer60, Sho39], quantum thermal transport in nanostructures [WWL08], and p-n junctions [BCYJH14, PFM14] which are key building blocks of modern semiconductor electronic devices. Besides, electronic transport in carbon nanotubes [LKS⁺15] and in molecular wires [NR03], which recently attracted a lot of interest, is often modeled by the junction of two semi-infinite systems with different chemical potentials. In recent years, studies of various quantum Hall effects and topological insulators focussed attention on 2D materials, see [HK10] and references therein. These 2D materials often possess periodicity in one dimension and can therefore be reduced to quasi 1D materials by momentum representation in the periodic direction [Hat93]. Furthermore, when studying edge states properties (see [Hat93, ASBVB13] and references therein) of 2D materials, these 2D materials can be seen as a junction with the vacuum: vacuum occupies one half of the 2D space, and the other half is occupied by a semi-infinite 2D material. The edge of the 2D materials is the junction surface between the vacuum and the 2D material, hence the edges states can be considered as states propagating alongside this junction surface.

The most prominent feature of quasi 1D materials (see Fig 1.5 for an illustration) is the presence of strong electron-electron interactions due to low screening effects [Bru10, Bru14] as electrons interact through the 3D space. For finite systems one can use an N -body Schrödinger model presented in Section 1.1.1 to describe electron-electron interactions. Nevertheless this is impossible for infinite systems. Mean-field approximations are good candidates to model infinite periodic systems as mentioned in Section 1.2. However, mean-field models are rarely available for quasi 1D periodic systems, as periodic systems are often considered either in the 3D space as in Section 1.2.2 (see also [LIE, CBL98] for Thomas–Fermi type models and [CLBL01] for Hartree–Fock type models), or in a strictly 1D geometry (see [BLB02] for Thomas–Fermi type models). The ground state of a 1D periodic system with interactions through the 3D space has been examined within a Thomas–Fermi type model [BLB00] for polymers. It is worth mentioning that for systems which are periodic in one direction, the ground state problem of periodic (in one direction) defects in the Schrödinger–Poisson model (rHF with positive temperature) has been treated in [Nie93a, Appendix] through a variational approach. Furthermore, a junction system is *a priori* a non-periodic infinite system. This gives rise to many mathematical challenges such as the definition of the ground state energy [BLBL03] and the justification of the model by a thermodynamic limit [HLS09b, HLS09c].

In this section we briefly describe the results obtained in [Cao19], which discusses mean-field stability of junctions of quasi 1D systems with Coulomb interactions. We start by introducing a rHF description for a periodic quasi 1D systems, in the same spirit as for the 3D periodic systems discussed in Section 1.2.2. We next introduce a junction model within the rHF framework and discuss the existence of a ground state for a junction system.

1.4.1 Mathematical models of quasi 1D systems

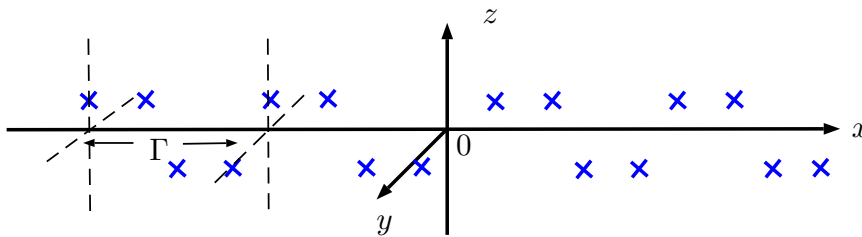


Figure 1.5: An example of nuclei configuration of a quasi 1D periodic system.

Consider a quasi 1D periodic system described by nuclei arranged periodically alongside the x -axis (see Fig. 1.5), with electrons occupying the 3D space. Its unit cell is denoted by $\Gamma := [-1/2, 1/2) \times \mathbb{R}^2$. We denote elements of \mathbb{R}^3 by $\mathbf{x} = (x, \mathbf{r})$ where $\mathbf{r} = (y, z)$ representing the other two directions. Assume that the periodic nuclear density is a smooth function μ_{per} which is \mathbb{Z} -translation invariant *only in the*

x-direction. We introduce a mixed Fourier transform \mathcal{F} consisting of a Fourier series transform in the *x*-direction and an integral Fourier transform in the *r*-direction. The operator \mathcal{F} is an isometry from $L^2_{\text{per},x}(\Gamma)$, the space of $L^2_{\text{loc}}(\mathbb{R}^3)$ functions that are \mathbb{Z} -periodic in the *x*-direction and square integrable in *r*-directions, to $\ell^2(\mathbb{Z}, L^2(\mathbb{R}^2))$ in the following sense:

$$\forall f, g \in L^2_{\text{per},x}(\Gamma), \quad \int_{\Gamma} \overline{f(x, \mathbf{r})} g(x, \mathbf{r}) dx d\mathbf{r} = \sum_{n \in \mathbb{Z}} \int_{\mathbb{R}^2} \overline{\mathcal{F}f(n, \mathbf{k})} \mathcal{F}g(n, \mathbf{k}) d\mathbf{k}. \quad (1.52)$$

In analogy to (1.29), we introduce the space of density matrices with finite kinetic energy per unit volume for the periodic quasi 1D systems

$$\mathcal{P}_{\text{per},x} := \left\{ \gamma \in \mathcal{S}(L^2(\mathbb{R}^3)) \mid 0 \leq \gamma \leq 1, \forall \mathbf{k} \in \mathbb{Z}, \tau_{\mathbf{k}}^x \gamma = \gamma \tau_{\mathbf{k}}^x, \int_{\Gamma^*} \text{Tr}_{L^2_{\text{per},x}}(\sqrt{1 - \Delta_{\xi}} \gamma_{\xi} \sqrt{1 - \Delta_{\xi}}) d\xi < \infty \right\},$$

as well as the Coulomb space

$$\mathcal{C}_{\Gamma} := \left\{ f \in \mathcal{S}'_{\text{per},x}(\Gamma) \mid \forall n \in \mathbb{Z}, \mathcal{F}(f)(n, \cdot) \in L^1_{\text{loc}}(\mathbb{R}^2), D_{\Gamma}(f, f) < +\infty \right\},$$

where

$$D_{\Gamma}(f, g) := 4\pi \sum_{n \in \mathbb{Z}} \int_{\mathbb{R}^2} \frac{\overline{\mathcal{F}(f)(n, \mathbf{k})} \mathcal{F}(g)(n, \mathbf{k})}{|\mathbf{k}|^2 + 4\pi^2 n^2} d\mathbf{k}$$

is the Coulomb energy associated with densities f, g interacting in the 3D space. The rHF energy functional for this \mathbb{Z} -periodic quasi 1D system associated with a trial density matrix γ can be defined, in the same spirit as for (1.30), as

$$\mathcal{E}_{\text{per},x}(\gamma) := \frac{1}{|\Gamma^*|} \int_{\Gamma^*} \text{Tr}_{L^2_{\text{per},x}(\Gamma)} \left(-\frac{1}{2} \Delta_{\xi} \gamma_{\xi} \right) d\xi + \frac{1}{2} D_{\Gamma}(\rho_{\gamma} - \mu_{\text{per}}, \rho_{\gamma} - \mu_{\text{per}}).$$

Denote by

$$\mathcal{F}_{\Gamma} = \{ \gamma \in \mathcal{P}_{\text{per},x} \mid \rho_{\gamma} - \mu_{\text{per}} \in \mathcal{C}_{\Gamma} \}$$

the space of states with finite kinetic energy per unit cell and finite Coulomb interaction energy per unit cell. The ground state of the quasi 1D system is given by

$$I_{\text{per}} = \inf \{ \mathcal{E}_{\text{per},x}(\gamma) \mid \gamma \in \mathcal{F}_{\Gamma} \}. \quad (1.53)$$

The following theorem ensures the existence of the rHF ground state for this quasi 1D periodic system.

Theorem 1.6 (Existence of a periodic rHF ground state. [Chapter 3, Theorem 3.6]). *The minimization problem (1.53) admits a minimizer γ_{per} with density $\rho_{\gamma_{\text{per}}}$ belonging to $L^p_{\text{per},x}(\Gamma)$ for $1 \leq p \leq 3$. Besides, all the minimizers share the same density.*

Remark that the above theorem is different from the results in [CLBL01, CDL08a] as the system is periodic only in the *x*-direction, so that the unit cell Γ is unbounded. Additional compactness estimates are therefore needed when dealing with the ground state problem. With an additional mild summability condition

$$\int_{\Gamma} |\mathbf{r}| \rho_{\gamma_{\text{per}}}(x, \mathbf{r}) dx d\mathbf{r} < +\infty \quad (1.54)$$

on the unique density of minimizers, we can prove that the system is characterized by a mean-field Hamiltonian

$$H_{\text{per}} = -\frac{1}{2} \Delta + V_{\text{per,sym}},$$

where $V_{\text{per,sym}}$ such that $-\Delta V_{\text{per,sym}} = 4\pi(\rho_{\gamma_{\text{per}}} - \mu_{\text{per}})$ is a mean-field potential tending to 0 in the *r*-direction. The reason why we require (1.54) is discussed in Remark 3.9 in Chapter 3. The main purpose is

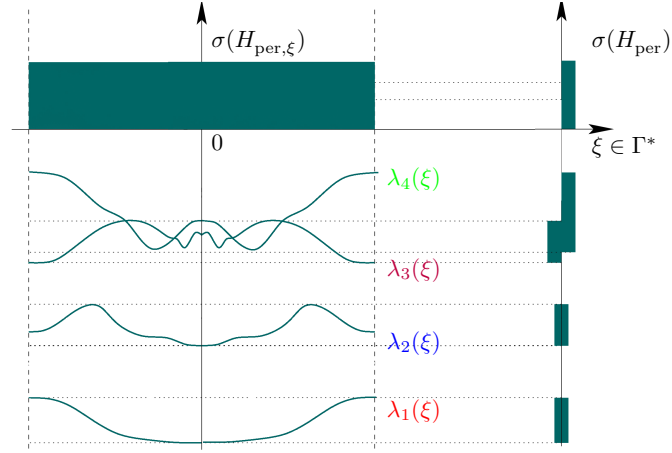


Figure 1.6: The spectrum of $H_{\text{per},\xi}$ and the band structure of H_{per} .

to define the mean-field potential $V_{\text{per},\text{sym}}$ and obtain some decay estimates of $V_{\text{per},\text{sym}}$ in the r -direction, given that the Green's kernel has log-growth in the r -direction.

We also obtain in [Theorem 3.7, Chapter 3] that there exists $N_H \in \mathbb{N}^*$ (which can be finite or infinite), and a sequence $\{\lambda_n(\xi)\}_{\xi \in \Gamma^*, 1 \leq n \leq N_H}$ such that

$$\sigma_{\text{ess}}(H_{\text{per},\xi}) = [0, +\infty), \quad \sigma_{\text{disc}}(H_{\text{per},\xi}) = \bigcup_{1 \leq n \leq N_H} \lambda_n(\xi) \subset [-\|V_{\text{per},\text{sym}}\|_{L^\infty}, 0).$$

Moreover, the following spectral decomposition holds (see Fig. 1.6):

$$\sigma(H_{\text{per}}) = \sigma_{\text{ess}}(H_{\text{per}}) = \bigcup_{\xi \in \Gamma^*} \sigma(H_{\text{per},\xi}), \quad \bigcup_{\xi \in \Gamma^*} \sigma_{\text{disc}}(H_{\text{per},\xi}) \subseteq \sigma_{\text{ac}}(H_{\text{per}}).$$

In particular, $[0, +\infty) \subset \sigma_{\text{ess}}(H_{\text{per}})$. The following theorem guarantees that the Fermi level of the quasi 1D system at its ground state is always negative under assumption (1.54).

Theorem 1.7 (Characterization of the ground state, [Chapter 3, Theorem 3.7]). *Suppose that the summability condition (1.54) holds. Then*

(1) *(The Fermi level is always negative) The energy level counting function*

$$F(\kappa) : \kappa \mapsto \frac{1}{|\Gamma^*|} \int_{\Gamma^*} \text{Tr}_{L^2_{\text{per},x}(\Gamma)} (\mathbb{1}_{(-\infty, \kappa]}(H_{\text{per},\xi})) d\xi = \frac{1}{|\Gamma^*|} \sum_{n=1}^{N_H} \int_{\Gamma^*} \mathbb{1}(\lambda_n(\xi) \leq \kappa) d\xi$$

is continuous and non-decreasing on $(-\infty, 0]$. The following inequality always holds:

$$N_H = F(0) \geq \int_{\Gamma} \mu_{\text{per},\text{sym}},$$

which means that there are always enough negative energy levels for the electrons. Moreover, there exists a real number $\epsilon_F < 0$ called Fermi level (chemical potential) such that $F(\epsilon_F) = \int_{\Gamma} \mu_{\text{per},\text{sym}} = Z$, which represents the highest occupied electronic energy level.

(2) *(The unique minimizer is a spectral projector) The minimizer of problem (3.17) is unique and satisfies the following self-consistent equation:*

$$\gamma_{\text{per}} = \mathbb{1}_{(-\infty, \epsilon_F]}(H_{\text{per}}) = \mathcal{B}^{-1} \left(\int_{\Gamma^*} \gamma_{\text{per},\xi} \frac{d\xi}{2\pi} \right) \mathcal{B}, \quad \gamma_{\text{per},\xi} := \mathbb{1}_{(-\infty, \epsilon_F]}(H_{\text{per},\xi}). \quad (1.55)$$

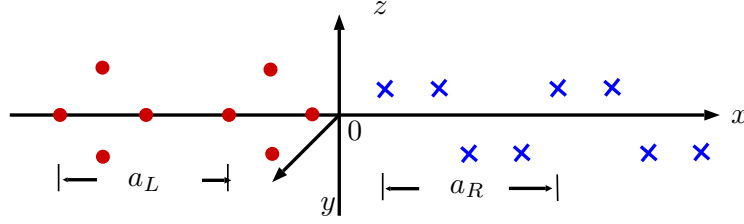


Figure 1.7: Nuclei configuration of the junction with period a_L on $(-\infty, 0] \times \mathbb{R}^2$ and a_R on $(0, +\infty) \times \mathbb{R}^2$.

1.4.2 Junction of quasi 1D systems.

In this section we describe the junction of two quasi 1D periodic systems with periods $a_L, a_R > 0$ such that $a_L \neq a_R$, and total charges of the nuclei per unit cell $Z_L, Z_R \in \mathbb{N} \setminus \{0\}$. We assume that the nuclear densities are described by

$$\mu_{\text{per},L}(x, \mathbf{r}) := \sum_{n \in \mathbb{Z}} Z_L m_L(x - a_L n, \mathbf{r}), \quad \mu_{\text{per},R}(x, \mathbf{r}) := \sum_{n \in \mathbb{Z}} Z_R m_R(x - a_R n, \mathbf{r}),$$

where $m_L(x, \mathbf{r})$ and $m_R(x, \mathbf{r})$ are non-negative C_c^∞ functions with supports respectively in $\Gamma_L := [-\frac{a_L}{2}, \frac{a_L}{2}] \times \mathbb{R}^2$ and $\Gamma_R := [-\frac{a_R}{2}, \frac{a_R}{2}] \times \mathbb{R}^2$, and such that $\int_{\mathbb{R}^3} m_L = 1$ and $\int_{\mathbb{R}^3} m_R = 1$.

In order to describe the junction of quasi 1D systems, more specifically to guarantee that the Coulomb energy generated by the perturbative state is finite, more assumptions on the integrability of the mean-field potential in the \mathbf{r} -direction are needed. We refer to the discussion preceding Lemma 3.10 in Chapter 3 for further details. A sufficient assumption is to require certain radial symmetry on the nuclear densities $\mu_{\text{per},L}$ and $\mu_{\text{per},R}$ of two different quasi 1D periodic systems. More precisely, we assume that there exist $m_{\text{sym},L}, m_{\text{sym},R} \in C_c^\infty(\mathbb{R})$ such that

$$\forall \mathbf{r} \in \mathbb{R}^2, \quad \int_{-a_L/2}^{a_L/2} m_L(x, \mathbf{r}) dx \equiv m_{\text{sym},L}(|\mathbf{r}|), \quad \int_{-a_R/2}^{a_R/2} m_R(x, \mathbf{r}) dx \equiv m_{\text{sym},R}(|\mathbf{r}|). \quad (1.56)$$

The junction system is described by considering the following nuclear configuration (see Fig. 1.7):

$$\mu_J := \mathbb{1}_{x \leq 0} \cdot \mu_{\text{per},L} + \mathbb{1}_{x > 0} \cdot \mu_{\text{per},R} + v,$$

where v is a local term around the origin describing how the nuclear configuration of the junction is initiated. We aim at establishing a quasi-particle description of this infinitely extended junction system with Coulomb interactions and show the existence of a ground state. As we do not assume any commensurability of the periods of the two quasi 1D systems, the junction system does not possess any translation-invariant symmetry. The main idea is to establish a well-suited reference system based on the linear combination of periodic systems, and use perturbative techniques described in Section 1.3.1 to justify the construction. More precisely, for $\mathbf{x} \in \mathbb{R}^3$, let us consider a set of smooth cut-off functions approximating $\mathbb{1}_{x \leq 0}$:

$$\mathcal{X} := \left\{ \chi \in C^2(\mathbb{R}^3) \mid 0 \leq \chi \leq 1; \chi(\mathbf{x}) = 1 \text{ if } \mathbf{x} \in \left(-\infty, -\frac{a_L}{2}\right] \times \mathbb{R}^2; \right. \\ \left. \chi(\mathbf{x}) = 0 \text{ if } \mathbf{x} \in \left[\frac{a_R}{2}, +\infty\right) \times \mathbb{R}^2 \right\}. \quad (1.57)$$

Fixing a function χ belonging to \mathcal{X} , we define a reference Hamiltonian and a reference state as

$$H_\chi = \chi H_{\text{per},L} \chi + \sqrt{1 - \chi^2} H_{\text{per},R} \sqrt{1 - \chi^2}, \quad \gamma_\chi := \mathbb{1}_{(-\infty, \epsilon_F)}(H_\chi),$$

where $H_{\text{per},L}$ and $H_{\text{per},R}$ are the mean-field Hamiltonians of the quasi 1D periodic systems. The following result shows that the definition of this reference state makes sense.

Proposition 1.8 ([Propositions 3.11 and 3.12, Chapter 3]). *Under the symmetry assumption (1.56) on the nuclear density,*

(1) (Spectral properties of the reference state H_χ) The essential spectrum of H_χ satisfies

$$\sigma_{\text{ess}}(H_\chi) = \sigma_{\text{ess}}(H_{\text{per},L}) \bigcup \sigma_{\text{ess}}(H_{\text{per},R}).$$

In particular, $[0, +\infty) \subset \sigma_{\text{ess}}(H_\chi)$ and $\sigma_{\text{ess}}(H_\chi)$ does not depend on the choice of the cut-off function $\chi \in \mathcal{X}$ defined in (1.57).

(2) (Exponential decay of the density difference) If ϵ_F is in the gap of H_χ , the spectral projector γ_χ is locally trace class, and its density ρ_χ is well defined in $L^1_{\text{loc}}(\mathbb{R}^3)$. Moreover,

$$\chi^2 \rho_{\text{per},L} + (1 - \chi^2) \rho_{\text{per},R} - \rho_\chi \in L^p(\mathbb{R}^3) \text{ for } 1 < p \leq 2.$$

Furthermore, denote by w_a the characteristic function of the unit cube centered at $a \in \mathbb{R}^3$. There exist positive constants C and t such that for all

$$\alpha = (\alpha_x, 0, 0) \in \mathbb{R}^3, \text{ with either } \text{supp}(w_\alpha) \subset (-\infty, a_L/2] \times \mathbb{R}^2 \text{ or } \text{supp}(w_\alpha) \subset [a_R/2, +\infty) \times \mathbb{R}^2,$$

it holds

$$\int_{\mathbb{R}^3} |w_\alpha (\chi^2 \rho_{\text{per},L} + (1 - \chi^2) \rho_{\text{per},R} - \rho_\chi) w_\alpha| \leq C e^{-t|\alpha|}.$$

The first result implies that the essential spectrum of the reference Hamiltonian is independent of the cut-off function χ . In particular, the linear junction preserves the scattering channels of the underlying systems, since the purely absolutely continuous spectrum of Hamiltonian has not been modified. The junction can be then used to study the electronic conductance with the Landauer-Büttiker formalism (see for example [BJLP15, BJLP16a, BJLP16b]) as well as the discussion following Proposition 3.11 in Chapter 3). The proof of the first result relies on an explicit construction of Weyl sequences associated with H_χ . The second result implies that the electronic density of the reference state γ_χ is exponential close to linear combinations of the original underlying densities. The proof of the results relies on Combes-Thomas estimates [CT73, Theorem 1].

The quasi-particle description of the nonlinear junction state can be constructed by considering

$$\gamma_J = \gamma_\chi + Q_\chi,$$

where Q_χ is a trial density matrix which encodes the nonlinear effects of the junction system. We associate Q_χ with some minimization problem and obtain a similar self-consistent equation [Proposition 3.15, Chapter 3] similar to (1.40). Denote by \overline{Q}_χ one of the minimizers. We show that the ground state of the junction system with Coulomb interactions exists and that its density is independent of the choice of the reference state.

Theorem 1.9 (Independence of the choice of reference states [Theorem 3.17, Chapter 3]). *Under the symmetry assumption (1.56) on the nuclear density, the density of the junction system $\rho_{\gamma_J} = \rho_\chi + \rho_{\overline{Q}_\chi}$ is unique and is independent of $\chi \in \mathcal{X}$.*

Extension to 2D materials. We briefly discuss the possible extension of the framework considered here to 2D materials in Section 3.3.5. We show that same techniques can be applied to treat the junctions of 2D materials, basically by combining the techniques used in [CCS18] and [Cao19]. This work is not finished.

1.5 Lattice dynamics in an adiabatic Born-Oppenheimer approximation

The previous sections discussed the ground-state electronic structures of materials, when the nuclear configurations are assumed to be fixed. In this section we focus on mathematical modeling of nuclear dynamics from first-principle, and describe our framework as well as results obtained at this stage for an on-going work on *adiabatic Born–Oppenheimer approximation* (ABO) [BO27, PLC⁺07] of nuclear dynamics in Chapter 4.

In this approximation, the dynamics of nuclei and electrons are decoupled. Furthermore, one assumes that electrons move instantaneously to their ground state when nuclei move. Electrons together with nuclei generate a Coulomb potential, which drives nuclear dynamics. Therefore nuclei obey an autonomous classical Hamiltonian dynamics on a potential energy surface obtained by electronic ground-state calculations. As discussed in Section 1.1, the electronic ground state problem itself needs to be approximated when the number of electrons becomes large. We choose in this work the rHF approximation of the electronic ground states introduced in Section 1.1.2.

One of our main motivations is to study the nonlinear collective excitations of nuclei (phonon modes) in a crystal. However rHF ground states associated with generic $\ell^\infty(\mathcal{R})$ -nuclear displacements with respect to the periodic configuration (where \mathcal{R} is the crystal lattice) are unknown. By relying on results from [CDL08a, CE11] for the rHF ground states of crystals with local defects, we instead focus on the fully nonlinear rHF Born-Oppenheimer dynamics of nuclei in the neighborhood of an equilibrium periodic configuration of a crystal. We define a Hilbert space \mathcal{H} of admissible nuclear displacements which is densely embedded in $\ell^2(\mathcal{R})$, and also introduce an infinite-dimensional Hamiltonian from $\mathcal{H} \times \ell^2(\mathcal{R})$ to \mathbb{R} describing the dynamics of nuclei. Our result is that for small initial data, the Cauchy problem associated with this Hamiltonian dynamics is well posed for short times. The existence and uniqueness for arbitrary initial data in $\mathcal{H} \times \ell^2(\mathcal{R})$, and/or for long time requires a perturbation analysis of the rHF model when the Fermi level is occupied. This will be addressed in future work. The result presented in Chapter 4 will be part of an article in preparation [CCS19].

This chapter describes results obtained in [CCS18].

Abstract. Studying the electronic structure of defects in materials is an important subject in condensed matter physics. From a mathematical point of view, nonlinear mean-field models of localized defects in insulators are well understood. We present here a mean-field model to study a particular instance of extended defects in metals. These extended defects typically correspond to taking out a slab of finite width in the three-dimensional homogeneous electron gas. We work in the framework of the reduced Hartree-Fock model with either Yukawa or Coulomb interactions. Using techniques developed in [FLLS11, FLLS13] to study local perturbations of the free-electron gas, we show that our model admits minimizers, and that Yukawa ground state energies and density matrices converge to ground state Coulomb energies and density matrices as the Yukawa parameter tends to zero. These minimizers are unique for Yukawa interactions, and are characterized by a self-consistent equation. We moreover present numerical simulations where we observe Friedel oscillations in the total electronic density.

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2.1 Introduction

In Section 2.2, we introduce a reduced Hartree-Fock model amenable to describe an extended two-dimensional defect in the three-dimensional Fermi sea, under the assumption that the defect is translation invariant in the (x, y) -directions. After introducing the functional setting in Section 2.2.1, we define renormalized free kinetic and potential energy functionals for an (x, y) -translation invariant defect in Section 2.2.2. In Section 2.2.3, we use these elementary bricks to define reduced Hartree-Fock (rHF) energy functionals for (x, y) -translation invariant defects, both for Coulomb and Yukawa interactions, and prove the existence of a ground state. We also show that the Yukawa ground states converge to the Coulomb ground states when the characteristic length of the Yukawa interaction goes to infinity, and uniquely characterize the minimizers for Yukawa interactions. The proof of the results presented in Section 2.2 can be read in Section 2.3. Finally, results of numerical simulations are reported in Section 2.4 for a model capacitor.

2.2 Construction of the model

Elements of \mathbb{R}^3 are denoted by $\mathbf{r} = (r, z)$, where $r = (x, y) \in \mathbb{R}^2$ and $z \in \mathbb{R}$.

2.2.1 Functional setting

In Section 2.2.1, we introduce a natural decomposition of (x, y) -translation invariant operators based on partial Fourier transform. In Section 2.2.1, we apply it to the special case of (x, y) -translation invariant one-body density matrices.

Decomposition of (x, y) -translation invariant operators

For $r = (x, y) \in \mathbb{R}^2$, we denote by τ_r the translation operator acting on $L^2_{\text{loc}}(\mathbb{R}^3)$ as

$$\forall u \in L^2_{\text{loc}}(\mathbb{R}^3), \quad (\tau_r u)(\cdot, z) = u(\cdot - r, z) \quad \text{for a.a. } z \in \mathbb{R}.$$

An operator A on $L^2(\mathbb{R}^3)$ is called (x, y) -translation invariant if it commutes with τ_r for all $r \in \mathbb{R}^2$. In order to decompose (x, y) -translation invariant operators on $L^2(\mathbb{R}^3)$, we introduce the constant fiber direct integral [RS78, Section XIII.16]

$$L^2(\mathbb{R}^2; L^2(\mathbb{R})) \equiv \int_{\mathbb{R}^2}^{\oplus} L^2(\mathbb{R}) dq$$

with base \mathbb{R}^2 , and the unitary operator $\mathcal{U} : L^2(\mathbb{R}^3) \rightarrow L^2(\mathbb{R}^2; L^2(\mathbb{R}))$ defined on the dense subspace $\mathcal{S}(\mathbb{R}^3)$ of $L^2(\mathbb{R}^3)$ by

$$(\mathcal{U}\Phi)_q(z) := \frac{1}{2\pi} \int_{\mathbb{R}^2} e^{-iq \cdot r} \Phi(r, z) dr. \quad (2.1)$$

The unitary \mathcal{U} is simply the partial Fourier transform along the x and y directions. It has the property that (x, y) -translation invariant operators on $L^2(\mathbb{R}^3)$ are decomposed by \mathcal{U} : for any $A \in \mathcal{L}(L^2(\mathbb{R}^3))$ such that $\tau_r A = A \tau_r$, there exists $A_\bullet \in L^\infty(\mathbb{R}^2; \mathcal{L}(L^2(\mathbb{R})))$ such that for all $u \in L^2(\mathbb{R}^3)$,

$$(\mathcal{U}(Au))_q = A_q(\mathcal{U}u)_q \quad \text{for a.a. } q \in \mathbb{R}^2.$$

Hence we use the following notation for the decomposition of (x, y) -translation invariant operator A

$$A = \mathcal{U}^{-1} \left(\int_{\mathbb{R}^2}^{\oplus} A_q dq \right) \mathcal{U}.$$

In addition, $\|A\|_{\mathcal{L}(L^2(\mathbb{R}^3))} = \|\|A_\bullet\|_{\mathcal{L}(L^2(\mathbb{R}))}\|_{L^\infty(\mathbb{R}^2)}$. Note that, formally, the kernel of A is related to the kernels of the operators A_q by the formula:

$$A(r, z; r', z') = \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} A_q(z, z') e^{iq(r-r')} dq.$$

In particular, if A is positive and locally trace-class, then for almost all $q \in \mathbb{R}^2$, A_q is locally trace-class. The densities of these operators are functions of the variable z only, and are related by the formula

$$\rho_A(z) = \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} \rho_{A_q}(z) dq.$$

Likewise, if A is a (not necessarily bounded) self-adjoint operator such that $\tau_r(A + i)^{-1} = (A + i)^{-1} \tau_r$ for all $r \in \mathbb{R}^2$, then A is decomposed by \mathcal{U} (see [RS78, Theorem XIII.84 and XIII.85]). In particular, the kinetic energy operator $T = -\frac{1}{2}\Delta$ on $L^2(\mathbb{R}^3)$ is decomposed by \mathcal{U} as follows:

$$T = \mathcal{U}^{-1} \left(\int_{\mathbb{R}^2}^{\oplus} T_q dq \right) \mathcal{U} \quad \text{with} \quad T_q := -\frac{1}{2} \frac{d^2}{dz^2} + \frac{|q|^2}{2}. \quad (2.2)$$

One-body density matrices

In Hartree-Fock and Kohn-Sham models, electronic states are described by one-body density matrices (see e.g. [Col63, CDL08a, FLLS13]). Recall that for a finite system with N electrons, a density matrix is a trace-class self-adjoint operator $\gamma \in \mathcal{S}(L^2(\mathbb{R}^3)) \cap \mathfrak{S}_1(L^2(\mathbb{R}^3))$ satisfying the Pauli principle $0 \leq \gamma \leq 1$ and the normalization condition $\text{Tr}(\gamma) = \int_{\mathbb{R}^3} \rho_\gamma = N$. The kinetic energy of γ is given by $\text{Tr}(-\frac{1}{2}\Delta\gamma) := \frac{1}{2}\text{Tr}(|\nabla|\gamma|\nabla|)$ (see [CLBL01, CDL08a]).

Let us from now on focus on the reduced Hartree-Fock(rHF) model, *i.e.* the Hartree-Fock model without exchange terms. In this case, the ground state density matrix of a homogeneous electron gas with density ρ_0 can be uniquely defined by a thermodynamic limit argument (relying on the strict convexity of the rHF model with respect to the density). It is given by

$$\gamma_0 := \mathbf{1}_{(-\infty, \epsilon_F]}(T), \quad (2.3)$$

with the Fermi level

$$\epsilon_F := \frac{1}{2}(6\pi^2\rho_0)^{2/3},$$

which is the chemical potential of the electrons. The calculations of expressions of $\rho_{0,q}$ and ρ_0 can be read in Appendix, Section 2.5.2. Although γ_0 is not trace-class, it is locally trace-class and its density is ρ_0 by construction. The operator γ_0 can be seen as the rHF ground-state density matrix of an infinite, locally neutral system, whose nuclear distribution is a jellium of uniform density $\rho_{\text{nuc}}^0 = \rho_0$.

Since T is decomposed by \mathcal{U} , so is γ_0 , and we have

$$\gamma_0 = \mathcal{U}^{-1} \left(\int_{\mathbb{R}^2}^{\oplus} \gamma_{0,q} dq \right) \mathcal{U}, \quad (2.4)$$

where $\{\gamma_{0,q}\}_{q \in \mathbb{R}^2}$ are orthogonal projectors acting on $L^2(\mathbb{R})$:

$$\gamma_{0,q} := \begin{cases} \mathbf{1}_{(-\infty, \epsilon_F]}(T_q) & \text{if } q \in \overline{\mathfrak{B}}_{\epsilon_F}, \\ 0 & \text{if } q \in \mathbb{R}^2 \setminus \overline{\mathfrak{B}}_{\epsilon_F}. \end{cases}$$

Here and in the sequel, $\mathfrak{B}_R := \left\{ q \in \mathbb{R}^2 \mid \frac{|q|^2}{2} < R \right\}$ and $\overline{\mathfrak{B}}_R := \left\{ q \in \mathbb{R}^2 \mid \frac{|q|^2}{2} \leq R \right\}$ respectively denote the open and closed balls of \mathbb{R}^2 of radius $\sqrt{2R}$ centered at the origin.

If we consider an (x, y) -translation invariant perturbation $\rho_{\text{nuc}} = \rho_{\text{nuc}}^0 + \nu$ of the nuclear distribution, and keep the Fermi level $\epsilon_F > 0$ fixed, we expect the perturbed ground state density matrix $\gamma_\nu = \gamma_0 + Q_\nu$ to be (x, y) -translation invariant as well, and therefore the operators γ_ν and Q_ν to be decomposed by \mathcal{U} :

$$\gamma_\nu = \mathcal{U}^{-1} \left(\int_{\mathbb{R}^2}^{\oplus} \gamma_{\nu,q} dq \right) \mathcal{U} \quad \text{and} \quad Q_\nu = \mathcal{U}^{-1} \left(\int_{\mathbb{R}^2}^{\oplus} Q_{\nu,q} dq \right) \mathcal{U}.$$

We will see that Q_ν can be characterized as the unique minimizer of a variational problem consisting in minimizing some renormalized free energy functional.

2.2.2 Renormalized free energy functionals

Defects that are (x, y) -translation invariant are extended (non-local) defects, and therefore, do not fall into the frameworks of [FLLS13, LS15] (nor *a fortiori* of [CDL08a] since the homogeneous electron gas is a metal). However, the approach consisting in characterizing the ground states as the minimizers of some renormalized free energy functional can still be used.

In Section 2.2.2, we define a renormalized kinetic free energy per unit area adapted to (x, y) -translation invariant perturbations of the homogeneous electron gas. In Section 2.2.2, we focus on the potential energy contributions, and define renormalized energies per unit area for (x, y) -translation invariant systems, both for Yukawa and Coulomb interactions.

Renormalized kinetic free energy functional

Let us start with a formal (non-rigorous) argument. The kinetic energy densities of the operator γ_0 and of an operator of the form $\gamma = \gamma_0 + Q$ can be defined as

$$\begin{aligned} t_{\gamma_0}(\mathbf{r}) &:= \rho_{T^{1/2}\gamma_0 T^{1/2}}(\mathbf{r}), \\ t_\gamma(\mathbf{r}) &:= \rho_{T^{1/2}\gamma T^{1/2}}(\mathbf{r}) = t_{\gamma_0}(\mathbf{r}) + t_Q(\mathbf{r}) \quad \text{with} \quad t_Q(\mathbf{r}) := \rho_{T^{1/2}Q T^{1/2}}(\mathbf{r}). \end{aligned}$$

By (x, y) -translation invariance, the functions t_{γ_0} , t_γ and t_Q are in fact functions of the transverse variable z only. Fixing the Fermi level $\epsilon_F > 0$, we can therefore define a renormalized kinetic free energy per unit area as

$$\begin{aligned} \underline{T}_{\text{ren}}(Q) &:= \left(\int_{\mathbb{R}} t_\gamma(z) dz - \epsilon_F \int_{\mathbb{R}} \rho_\gamma(z) dz \right) - \left(\int_{\mathbb{R}} t_{\gamma_0}(z) dz - \epsilon_F \int_{\mathbb{R}} \rho_{\gamma_0}(z) dz \right) \\ &= \int_{\mathbb{R}} (t_Q(z) - \epsilon_F \rho_Q(z)) dz. \end{aligned}$$

Decomposing by \mathcal{U} and using the fact that $\gamma_{0,q}$ is an orthogonal projector commuting with T_q and such that

$$(T_q - \epsilon_F)\gamma_{0,q} = -|T_q - \epsilon_F|\gamma_{0,q}, \quad (T_q - \epsilon_F)(1 - \gamma_{0,q}) = |T_q - \epsilon_F|(1 - \gamma_{0,q}),$$

we obtain

$$\begin{aligned} \underline{T}_{\text{ren}}(Q) &= \int_{\mathbb{R}} (\rho_{T^{1/2}Q T^{1/2}}(\mathbf{r}) - \epsilon_F \rho_Q(z)) dz \\ &= \int_{\mathbb{R}} \left[\frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} (\rho_{T_q^{1/2}Q_q T_q^{1/2}}(z) - \epsilon_F \rho_{Q_q}(z)) dq \right] dz \\ &= \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} \left(\text{Tr}(T_q^{1/2}Q_q T_q^{1/2}) - \epsilon_F \text{Tr}(Q_q) \right) dq \\ &= \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} \text{Tr}((T_q - \epsilon_F)Q_q) dq \\ &= \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} \text{Tr}[(T_q - \epsilon_F)(\gamma_{0,q} + (1 - \gamma_{0,q}))Q_q] dq \\ &= \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} \text{Tr}(|T_q - \epsilon_F|^{1/2}(Q_q^{++} - Q_q^{--})|T_q - \epsilon_F|^{1/2}) dq, \end{aligned} \tag{2.5}$$

where

$$Q_q^{++} := (1 - \gamma_{0,q})Q_q(1 - \gamma_{0,q}) \geq 0 \quad \text{and} \quad Q_q^{--} := \gamma_{0,q}Q_q\gamma_{0,q} \leq 0.$$

It follows that the integrand in the right-hand side of (2.5) is non-negative. We also observe that

$$0 \leq \gamma_0 + Q \leq 1 \quad \Leftrightarrow \quad (-\gamma_{0,q} \leq Q_q \leq 1 - \gamma_{0,q} \quad \text{a.e.}) \quad \Leftrightarrow \quad (Q_q^2 \leq Q_q^{++} - Q_q^{--} \quad \text{a.e.}),$$

so that

$$\begin{aligned} \int_{\mathbb{R}^2} \left\| |T_q - \epsilon_F|^{1/2} Q_q \right\|_{\mathfrak{S}_2(L^2(\mathbb{R}))}^2 dq &= \int_{\mathbb{R}^2} \text{Tr} \left(|T_q - \epsilon_F|^{1/2} Q_q^2 |T_q - \epsilon_F|^{1/2} \right) dq \\ &\leq \int_{\mathbb{R}^2} \text{Tr} \left(|T_q - \epsilon_F|^{1/2} (Q_q^{++} - Q_q^{--}) |T_q - \epsilon_F|^{1/2} \right) dq. \end{aligned}$$

Reasoning as in [FLLS13, LS15], the above formal manipulations lead us to introduce

- the functional space

$$\begin{aligned} \mathcal{X}_q := \left\{ Q_q \in \mathcal{S}(L^2(\mathbb{R})) \mid |T_q - \epsilon_F|^{1/2} Q_q \in \mathfrak{S}_2(L^2(\mathbb{R})), \right. \\ \left. |T_q - \epsilon_F|^{1/2} Q_q^{\pm\pm} |T_q - \epsilon_F|^{1/2} \in \mathfrak{S}_1(L^2(\mathbb{R})) \right\}, \end{aligned}$$

which, equipped with the norm

$$\begin{aligned} \|Q_q\|_{\mathcal{X}_q} := & \|Q_q\|_{\mathcal{L}(L^2(\mathbb{R}))} + \left\| |T_q - \epsilon_F|^{1/2} Q_q \right\|_{\mathfrak{S}_2(L^2(\mathbb{R}))} \\ & + \sum_{\alpha \in \{+, -\}} \left\| |T_q - \epsilon_F|^{1/2} Q_q^{\alpha\alpha} |T_q - \epsilon_F|^{1/2} \right\|_{\mathfrak{S}_1(L^2(\mathbb{R}))}, \end{aligned}$$

is a Banach space;

- the convex set $\mathcal{K}_q := \left\{ Q_q \in \mathcal{X}_q \mid -\gamma_{0,q} \leq Q_q \leq 1 - \gamma_{0,q} \right\}$;
- the linear form

$$\underline{\text{Tr}}((T - \epsilon_F)Q) := \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} \text{Tr} \left(|T_q - \epsilon_F|^{1/2} (Q_q^{++} - Q_q^{--}) |T_q - \epsilon_F|^{1/2} \right) dq, \quad (2.6)$$

which is well-defined with values in $[0, +\infty]$ whenever $\mathbb{R}^2 \ni q \mapsto Q_q \in \mathcal{S}(L^2(\mathbb{R}))$ is measurable with $Q_q \in \mathcal{K}_q$ for almost all $q \in \mathbb{R}^2$.

Definition 2.1. (*Density matrices with finite renormalized kinetic free energy per unit area*) An (x, y) -translation invariant density matrix

$$\gamma = \gamma_0 + Q$$

has a finite renormalized kinetic free energy per unit area if $Q \in \mathcal{K}$, where

$$\begin{aligned} \mathcal{K} := \left\{ Q = \mathcal{U}^{-1} \left(\int_{\mathbb{R}^2}^{\oplus} Q_q dq \right) \mathcal{U} \mid q \mapsto Q_q \in L^\infty(\mathbb{R}^2; \mathcal{S}(L^2(\mathbb{R}))), \right. \\ \left. Q_q \in \mathcal{K}_q \text{ a.e.}, \underline{\text{Tr}}((T - \epsilon_F)Q) < \infty \right\}. \end{aligned} \quad (2.7)$$

It is not obvious *a priori* that operators in \mathcal{K} , which are not trace-class, nor even compact, have densities. However, it is in fact possible to define the density ρ_Q of any state $Q \in \mathcal{K}$, which will be useful to define renormalized rHF free energy functionals involving Yukawa or Coulomb interactions (see Section 2.2.3).

Proposition 2.2. (Densities of operators in \mathcal{K}) Any $Q \in \mathcal{K}$ is locally trace-class, its density ρ_Q is a function of the variable z only, and $\rho_Q \in L^p(\mathbb{R}) + L^2(\mathbb{R})$ for any $1 < p < 5/3$.

In addition, for all $1 < p < 5/3$ and all $c > 0$, there exists two positive constants $\eta_{c,-}, \eta_{p,c,+}$ such that

$$\forall Q \in \mathcal{K}, \quad \eta_{c,-} \|\rho_Q^{c,-}\|_{L^2(\mathbb{R})}^2 + \eta_{p,c,+} \|\rho_Q^{c,+}\|_{L^p(\mathbb{R})}^p \leq \text{Tr}((T - \epsilon_F)Q), \quad (2.8)$$

where $\rho_Q = \rho_Q^{c,-} + \rho_Q^{c,+}$ with

$$\rho_Q^{c,-} := \frac{1}{(2\pi)^2} \int_{\mathfrak{B}_{\epsilon_F+c}} \rho_{Q_q} dq \in L^2(\mathbb{R}), \quad \text{and} \quad \rho_Q^{c,+} := \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2 \setminus \mathfrak{B}_{\epsilon_F+c}} \rho_{Q_q} dq \in L^p(\mathbb{R}).$$

The proof of this result is based on Lieb–Thirring type inequalities and can be read in Section 2.3.1.

Coulomb and Yukawa energy functionals

The extended defect being (x, y) -translation invariant, the renormalized total charge density

$$\rho := \rho_{\gamma_0+Q} - (\rho_{\text{nuc}}^0 + \nu) = \rho_Q - \nu$$

is a function of the variable z only. The Coulomb potential generated by this density is therefore obtained by solving the 1D Poisson equation $-v''_{\rho,0} = 2\rho$, which also reads in Fourier representation $|k|^2 \hat{v}_{\rho,0}(k) = 2\hat{\rho}(k)$. Formally, the Coulomb energy of ρ per unit area is thus given by

$$\int_{\mathbb{R}} \rho(z) v_{\rho,0}(z) dz = \int_{\mathbb{R}} \overline{\hat{\rho}(k)} \hat{v}_{\rho,0}(k) = 2 \int_{\mathbb{R}} \frac{|\hat{\rho}(k)|^2}{|k|^2} dk.$$

This motivates the following definition of the 1D Coulomb space

$$\underline{\mathcal{C}} := \left\{ \rho \in \mathcal{S}'(\mathbb{R}) \mid \hat{\rho} \in L^1_{\text{loc}}(\mathbb{R}), \frac{\hat{\rho}(k)}{|k|} \in L^2(\mathbb{R}) \right\}, \quad (2.9)$$

endowed with the inner product

$$\underline{D}(\rho_1, \rho_2) := 2 \int_{\mathbb{R}} \frac{\overline{\hat{\rho}_1(k)} \hat{\rho}_2(k)}{|k|^2} dk. \quad (2.10)$$

Let us prove that $\underline{\mathcal{C}}$ is a Hilbert space. It suffices to prove that $\underline{\mathcal{C}}$ is complete. Consider to this end a Cauchy sequence $\{u_n\}_{n \geq 1}$ in $\underline{\mathcal{C}}$. By definition, the sequence $\left\{ \frac{\hat{u}_n(k)}{|k|} \right\}_{n \geq 1}$ is a Cauchy sequence in $L^2(\mathbb{R})$. Denote by $w \in L^2(\mathbb{R})$ its limit and define $f(k) := \frac{|k|w(k)}{1+|k|^2} \in L^2(\mathbb{R})$. Note that $\check{f} \in L^2(\mathbb{R})$. Introduce next $u = (1 - \Delta)\check{f} \in H^{-2}(\mathbb{R}) \subset \mathcal{S}'(\mathbb{R})$. By the stability of Fourier transform in $\mathcal{S}'(\mathbb{R})$, it holds $\hat{u} = (1 + |k|^2)f = |k|w \in \mathcal{S}'(\mathbb{R})$. Therefore $\left\{ \frac{\hat{u}_n(k)}{|k|} \right\}_{n \geq 1}$ converges in $L^2(\mathbb{R})$ to $w(k) = \frac{\hat{u}(k)}{|k|}$. Since $u \in \mathcal{S}'(\mathbb{R})$, and $\hat{u} = |\cdot|w \in L^1_{\text{loc}}(\mathbb{R})$, we can conclude that $u \in \underline{\mathcal{C}}$ and that $\|u - u_n\|_{\underline{\mathcal{C}}} \rightarrow 0$, which proves the completeness of $\underline{\mathcal{C}}$.

The quantity $\frac{1}{2}\underline{D}(\rho, \rho) \in [0, +\infty]$ represents the Coulomb energy per unit area of the (x, y) -translation invariant renormalized charge density ρ .

Remark 2.3. Note that charge densities in $\underline{\mathcal{C}}$ are neutral in some weak sense. In particular, if $\rho \in \underline{\mathcal{C}} \cap L^1(\mathbb{R})$, then $\int_{\mathbb{R}} \rho = (2\pi)^{1/2} \hat{\rho}(0) = 0$ since the function $k \mapsto \frac{|\hat{\rho}(k)|^2}{|k|^2}$ has to be integrable in the vicinity of 0.

Likewise, the Yukawa potential of parameter $m > 0$ generated by the renormalized charge density ρ of the extended defect is obtained by solving the 1D Yukawa equation $-v''_{\rho,m} + m^2 v_{\rho,m} = 2\rho$, and its Yukawa energy per unit area is formally given by

$$\int_{\mathbb{R}} \frac{|\hat{\rho}(k)|^2}{|k|^2 + m^2} dk.$$

This leads us to introduce the Yukawa space of parameter m

$$\underline{\mathcal{C}}_m := \left\{ \rho \in \mathcal{S}'(\mathbb{R}) \mid \widehat{\rho} \in L^1_{\text{loc}}(\mathbb{R}), \frac{\widehat{\rho}(k)}{\sqrt{|k|^2 + m^2}} \in L^2(\mathbb{R}) \right\}, \quad (2.11)$$

endowed with the inner product

$$\underline{D}_m(\rho_1, \rho_2) := 2 \int_{\mathbb{R}} \frac{\widehat{\rho}_1(k) \widehat{\rho}_2(k)}{|k|^2 + m^2} dk. \quad (2.12)$$

We will use in the sequel the consistent notation $\underline{D}_0 := \underline{D}$ for Coulomb interactions.

Remark 2.4. For any $m > 0$, the Yukawa space $\underline{\mathcal{C}}_m$ actually coincides with the Sobolev space $H^{-1}(\mathbb{R})$ and the norms $\|\cdot\|_{H^{-1}}$ and $\underline{D}_m(\cdot, \cdot)^{1/2}$ are equivalent. However we will consider in the following m as a parameter and will pass to limit $m \rightarrow 0$ to make a connection with the Coulomb interaction. We therefore prefer to keep the notation $\underline{\mathcal{C}}_m$.

Remark 2.5. For any $1 < p < 5/3$, we have $L^p(\mathbb{R}) + L^2(\mathbb{R}) \hookrightarrow H^{-1}(\mathbb{R})$. It therefore follows from Proposition 2.2 that the density associated to any $Q \in \mathcal{K}$ has a finite renormalized Yukawa energy per unit area. On the other hand, its renormalized Coulomb energy can be either finite or infinite.

2.2.3 Formulation and mathematical properties of the model

We now consider an (x, y) -translation invariant nuclear defect ν , typically a sharp trench

$$\nu = -\rho_{\text{nuc}}^0 \mathbb{1}_{[-a, a]}(z)$$

for some $a > 0$, where $\mathbb{1}_{[-a, a]} : \mathbb{R} \rightarrow \mathbb{R}$ is the characteristic function of the range $[-a, a]$. Mollified versions of this indicator function can also be considered.

Based on the content of Section 2.2.2, we can define the renormalized free energy per unit area associated with a trial density matrix $\gamma = \gamma_0 + Q$ by

$$\mathcal{E}_{\nu, m}(Q) = \underline{\text{Tr}}((T - \epsilon_F) Q) + \frac{1}{2} \underline{D}_m(\rho_Q - \nu, \rho_Q - \nu), \quad (2.13)$$

where the renormalized kinetic free energy per unit area is given by (2.6), and when the Yukawa ($m > 0$) or Coulomb ($m = 0$) potential energy functional per unit area is given by (2.12). For any $Q \in \mathcal{K}$, the right-hand side of (2.13) is the sum of two non-negative terms. The former is always finite. The latter is always finite for Yukawa interactions as soon as $\nu \in H^{-1}(\mathbb{R})$, but can a priori be infinite for Coulomb interactions. For this reason, we introduce the (possibly empty) set

$$\mathcal{F}_\nu := \{Q \in \mathcal{K} \mid \rho_Q - \nu \in \underline{\mathcal{C}}\}.$$

We can then state the following result.

Theorem 2.6 (Existence of minimizers).

(1) *Yukawa interaction: for any $\nu \in H^{-1}(\mathbb{R})$, the minimization problem*

$$\boxed{I_{\nu, m} = \inf\{\mathcal{E}_{\nu, m}(Q), Q \in \mathcal{K}\}} \quad (2.14)$$

has a minimizer $Q_{\nu, m}$ and all the minimizers share the same density $\rho_{\nu, m}$.

(2) *Coulomb interaction: for any $\nu \in L^1(\mathbb{R})$ such that $|\cdot| \nu(\cdot) \in L^1(\mathbb{R})$, the set \mathcal{F}_ν is non-empty, the minimization problem*

$$\boxed{I_{\nu, 0} = \inf\{\mathcal{E}_{\nu, 0}(Q), Q \in \mathcal{F}_\nu\}} \quad (2.15)$$

has a minimizer $Q_{\nu, 0}$, and all the minimizers share the same density $\rho_{\nu, 0}$.

(3) For any $\nu \in H^{-1}(\mathbb{R})$, the function $(0, +\infty) \ni m \mapsto I_{\nu, m} \in \mathbb{R}_+$ is continuous, non-increasing,

$$\lim_{m \rightarrow 0} I_{\nu, m} \leq I_{\nu, 0} \quad \text{and} \quad \lim_{m \rightarrow +\infty} I_{\nu, m} = 0,$$

with the convention that $I_{\nu, 0} = +\infty$ if \mathcal{F}_ν is empty. When $\nu \in L^1(\mathbb{R})$ and $|\cdot| \nu(\cdot) \in L^1(\mathbb{R})$,

$$\lim_{m \rightarrow 0} I_{\nu, m} = I_{\nu, 0}.$$

Moreover, if $\nu \in L^1(\mathbb{R})$ and $|\cdot| \nu(\cdot) \in L^1(\mathbb{R})$, there exists a sequence $(m_k)_{k \in \mathbb{N}}$ of positive real numbers decreasing to zero, and a sequence $(Q_{\nu, m_k})_{k \in \mathbb{N}}$ of elements of \mathcal{K} such that, for each $k \in \mathbb{N}$, Q_{ν, m_k} is a minimizer of (2.14) for $m = m_k$, converging to a minimizer $Q_{\nu, 0}$ of (2.15) in the following sense:

$$\mathcal{U} Q_{\nu, m_k} \mathcal{U}^{-1} \xrightarrow[k \rightarrow \infty]{} \mathcal{U} Q_{\nu, 0} \mathcal{U}^{-1} \quad \text{for the weak-* topology of } L^\infty(\mathbb{R}^2; \mathcal{S}(L^2(\mathbb{R}))); \quad (2.16)$$

$$\mathcal{U} |T - \epsilon_F|^{1/2} Q_{\nu, m_k} \mathcal{U}^{-1} \xrightarrow[k \rightarrow \infty]{} \mathcal{U} |T - \epsilon_F|^{1/2} Q_{\nu, 0} \mathcal{U}^{-1} \quad \text{weakly in } L^2(\mathbb{R}^2; \mathfrak{S}_2(L^2(\mathbb{R}))). \quad (2.17)$$

The proof of Theorem 2.6 can be read in Section 2.3.4.

Remark 2.7. The convergence of (2.16) can be stated as follows: for any operator-valued function $q \mapsto U_q \in L^1(\mathbb{R}^2; \mathfrak{S}_1(L^2(\mathbb{R})))$,

$$\int_{\mathbb{R}^2} \text{Tr}_{L^2(\mathbb{R})} \left(U_q (Q_{\nu, m_k})_q \right) dq \xrightarrow[k \rightarrow \infty]{} \int_{\mathbb{R}^2} \text{Tr}_{L^2(\mathbb{R})} \left(U_q (Q_{\nu, 0})_q \right) dq.$$

Similarly, the convergence of (2.17) can be stated as follows: for any operator-valued function $q \mapsto M_q \in L^2(\mathbb{R}^2; \mathfrak{S}_2(L^2(\mathbb{R})))$,

$$\int_{\mathbb{R}^2} \text{Tr}_{L^2(\mathbb{R})} \left(|T_q - \epsilon_F|^{1/2} (Q_{\nu, m_k})_q M_q \right) dq \xrightarrow[n \rightarrow \infty]{} \int_{\mathbb{R}^2} \text{Tr}_{L^2(\mathbb{R})} \left(|T_q - \epsilon_F|^{1/2} (Q_{\nu, 0})_q M_q \right) dq,$$

where $(Q_{\nu, m_k})_q$ and $(Q_{\nu, 0})_q$ are respectively the \mathcal{U} decompositions of Q_{ν, m_k} and $Q_{\nu, 0}$.

In the Yukawa case ($m > 0$), we are able to characterize the minimizers of (2.14). By Theorem 2.6, all the minimizers of the problem (2.14) share the same density $\rho_{\nu, m} \in \mathcal{K}$. In view of Proposition 2.2, the function $\rho_{\nu, m}$ is in $L^p(\mathbb{R}) + L^2(\mathbb{R})$ for some $1 < p < 5/3$, thus in $H^{-1}(\mathbb{R})$ (see Remark 2.5). The Yukawa potential

$$V_{\nu, m} := \left(-\frac{d^2}{dz^2} + m^2 \right)^{-1} (\rho_{\nu, m} - \nu) = \frac{e^{-m|\cdot|}}{m} \star (\rho_{\nu, m} - \nu), \quad (2.18)$$

is therefore well-defined in $H^1(\mathbb{R})$. In particular, $V_{\nu, m}$ is a continuous function vanishing at infinity. The following result shows that this is sufficient to ensure the uniqueness of the ground-state density matrix in (2.14).

Theorem 2.8 (Uniqueness and characterization of the minimizer for the Yukawa case). *Let $\nu \in H^{-1}(\mathbb{R})$ and $m > 0$. The minimizer $Q_{\nu, m}$ of the problem (2.14) is unique and is the unique solution in \mathcal{K} to the self-consistent equations:*

$$\begin{cases} \gamma_{\nu, m} := \mathbb{1}_{(-\infty, \epsilon_F]}(T + V_{\nu, m}), \\ V_{\nu, m} := \frac{e^{-m|\cdot|}}{m} \star (\rho_{Q_{\nu, m}} - \nu), \\ Q_{\nu, m} := \gamma_{\nu, m} - \gamma_0. \end{cases} \quad (2.19)$$

The proof of Theorem 2.8 can be read in Section 2.3.5.

Remark 2.9. Proving that self-consistent equations similar to (2.19) hold for Coulomb interactions is much more challenging. The first step would be to properly define the potential $V_{\nu, 0} = \rho_{\nu, 0} \star |\cdot|$, as well as the self-adjoint extension of the operator $T + V_{\nu, 0}$ (see [DOV09]). The technique of proof we use in the Yukawa case relies on the fact that the potential is bounded and in $L^2(\mathbb{R})$ (although it would be possible to work in more general Lebesgue spaces). It is not obvious at all that $V_{\nu, 0}$ satisfies these properties.

2.3 Proofs of the results

Unless otherwise specified, we simply write \mathfrak{S}_p instead of $\mathfrak{S}_p(L^2(\mathbb{R}))$ in all the proofs.

2.3.1 Proof of Proposition 2.2

The proof of Proposition 2.2 is based on the following technical results, which show that the decomposed kinetic energy of defects actually satisfies Lieb–Thirring-like inequalities [LT91]. The density associated with the state of the defect can therefore be controlled by the kinetic energy of the defect.

For $q \in \overline{\mathfrak{B}}_{\epsilon_F}$, Lemma 2.10 (resp. 2.11) provides a lower bound of the densities of diagonal blocks (resp. off-diagonal blocks) of operators in \mathcal{K}_q . The proof of these results, obtained by the same techniques as in [FLLS13], can be read in Section 2.3.2 (resp. Section 2.3.3).

Lemma 2.10. *There exist positive constants $C_{1,\text{diag}}, C_{2,\text{diag}}$ such that, for all $q \in \overline{\mathfrak{B}}_{\epsilon_F}$ and $Q_q \in \mathcal{K}_q$,*

$$\begin{aligned} \pm \text{Tr}_{L^2(\mathbb{R})} \left(|T_q - \epsilon_F|^{1/2} Q_q^{\pm\pm} |T_q - \epsilon_F|^{1/2} \right) &\geq C_{1,\text{diag}} \int_{\mathbb{R}} \left| \rho_{Q_q^{\pm\pm}}(z) \right|^3 dz \\ &+ C_{2,\text{diag}} \sqrt{2\epsilon_F - |q|^2} \int_{\mathbb{R}} \rho_{Q_q^{\pm\pm}}^2(z) dz. \end{aligned} \quad (2.20)$$

The absolute value in the integrand of the first integral on the right-hand side is motivated by the fact that $Q_q^{--} \leq 0$, so that $\rho_{Q_q^{--}} \leq 0$.

Lemma 2.11. *There exist $C_{+-} \in \mathbb{R}_+$ such that, for all $q \in \overline{\mathfrak{B}}_{\epsilon_F}$ and $Q_q \in \mathcal{K}_q$,*

$$\begin{aligned} \text{Tr}_{L^2(\mathbb{R})} \left(|T_q - \epsilon_F|^{1/2} (Q_q^{++} - Q_q^{--}) |T_q - \epsilon_F|^{1/2} \right) \\ \geq C_{+-} (2\epsilon_F - |q|^2)^{1/4} \int_{\mathbb{R}} \left| \widehat{\rho_{Q_q^{\pm\mp}}}(k) \right|^2 \left| |k| - 2\sqrt{2\epsilon_F - |q|^2} \right|^{1/2} dk. \end{aligned} \quad (2.21)$$

For $q \in \mathbb{R}^2 \setminus \overline{\mathfrak{B}}_{\epsilon_F}$, it holds $\gamma_{0,q} \equiv 0$ and $0 \leq Q_q \leq 1$, so that $Q_q^{++} \equiv Q_q$ and $Q_q^{--} \equiv 0$. In particular, $\rho_{Q_q} \geq 0$. The following estimate therefore follows from the one dimensional Lieb–Thirring inequality [LT91].

Lemma 2.12. *There exists a positive constant C such that, for all $q \in \mathbb{R}^2 \setminus \overline{\mathfrak{B}}_{\epsilon_F}$ and $Q_q \in \mathcal{K}_q$,*

$$\text{Tr}_{L^2(\mathbb{R})} \left(|T_q - \epsilon_F|^{1/2} (Q_q^{++} - Q_q^{--}) |T_q - \epsilon_F|^{1/2} \right) \geq C \int_{\mathbb{R}} \rho_{Q_q}^3(z) dz + \left(\frac{|q|^2}{2} - \epsilon_F \right) \int_{\mathbb{R}} \rho_{Q_q}(z) dz. \quad (2.22)$$

We are now in position to prove Proposition 2.2. Fix $Q \in \mathcal{K}$. Bounds on the densities are obtained by separating the estimates for $q \in \mathbb{R}^2 \setminus \overline{\mathfrak{B}}_{\epsilon_F}$ and $q \in \overline{\mathfrak{B}}_{\epsilon_F}$. More precisely, defining

$$f(q) := \left| |q|^2 - 2\epsilon_F \right| = \begin{cases} |q|^2 - 2\epsilon_F > 0 & \text{if } q \in \mathbb{R}^2 \setminus \overline{\mathfrak{B}}_{\epsilon_F}, \\ 2\epsilon_F - |q|^2 \geq 0 & \text{if } q \in \overline{\mathfrak{B}}_{\epsilon_F}, \end{cases} \quad (2.23)$$

the key ingredient in our proof is the following Hölder inequality, written in a generic form for real numbers $\beta > 1$, $\alpha > 0$ and an integration domain $A \subset \mathbb{R}^2$:

$$\int_{\mathbb{R}} \left(\int_A |\rho_{Q_q}(z)| dq \right)^\beta dz \leq \int_{\mathbb{R}} \left(\int_A |\rho_{Q_q}(z)|^\beta f^{\alpha\beta}(q) dq \right) \left(\int_A f^{-\alpha\beta/(\beta-1)}(q) dq \right)^{\beta-1} dz. \quad (2.24)$$

We successively consider three situations: total density for $q \in \overline{\mathfrak{B}}_{\epsilon_F}$, density associated with the diagonal blocks of Q for $q \in \overline{\mathfrak{B}}_{\epsilon_F}$, and density associated with the off-diagonal blocks of Q for $q \in \overline{\mathfrak{B}}_{\epsilon_F}$.

Estimates for the total density on $\mathbb{R}^2 \setminus \overline{\mathfrak{B}}_{\epsilon_F}$. Lemma 2.12 shows that

$$\begin{aligned} & \int_{\mathbb{R}^2 \setminus \overline{\mathfrak{B}}_{\epsilon_F}} \left(C \int_{\mathbb{R}} \rho_{Q_q}^3(z) dz + \left(\frac{|q|^2}{2} - \epsilon_F \right) \int_{\mathbb{R}} \rho_{Q_q}(z) dz \right) dq \\ & \leq \int_{\mathbb{R}^2 \setminus \overline{\mathfrak{B}}_{\epsilon_F}} \text{Tr}_{L^2(\mathbb{R})} \left(|T_q - \epsilon_F|^{1/2} (Q_q^{++} - Q_q^{--}) |T_q - \epsilon_F|^{1/2} \right) dq \leq \underline{\text{Tr}}((T - \epsilon_F)Q) < +\infty. \end{aligned}$$

The above inequality implies that

$$\int_{\mathbb{R}^2 \setminus \overline{\mathfrak{B}}_{\epsilon_F}} \int_{\mathbb{R}} \rho_{Q_q}^3(z) dz dq \leq \frac{1}{C} \underline{\text{Tr}}((T - \epsilon_F)Q), \quad \int_{\mathbb{R}^2 \setminus \overline{\mathfrak{B}}_{\epsilon_F}} \int_{\mathbb{R}} f(q) \rho_{Q_q}(z) dz dq \leq 2 \underline{\text{Tr}}((T - \epsilon_F)Q). \quad (2.25)$$

In order to obtain bounds on the density, we separate the integration domain in two pieces: large values of $|q|$, and values close to $\{|q|^2 = 2\epsilon_F\}$ where $f(q)$ vanishes. More precisely, for a given $c > 0$, we decompose the integration domain as $\mathbb{R}^2 \setminus \overline{\mathfrak{B}}_{\epsilon_F} = (\mathbb{R}^2 \setminus \overline{\mathfrak{B}}_{\epsilon_F+c}) \cup (\overline{\mathfrak{B}}_{\epsilon_F+c} \setminus \overline{\mathfrak{B}}_{\epsilon_F})$.

We first set $A = \mathbb{R}^2 \setminus \overline{\mathfrak{B}}_{\epsilon_F+c}$ in (2.24). The last integral in this inequality reads

$$\int_A f^{-\alpha\beta/(\beta-1)}(q) dq = \int_{\mathbb{R}^2 \setminus \overline{\mathfrak{B}}_{\epsilon_F+c}} (|q|^2 - 2\epsilon_F)^{-\alpha\beta/(\beta-1)} dq = 2\pi \int_{\sqrt{2(\epsilon_F+c)}}^{+\infty} r (r^2 - 2\epsilon_F)^{-\alpha\beta/(\beta-1)} dr.$$

The latter integral is finite if and only if $\alpha\beta/(\beta-1) > 1$. Moreover, a Hölder inequality combined with (2.25) implies that the following integral is finite for $a > 1$:

$$\begin{aligned} & \int_{\mathbb{R}^2 \setminus \overline{\mathfrak{B}}_{\epsilon_F+c}} \int_{\mathbb{R}} \rho_{Q_q}^{3-\frac{2}{a}}(z) f^{1/a}(q) dz dq \\ & \leq \left(\int_{\mathbb{R}^2 \setminus \overline{\mathfrak{B}}_{\epsilon_F+c}} \int_{\mathbb{R}} f(q) \rho_{Q_q}(z) dz dq \right)^{1/a} \left(\int_{\mathbb{R}^2 \setminus \overline{\mathfrak{B}}_{\epsilon_F+c}} \int_{\mathbb{R}} \rho_{Q_q}^3(z) dz dq \right)^{(a-1)/a} \\ & \leq \max \left(2, \frac{1}{C} \right) \underline{\text{Tr}}((T - \epsilon_F)Q). \end{aligned}$$

In view of (2.24), this suggests taking $\alpha\beta = 1/a$ and $\beta = 3 - 2/a$. The condition $\alpha\beta/(\beta-1) > 1$ can be rephrased as $1/(2a-2) > 1$. The latter inequality is satisfied for $1 < a < 3/2$, which is equivalent to $1 < \beta < 5/3$. For the latter choice, inequality (2.24) combined with (2.25) then shows that there exists $K_{\beta, \mathbb{R}^2 \setminus \overline{\mathfrak{B}}_{\epsilon_F+c}} \in \mathbb{R}_+$ such that

$$\int_{\mathbb{R}} \left(\int_{\mathbb{R}^2 \setminus \overline{\mathfrak{B}}_{\epsilon_F+c}} \rho_{Q_q}(z) dz \right)^\beta dz \leq K_{\beta, \mathbb{R}^2 \setminus \overline{\mathfrak{B}}_{\epsilon_F+c}} \underline{\text{Tr}}((T - \epsilon_F)Q). \quad (2.26)$$

We next set $A = \overline{\mathfrak{B}}_{\epsilon_F+c} \setminus \overline{\mathfrak{B}}_{\epsilon_F}$ in (2.24) and follow the same strategy as in the previous case. We still take $\alpha\beta = 1/a$ and $\beta = 3 - 2/a$, but need now that $\alpha\beta/(\beta-1) < 1$ in order to ensure that the last integral in (2.24) is finite. This condition is equivalent to $a > 3/2$, i.e. $5/3 < \beta < 3$. We therefore consider $\beta = 2$. The inequality (2.24) combined with (2.25) then shows that there exists $K_{\overline{\mathfrak{B}}_{\epsilon_F+c} \setminus \overline{\mathfrak{B}}_{\epsilon_F}} \in \mathbb{R}_+$ such that

$$\int_{\mathbb{R}} \left(\int_{\overline{\mathfrak{B}}_{\epsilon_F+c} \setminus \overline{\mathfrak{B}}_{\epsilon_F}} \rho_{Q_q}(z) dz \right)^2 dz \leq K_{\overline{\mathfrak{B}}_{\epsilon_F+c} \setminus \overline{\mathfrak{B}}_{\epsilon_F}} \underline{\text{Tr}}((T - \epsilon_F)Q). \quad (2.27)$$

Estimates for $q \in \overline{\mathfrak{B}}_{\epsilon_F}$, diagonal blocks. We write the estimates for $\rho_{Q_q^{++}}$ only, the bounds for $\rho_{Q_q^{--}}$ being similar. Lemma 2.10 shows that

$$\begin{aligned} & \int_{\overline{\mathfrak{B}}_{\epsilon_F}} \int_{\mathbb{R}} \rho_{Q_q^{++}}^3(z) dz dq \leq \frac{1}{C_{1,\text{diag}}} \underline{\text{Tr}}((T - \epsilon_F)Q), \\ & \int_{\overline{\mathfrak{B}}_{\epsilon_F}} \int_{\mathbb{R}} f^{1/2}(q) \rho_{Q_q^{++}}^2(z) dz dq \leq \frac{1}{C_{2,\text{diag}}} \underline{\text{Tr}}((T - \epsilon_F)Q), \end{aligned} \quad (2.28)$$

so that, by a Hölder inequality for $a > 1$,

$$\begin{aligned} & \int_{\overline{\mathfrak{B}}_{\epsilon_F}} \int_{\mathbb{R}} \rho_{Q_q^{++}}^{3-1/a}(z) f^{1/(2a)}(q) dz dq \\ & \leq \left(\int_{\overline{\mathfrak{B}}_{\epsilon_F}} \int_{\mathbb{R}} f^{1/2}(q) \rho_{Q_q^{++}}^2(z) dz dq \right)^{1/a} \left(\int_{\overline{\mathfrak{B}}_{\epsilon_F}} \int_{\mathbb{R}} \rho_{Q_q^{++}}^3(z) dz dq \right)^{(a-1)/a} \\ & \leq C_{1,\text{diag}}^{1/a-1} C_{2,\text{diag}}^{-1/a} \underline{\text{Tr}}((T - \epsilon_F)Q) < +\infty. \end{aligned} \quad (2.29)$$

We now consider (2.24) with $A = \overline{\mathfrak{B}}_{\epsilon_F}$ and ρ_{Q_q} replaced by $\rho_{Q_q^{++}}$. The previous inequality suggests choosing $\beta = 3 - 1/a$ and $\alpha\beta = 1/(2a)$. The last integral in (2.24) is finite if and only if $\alpha\beta/(\beta - 1) < 1$, which is equivalent to $1/(4a - 2) < 1$, i.e. $a > 3/4$ and $5/3 < \beta < 3$. We therefore choose $\beta = 2$. The inequality (2.24) combined with (2.25) then shows that there exists $K_{\overline{\mathfrak{B}}_{\epsilon_F}, ++} \in \mathbb{R}_+$ such that

$$\int_{\mathbb{R}} \left(\int_{\overline{\mathfrak{B}}_{\epsilon_F}} \rho_{Q_q^{++}}(z) dz \right)^2 dq \leq K_{\overline{\mathfrak{B}}_{\epsilon_F}, ++} \underline{\text{Tr}}((T - \epsilon_F)Q). \quad (2.30)$$

Estimates for $q \in \overline{\mathfrak{B}}_{\epsilon_F}$, off-diagonal blocks. Define, for $k \in \mathbb{R}$ and $q \in \overline{\mathfrak{B}}_{\epsilon_F}$,

$$g(k, q) = \left| |k| - 2\sqrt{2\epsilon_F - |q|^2} \right|^{1/2} (2\epsilon_F - |q|^2)^{1/4}.$$

In view of Lemma 2.11 and the inequality $\left| \widehat{\rho_{Q_q^{+-}}}(k) + \widehat{\rho_{Q_q^{-+}}}(k) \right| = \left| 2\Re \widehat{\rho_{Q_q^{+-}}}(k) \right| \leq 2 \left| \widehat{\rho_{Q_q^{+-}}}(k) \right|$, it holds

$$\int_{\overline{\mathfrak{B}}_{\epsilon_F}} \int_{\mathbb{R}} \left| \widehat{\rho_{Q_q^{+-}}}(k) + \widehat{\rho_{Q_q^{-+}}}(k) \right|^2 g(k, q) dk dq \leq \frac{4}{C_{+-}} \underline{\text{Tr}}((T - \epsilon_F)Q). \quad (2.31)$$

Note that, by the change of variables $t = |q|/\sqrt{2\epsilon_F}$ and $w = \sqrt{1 - t^2}$,

$$\begin{aligned} G(k) & := \int_{\overline{\mathfrak{B}}_{\epsilon_F}} g(k, q)^{-1} dq = 2\pi \int_0^1 \frac{\sqrt{2\epsilon_F} t}{\left| (2\epsilon_F)^{-1/2} |k| - 2\sqrt{1 - t^2} \right|^{1/2} (1 - t^2)^{1/4}} dt \\ & = 2\pi \int_0^1 \frac{\sqrt{2\epsilon_F} \sqrt{w}}{\left| (2\epsilon_F)^{-1/2} |k| - 2w \right|^{1/2}} dw, \end{aligned}$$

from which it is easy to see that G is a bounded positive function tending to 0 as $|k| \rightarrow \infty$. Define

$$\rho_{Q^{\text{offdiag}}}(z) := \frac{1}{(2\pi)^2} \int_{\overline{\mathfrak{B}}_{\epsilon_F}} \left(\rho_{Q_q^{+-}}(z) + \rho_{Q_q^{-+}}(z) \right) dq.$$

Using the isometry property of the Fourier transform, the Cauchy–Schwarz inequality and (2.31), we obtain the following bound on the L^2 norm of $\rho_{Q^{\text{offdiag}}}$:

$$\begin{aligned} \|\rho_{Q^{\text{offdiag}}}\|_{L^2(\mathbb{R})}^2 & = \int_{\mathbb{R}} \left| \widehat{\rho_{Q^{\text{offdiag}}}}(k) \right|^2 dk = \frac{1}{(2\pi)^4} \int_{\mathbb{R}} \left| \int_{\overline{\mathfrak{B}}_{\epsilon_F}} \left(\widehat{\rho_{Q_q^{+-}}}(k) + \widehat{\rho_{Q_q^{-+}}}(k) \right) dq \right|^2 dk \\ & \leq \frac{1}{(2\pi)^4} \int_{\mathbb{R}} \left[\int_{\overline{\mathfrak{B}}_{\epsilon_F}} \left| \widehat{\rho_{Q_q^{+-}}}(k) + \widehat{\rho_{Q_q^{-+}}}(k) \right|^2 g(k, q) dq \right] G(k) dk \\ & \leq \frac{1}{(2\pi)^4} \|G\|_{L^\infty(\mathbb{R})} \int_{\mathbb{R}} \int_{\overline{\mathfrak{B}}_{\epsilon_F}} \left| \widehat{\rho_{Q_q^{+-}}}(k) + \widehat{\rho_{Q_q^{-+}}}(k) \right|^2 g(k, q) dq dk \\ & \leq \frac{1}{4\pi^4 C_{+-}} \|G\|_{L^\infty(\mathbb{R})} \underline{\text{Tr}}((T - \epsilon_F)Q). \end{aligned} \quad (2.32)$$

Conclusion of the proof. The estimate (2.8) finally follows from (2.26), (2.27), (2.30) and (2.32).

2.3.2 Proof of Lemma 2.10

Let us first state a useful technical result showing that finite-rank operators are dense in \mathcal{X}_q and \mathcal{K}_q . It is a direct adaptation of [FLLS13, Lemma 3.2].

Lemma 2.13. Fix $q \in \mathbb{R}^2$ and consider $Q_q \in \mathcal{X}_q$. There exists a sequence $(Q_{n,q})_{n \geq 1} \subset \mathcal{X}_q$ of finite-rank operators such that $T_q Q_{n,q} \in \mathcal{L}(L^2(\mathbb{R}))$, and

- $Q_{n,q} \rightarrow Q_q$ strongly (i.e., $Q_{n,q} f \rightarrow Q_q f$ strongly in $L^2(\mathbb{R})$ for any $f \in L^2(\mathbb{R})$);
- $\lim_{n \rightarrow +\infty} \left\| |T_q - \epsilon_F|^{1/2} (Q_{n,q}^{\pm\pm} - Q_q^{\pm\pm}) |T_q - \epsilon_F|^{1/2} \right\|_{\mathfrak{S}_1(L^2(\mathbb{R}))} = 0$.

Moreover, if $Q_q \in \mathcal{K}_q$, the sequence $(Q_{n,q})_{n \geq 1}$ can be chosen in \mathcal{K}_q .

We can now provide the proof of Lemma 2.10, which follows the proof of [FLLS13, Lemma 3.3] and uses in particular ideas from [Rum11]. Let $0 \leq \gamma \leq 1$ be a smooth enough self-adjoint finite-rank operator on $L^2(\mathbb{R})$ (with density ρ_γ). For $q \in \partial \mathfrak{B}_{\epsilon_F}$, $T_q - \epsilon_F = -\frac{1}{2} \frac{d^2}{dz^2}$ and (2.20) boils down to the one-dimensional Lieb–Thirring inequality [LT91]. For $q \in \mathfrak{B}_{\epsilon_F}$, denote by $\rho_{e,q}$ is the density of the finite-rank operator $P_{e,q} \gamma P_{e,q}$ where $P_{e,q} := \mathbb{1}_{[e, +\infty)}(|T_q - \epsilon_F|)$. Then, by the same manipulations as in [FLLS13],

$$\mathrm{Tr}_{L^2(\mathbb{R})} \left(|T_q - \epsilon_F|^{1/2} \gamma |T_q - \epsilon_F|^{1/2} \right) = \int_0^{+\infty} \left(\int_{\mathbb{R}} \rho_{e,q}(z) dz \right) de \geq \int_{\mathbb{R}} R_q(\rho_\gamma(z)) dz,$$

with

$$R_q(t) = \int_0^{f_q^{-1}(t)} \left(\sqrt{t} - \sqrt{f_q(e)} \right)^2 de,$$

where (introducing $a_+ = \max(0, a)$) the nonnegative function

$$\begin{aligned} f_q(e) &= (2\pi)^{-1} \left| \left\{ p \in \mathbb{R}, \left| \frac{|p|^2}{2} + \frac{|q|^2}{2} - \epsilon_F \right| \leq e \right\} \right| \\ &= (2\pi)^{-1} \left(\sqrt{2e + 2\epsilon_F - |q|^2} - \sqrt{(-2e + 2\epsilon_F - |q|^2)_+} \right) \end{aligned}$$

is increasing, hence invertible.

Let us now provide a global lower bound on the function $t \mapsto R_q(t)$ by considering the asymptotic behavior of this function in the regimes $t \rightarrow 0$ and $t \rightarrow +\infty$. We work in fact with the rescaled parameter $T = t/\omega_q$ and the rescaled energy $E = e/\omega_q^2$ with $\omega_q = \sqrt{2\epsilon_F - |q|^2} > 0$ (since $q \in \mathfrak{B}_{\epsilon_F}$). Note indeed that

$$f_q(e) = \omega_q F \left(\frac{e}{\omega_q^2} \right), \quad F(E) = \frac{1}{2\pi} \left(\sqrt{1 + 2E} - \sqrt{(1 - 2E)_+} \right),$$

and

$$R_q(t) = \int_0^{+\infty} \left[\left(\sqrt{t} - \sqrt{f_q(e)} \right)_+ \right]^2 de = \omega_q^3 \int_0^{+\infty} \left[\left(\sqrt{\frac{t}{\omega_q}} - \sqrt{F(E)} \right)_+ \right]^2 dE.$$

Since $F(E) \sim \pi^{-1}E$ as $E \rightarrow 0$ and $F(E) \sim \pi^{-1}\sqrt{E}/2$ as $E \rightarrow +\infty$, a simple computation shows that

$$\int_0^{+\infty} \left[\left(\sqrt{T} - \sqrt{F(E)} \right)_+ \right]^2 dE \underset{T \rightarrow 0}{\sim} \frac{\pi}{6} T^2, \quad \int_0^{+\infty} \left[\left(\sqrt{T} - \sqrt{F(E)} \right)_+ \right]^2 dE \underset{T \rightarrow \infty}{\sim} \frac{2\pi^2}{15} T^3.$$

There exist therefore two positive constants $C_{1,\mathrm{diag}}, C_{2,\mathrm{diag}}$ such that

$$\forall T \geq 0, \quad \int_0^{+\infty} \left[\left(\sqrt{T} - \sqrt{F(E)} \right)_+ \right]^2 dE \geq C_{1,\mathrm{diag}} T^2 + C_{2,\mathrm{diag}} T^3,$$

from which we deduce that

$$\forall t \geq 0, \quad R_q(t) \geq C_{1,\mathrm{diag}} \omega_q t^2 + C_{2,\mathrm{diag}} t^3.$$

The final result is obtained by a continuity argument and the density result of Lemma 2.13.

2.3.3 Proof of Lemma 2.11

We follow the proofs of [FLLS13, Theorem 2.1 and Lemma 3.4]. Inequality (2.21) is trivial for $q \in \partial \overline{\mathfrak{B}}_{\epsilon_F}$. Fix $q \in \mathfrak{B}_{\epsilon_F}$ and $Q_q \in \mathcal{K}_q$. Since $Q_q^{+-} = (Q_q^{-+})^*$, it holds $\rho_{Q_q^{+-}} + \rho_{Q_q^{-+}} = 2\Re \rho_{Q_q^{-+}}$. It suffices therefore to obtain estimates for $\rho_{Q_q^{-+}}$. We rely on a duality argument. Consider to this end $V \in L^2(\mathbb{R})$. By Hölder-type inequalities in Schatten spaces,

$$\begin{aligned} \left| \int_{\mathbb{R}} V \rho_{Q_q^{-+}} \right| &= \left| \text{Tr}_{L^2(\mathbb{R})} \left(\frac{1 - \gamma_{0,q}}{|T_q - \epsilon_F|^{1/4}} V \frac{\gamma_{0,q}}{|T_q - \epsilon_F|^{1/4}} |T_q - \epsilon_F|^{1/4} Q_q |T_q - \epsilon_F|^{1/4} \right) \right| \\ &\leq \left\| \frac{1 - \gamma_{0,q}}{|T_q - \epsilon_F|^{1/4}} V \frac{\gamma_{0,q}}{|T_q - \epsilon_F|^{1/4}} \right\|_{\mathfrak{S}_2} \left\| |T_q - \epsilon_F|^{1/4} Q_q |T_q - \epsilon_F|^{1/4} \right\|_{\mathfrak{S}_2} \\ &\leq \left\| \frac{1 - \gamma_{0,q}}{|T_q - \epsilon_F|^{1/4}} V \frac{\gamma_{0,q}}{|T_q - \epsilon_F|^{1/4}} \right\|_{\mathfrak{S}_2} \left\| |T_q - \epsilon_F|^{1/4} |Q_q|^{1/2} \right\|_{\mathfrak{S}_4}^2 \\ &\leq \left\| \frac{1 - \gamma_{0,q}}{|T_q - \epsilon_F|^{1/4}} V \frac{\gamma_{0,q}}{|T_q - \epsilon_F|^{1/4}} \right\|_{\mathfrak{S}_2} \left\| |T_q - \epsilon_F|^{1/2} Q_q \right\|_{\mathfrak{S}_2}, \end{aligned}$$

where we used the Araki-Lieb-Thirring inequality for operators [Ara90] (as in [LT91, LS15]) to obtain the last estimate.

$$\left\| |T_q - \epsilon_F|^{1/4} |Q_q|^{1/2} \right\|_{\mathfrak{S}_4}^2 \leq \left\| |T_q - \epsilon_F|^{1/2} Q_q \right\|_{\mathfrak{S}_2}.$$

Since $0 \leq Q_q^2 \leq Q_q^{++} - Q_q^{--}$, it finally holds,

$$\left| \int_{\mathbb{R}} V \rho_{Q_q^{-+}} \right| \leq \left\| \frac{1 - \gamma_{0,q}}{|T_q - \epsilon_F|^{1/4}} V \frac{\gamma_{0,q}}{|T_q - \epsilon_F|^{1/4}} \right\|_{\mathfrak{S}_2} \sqrt{\text{Tr}_{L^2(\mathbb{R})} (|T_q - \epsilon_F|^{1/2} (Q_q^{++} - Q_q^{--}) |T_q - \epsilon_F|^{1/2})}. \quad (2.33)$$

Now we calculate the kernel $K(z, z')$ of operator $(1 - \gamma_{0,q})|T_q - \epsilon_F|^{-1/4} V \gamma_{0,q} |T_q - \epsilon_F|^{-1/4}$. Remark that

$$\left\| \frac{1 - \gamma_{0,q}}{|T_q - \epsilon_F|^{1/4}} V \frac{\gamma_{0,q}}{|T_q - \epsilon_F|^{1/4}} \right\|_{\mathfrak{S}_2}^2 = \int_{z \in \mathbb{R}, z' \in \mathbb{R}} |K(z, z')|^2 dx dy.$$

We have, for $f \in L^2(\mathbb{R})$

$$\left(\frac{\gamma_{0,q}}{|T_q - \epsilon_F|^{1/4}} f \right) (z) = \frac{1}{2\pi} \int_{\frac{|q|^2}{2} - \epsilon_F + \frac{p^2}{2} \leq 0} \int_{\mathbb{R}} \frac{\mathbb{1}(|p|^2 + |q|^2 \leq 2\epsilon_F)}{\left| \frac{|p|^2}{2} + \frac{|q|^2}{2} - \epsilon_F \right|^{1/4}} e^{ip(z-z')} f(z') dz' dp.$$

We also have

$$\begin{aligned} \left(\frac{1 - \gamma_{0,q}}{|T_q - \epsilon_F|^{1/4}} V \frac{\gamma_{0,q}}{|T_q - \epsilon_F|^{1/4}} f \right) (z) &= \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}} \int_{\substack{\frac{|q|^2}{2} - \epsilon_F + \frac{p^2}{2} \leq 0 \\ \frac{|q|^2}{2} - \epsilon_F + \frac{s^2}{2} \geq 0}} e^{isz} \widehat{V}(s - p) \\ &\quad \cdot \frac{\mathbb{1}(|p|^2 + |q|^2 \leq 2\epsilon_F) \mathbb{1}(|s|^2 + |q|^2 \geq 2\epsilon_F)}{\left| \frac{|p|^2}{2} + \frac{|q|^2}{2} - \epsilon_F \right|^{1/4} \left| \frac{|s|^2}{2} + \frac{|q|^2}{2} - \epsilon_F \right|^{1/4}} e^{-ipz'} f(z') ds dp dz', \end{aligned}$$

therefore

$$\begin{aligned} K(z, z') &= \frac{1}{(2\pi)^{3/2}} \int_{\substack{\frac{|q|^2}{2} - \epsilon_F + \frac{p^2}{2} \leq 0 \\ \frac{|q|^2}{2} - \epsilon_F + \frac{s^2}{2} \geq 0}} e^{isz} \widehat{V}(s - p) \cdot \frac{\mathbb{1}(|p|^2 + |q|^2 \leq 2\epsilon_F) \mathbb{1}(|s|^2 + |q|^2 \geq 2\epsilon_F)}{\left| \frac{|p|^2}{2} + \frac{|q|^2}{2} - \epsilon_F \right|^{1/4} \left| \frac{|s|^2}{2} + \frac{|q|^2}{2} - \epsilon_F \right|^{1/4}} e^{-ipz'} ds dp. \end{aligned}$$

By consequence,

$$\begin{aligned} & \int_{z \in \mathbb{R}, z' \in \mathbb{R}} |K(z, z')|^2 dz dz' \\ &= \frac{1}{2\pi} \int_{\substack{|q|^2 - \epsilon_F + \frac{p^2}{2} \leq 0 \\ \frac{|q|^2}{2} - \epsilon_F + \frac{s^2}{2} \geq 0}} |\widehat{V}(s-p)|^2 \cdot \frac{\mathbb{1}(|p|^2 + |q|^2 \leq 2\epsilon_F) \mathbb{1}(|s|^2 + |q|^2 \geq 2\epsilon_F)}{\left| \frac{|p|^2}{2} + \frac{|q|^2}{2} - \epsilon_F \right|^{1/2} \left| \frac{|s|^2}{2} + \frac{|q|^2}{2} - \epsilon_F \right|^{1/2}} ds dp. \end{aligned}$$

Therefore by denoting

$$\Phi_q(k) := \int_{\substack{|q|^2 + \frac{(s-k)^2}{2} \geq \epsilon_F \\ \frac{|q|^2}{2} + \frac{s^2}{2} \leq \epsilon_F}} \frac{ds}{\sqrt{\left(\frac{|q|^2}{2} + \frac{(s-k)^2}{2} - \epsilon_F \right) \left(\epsilon_F - \frac{|q|^2}{2} - \frac{s^2}{2} \right)}},$$

we obtain that

$$\left\| \frac{1 - \gamma_{0,q}}{|T_q - \epsilon_F|^{1/4}} V \frac{\gamma_{0,q}}{|T_q - \epsilon_F|^{1/4}} \right\|_{\mathfrak{S}_2}^2 = \frac{1}{2\pi} \int_{\mathbb{R}} |\widehat{V}(k)|^2 \Phi_q(k) dk. \quad (2.34)$$

In fact, denoting by $\omega_q = \sqrt{2\epsilon_F - |q|^2} > 0$ (since $q \in \mathfrak{B}_{\epsilon_F}$),

$$\Phi_q(k) = \frac{1}{\omega_q} \Psi\left(\frac{k}{\omega_q}\right), \quad \Psi(t) = 2 \int_{\substack{(m-t)^2 \geq 1 \\ m^2 \leq 1}} \frac{dm}{\sqrt{((m-t)^2 - 1)(1 - m^2)}}.$$

The bounds (2.33) and (2.34) then lead to

$$\left| \int_{\mathbb{R}} V \rho_{Q_q^-} \right|^2 \leq \frac{1}{2\pi} \left(\int_{\mathbb{R}} |\widehat{V}(k)|^2 \Phi_q(k) dk \right) \text{Tr}_{L^2(\mathbb{R})} \left(|T_q - \epsilon_F|^{1/2} (Q_q^{++} - Q_q^{--}) |T_q - \epsilon_F|^{1/2} \right).$$

From the estimates on Ψ provided by [FLLS13, Lemma 3.4] (namely $\Psi(t) \sim -\log|t-2|$ as $t \rightarrow 2$ and $\Psi(t) \sim 2\pi/t$ as $t \rightarrow +\infty$), there exists a positive constant R such that

$$\forall 0 < w_q \leq \sqrt{2\epsilon_F}, \forall k \in \mathbb{R}, \quad 0 \leq \Phi_q(k) \leq \frac{R}{\left| |k| - 2\omega_q \right|^{1/2} \sqrt{\omega_q}}, \quad (2.35)$$

which implies

$$\begin{aligned} \frac{2\pi}{R} \sqrt{\omega_q} \int_{\mathbb{R}} |\widehat{\rho}_{Q_q^-}(k)|^2 \left| |k| - 2\omega_q \right|^{1/2} dk &\leq 2\pi \int_{\mathbb{R}} \frac{|\widehat{\rho}_{Q_q^-}(k)|^2}{\Phi_q(k)} dk \\ &\leq \text{Tr}_{L^2(\mathbb{R})} \left(|T_q - \epsilon_F|^{1/2} (Q_q^{++} - Q_q^{--}) |T_q - \epsilon_F|^{1/2} \right). \end{aligned}$$

This gives the claimed result.

2.3.4 Proof of Theorem 2.6

We first show in Section 2.3.4 that the minimization set \mathcal{F}_ν for Coulomb interactions is not empty. We then prove in Section 2.3.4 the existence of minimizers for Yukawa and Coulomb interactions. The uniqueness of the densities relies on a technical result whose proof is postponed to Section 2.3.4. Finally, we show in Section 2.3.4 that the Yukawa ground state converges to the Coulomb ground state when $m \rightarrow 0$.

Step 1. The set \mathcal{F}_ν is not empty.

We prove in this section that the set $\mathcal{F}_\nu = \{Q \in \mathcal{K} \mid \rho_Q - \nu \in \mathcal{C}\}$ is non-empty for all $\nu \in L^1(\mathbb{R})$ such that $|\cdot| \nu(\cdot) \in L^1(\mathbb{R})$. We do so by explicitly constructing an element in \mathcal{F}_ν . We distinguish the cases $\kappa \geq 0$ and $\kappa < 0$, where ν is the total charge per unit area of the defect:

$$\kappa = \int_{-\infty}^{+\infty} \nu(z) dz.$$

Non-negative total charge per unit area. Consider first the case when $\kappa \geq 0$. We introduce an even cut-off function $\chi \in C_c^\infty(\mathbb{R})$ such that

$$0 \leq \chi \leq 1, \quad \int_{\mathbb{R}} \chi^2 = 1.$$

For a parameter $\mu \in (\epsilon_F, +\infty)$ to be specified and almost all $q \in \mathbb{R}^2$, we then define the self-adjoint operator

$$Q_\mu := \mathcal{U} \left(\int_{\mathbb{R}^2}^\oplus Q_{\mu,q} dq \right) \mathcal{U}^{-1}, \quad Q_{\mu,q} := \mathbb{1}_{(\epsilon_F, \mu]}(T_q) \chi^2 \mathbb{1}_{(\epsilon_F, \mu]}(T_q). \quad (2.36)$$

Note first that $Q_{\mu,q} = 0$ when $|q|^2 > 2\mu$. The operator inequality $0 \leq \mathbb{1}_{(\epsilon_F, \mu]}(T_q) \leq \mathbb{1}_{(\epsilon_F, +\infty)}(T_q) = 1 - \gamma_{0,q}$ also implies that $0 \leq Q_{\mu,q} \equiv Q_{\mu,q}^{++} \leq 1 - \gamma_{0,q}$. Therefore, $q \mapsto Q_{\mu,q} \in L^\infty(\mathbb{R}^2; \mathcal{S}(L^2(\mathbb{R})))$. Moreover, the Kato–Seiler–Simon inequality [Sim79, Theorem 4.1]

$$\forall p \geq 2, \quad \|f(-i\nabla)g\|_{\mathfrak{S}_p(L^2(\mathbb{R}))} \leq (2\pi)^{-1/p} \|g\|_{L^p} \|f\|_{L^p}, \quad (2.37)$$

shows that

$$|T_q - \epsilon_F|^{1/2} Q_{\mu,q} |T_q - \epsilon_F|^{1/2} = \left(|T_q - \epsilon_F|^{1/2} \mathbb{1}_{(\epsilon_F, \mu]}(T_q) \chi \right) \left(\chi \mathbb{1}_{(\epsilon_F, \mu]}(T_q) |T_q - \epsilon_F|^{1/2} \right) \in \mathfrak{S}_1 \quad (2.38)$$

as the product of two Hilbert–Schmidt operators. We have therefore proven at this stage that $Q_{\mu,q} \in \mathcal{K}_q$ for all $q \in \mathbb{R}^2$.

In addition, since the kernel of the operator $|T_q - \epsilon_F|^{1/2} \mathbb{1}_{(\epsilon_F, \mu]}(T_q) \chi$ is $(z, z') \mapsto g_q(z - z') \chi(z')$ with

$$g_q(z) = \frac{1}{2\pi} \int_{\mathbb{R}} \left| \frac{k^2 + |q|^2}{2} - \epsilon_F \right|^{1/2} \mathbb{1}_{\left\{ \frac{k^2 + |q|^2}{2} \in (\epsilon_F, \mu] \right\}} e^{ikz} dk,$$

we obtain

$$\begin{aligned} \underline{\text{Tr}}((T - \epsilon_F)Q_\mu) &= \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} \underline{\text{Tr}}_{L^2(\mathbb{R})} \left(|T_q - \epsilon_F|^{1/2} Q_{\mu,q} |T_q - \epsilon_F|^{1/2} \right) dq \\ &= \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} \left(\int_{\mathbb{R}} \chi^2 \right) \left(\int_{\mathbb{R}} |g_q|^2 \right) dq \\ &= \frac{1}{(2\pi)^3} \int_{\mathbb{R}^2} \int_{\epsilon_F < \frac{|q|^2}{2} + \frac{k^2}{2} \leq \mu} \left(\frac{k^2 + |q|^2}{2} - \epsilon_F \right) dk dq < \infty, \end{aligned} \quad (2.39)$$

which shows that $Q_\mu \in \mathcal{K}$.

It remains to prove that $\rho_{Q_\mu} - \nu \in \underline{\mathcal{C}}$. First, it easily follows from (2.36) that ρ_{Q_μ} is smooth and compactly supported. By computations similar to the ones used to establish (2.39), and noting that $Q_{\mu,q} \in \mathfrak{S}_1$ by a decomposition similar to (2.38),

$$\underline{\text{Tr}}(Q_\mu) = \int_{\mathbb{R}} \rho_{Q_\mu} = \frac{1}{(2\pi)^3} \int_{\mathbb{R}^2} \int_{\epsilon_F < \frac{|q|^2}{2} + \frac{k^2}{2} \leq \mu} dk dq = \frac{\sqrt{2}}{3\pi^2} \left(\mu^{3/2} - \epsilon_F^{3/2} \right).$$

There exists therefore a (unique) value $\mu(\kappa)$ such that $\int_{\mathbb{R}} \rho_{Q_{\mu(\kappa)}}(z) dz = \kappa$. The latter equality is equivalent to $\widehat{\rho_{Q_{\mu(\kappa)}}}(0) - \widehat{\nu}(0) = 0$. Since $\widehat{\rho_{Q_{\mu(\kappa)}}} - \widehat{\nu}$ is C^1 and bounded, we can therefore conclude that the function $k \mapsto |k|^{-1}(\widehat{\rho_{Q_{\mu(\kappa)}}}(k) - \widehat{\nu}(k))$ is in $L^2(\mathbb{R})$, i.e. $\rho_{Q_\mu} - \nu \in \underline{\mathcal{C}}$. This allows to conclude that $Q_{\mu(\kappa)} \in \mathcal{F}_\nu$, and so \mathcal{F}_ν is not empty.

Negative total charge per unit area. We now consider the case when $\kappa < 0$. We define the following self-adjoint operator, for a parameter $\alpha \in (0, +\infty)$ to be specified later on:

$$Q_\alpha := \mathcal{U} \left(\int_{\mathbb{R}^2}^{\oplus} Q_{\alpha,q} dq \right) \mathcal{U}^{-1}, \quad Q_{\alpha,q} := -\alpha \gamma_{0,q} \chi^2 \gamma_{0,q}.$$

It is easy to see that $-\gamma_{0,q} \leq Q_{\alpha,q} = Q_{\alpha,q}^- \leq 0$ and that $Q_{\alpha,q} = 0$ when $|q|^2 > 2\epsilon_F$, so that $q \mapsto Q_{\alpha,q} \in L^\infty(\mathbb{R}^2; \mathcal{S}(L^2(\mathbb{R})))$. Moreover, $|T_q - \epsilon_F|^{1/2} Q_{\alpha,q} \in \mathfrak{S}_2$ by the Kato–Seiler–Simon inequality (2.37), so that $|T_q - \epsilon_F|^{1/2} Q_{\alpha,q} |T_q - \epsilon_F|^{1/2} \in \mathfrak{S}_1$. This shows that $Q_{\alpha,q} \in \mathcal{K}_q$ for all $q \in \mathbb{R}^2$. In addition, by computations similar to the ones performed for the case $\kappa \geq 0$,

$$\underline{\text{Tr}}((T - \epsilon_F) Q_\mu) = \frac{\alpha}{(2\pi)^3} \int_{\mathbb{R}^2} \int_{0 \leq k^2 + |q|^2 \leq 2\epsilon_F} \left(\epsilon_F - \frac{k^2 + |q|^2}{2} \right) dk dq < \infty,$$

so that $Q_\alpha \in \mathcal{K}$.

It can be shown same as for the case $\kappa \geq 0$ that ρ_{Q_α} is smooth and compactly supported. Moreover,

$$\int_{\mathbb{R}} \rho_{Q_\alpha} = -\frac{\alpha}{(2\pi)^3} \int_{\mathbb{R}^2} \int_{\frac{|q|^2}{2} + \frac{k^2}{2} \leq \epsilon_F} dk dq = -\frac{\alpha \sqrt{2} \epsilon_F^{3/2}}{3\pi^2},$$

so that the choice $\alpha(\kappa) = 3\pi^2 \epsilon_F^{-3/2} |\kappa| / \sqrt{2}$ ensures that $\int_{\mathbb{R}} \rho_{Q_{\alpha(\kappa)}} = \kappa$. We can then conclude, by the same reasoning as for the case $\kappa \geq 0$, that $\rho_{Q_{\alpha(\kappa)}} - \nu \in \underline{\mathcal{C}}$, and finally that \mathcal{F}_ν is not empty.

Step 2. Existence of ground state for Yukawa (resp. Coulomb) interactions.

We write a detailed proof for Coulomb interactions, the result for Yukawa interactions following the same lines. We first construct a candidate minimizer \bar{Q} by as the limit of some minimizing sequence for (2.14) and next show that \bar{Q} is an admissible state (i.e. $\bar{Q} \in \mathcal{K}$). We finally prove that \bar{Q} is a minimizer and that all minimizers share the same density.

Construction of a candidate minimizer. It is easy to see that the functional $\mathcal{E}_{\nu,0}(Q)$ is well defined on the non-empty set \mathcal{F}_ν . Consider a minimizing sequence $\{Q_n\}_{n \geq 1} \subset \mathcal{F}_\nu$. There exists $C \in \mathbb{R}_+$ such that

$$\forall n \geq 1, \quad \underline{\text{Tr}}((T - \epsilon_F) Q_n) \leq C, \quad \underline{D}(\rho_{Q_n} - \nu, \rho_{Q_n} - \nu) \leq C. \quad (2.40)$$

Consider any exponent $1 < p < 5/3$. Inequality (2.8) shows that the sequence of densities $\{\rho_{Q_n}\}_{n \geq 1}$ is uniformly bounded in $L^2(\mathbb{R}) + L^p(\mathbb{R})$. Up to extraction, there exist

$$\bar{Q} := \mathcal{U}^{-1} \left(\int_{\mathbb{R}^2}^{\oplus} \bar{Q}_q dq \right) \mathcal{U}, \quad \bar{\rho}_Q \in L^2(\mathbb{R}) + L^p(\mathbb{R}), \quad \tilde{\rho}_Q - \nu \in \underline{\mathcal{C}}$$

such that $\rho_{Q_n} \rightharpoonup \bar{\rho}_Q$ weakly in $L^2(\mathbb{R}) + L^p(\mathbb{R})$ and $\rho_{Q_n} - \nu \rightharpoonup \tilde{\rho}_Q - \nu$ weakly in $\underline{\mathcal{C}}$, while $-\gamma_0 \leq \bar{Q} \leq 1 - \gamma_0$ and $Q_n \xrightarrow{*} \bar{Q}$ in the following sense:

- for any operator-valued function $q \mapsto U_q \in L^1(\mathbb{R}^2; \mathfrak{S}_1)$,

$$\int_{\mathbb{R}^2} \text{Tr}_{L^2(\mathbb{R})} (U_q Q_{n,q}) dq \xrightarrow{n \rightarrow \infty} \int_{\mathbb{R}^2} \text{Tr}_{L^2(\mathbb{R})} (U_q \bar{Q}_q) dq; \quad (2.41)$$

- for any operator-valued function $q \mapsto M_q \in L^2(\mathbb{R}^2; \mathfrak{S}_2)$,

$$\int_{\mathbb{R}^2} \text{Tr}_{L^2(\mathbb{R})} (|T_q - \epsilon_F|^{1/2} Q_{n,q} M_q) dq \xrightarrow{n \rightarrow \infty} \int_{\mathbb{R}^2} \text{Tr}_{L^2(\mathbb{R})} (|T_q - \epsilon_F|^{1/2} \bar{Q}_q M_q) dq; \quad (2.42)$$

$$\int_{\mathbb{R}^2} \text{Tr}_{L^2(\mathbb{R})} (M_q |T_q - \epsilon_F|^{1/2} Q_{n,q}) dq \xrightarrow{n \rightarrow \infty} \int_{\mathbb{R}^2} \text{Tr}_{L^2(\mathbb{R})} (M_q |T_q - \epsilon_F|^{1/2} \bar{Q}_q) dq; \quad (2.43)$$

$$\int_{\mathbb{R}^2} \text{Tr}_{L^2(\mathbb{R})} (M_q Q_{n,q} |T_q - \epsilon_F|^{1/2}) dq \xrightarrow{n \rightarrow \infty} \int_{\mathbb{R}^2} \text{Tr}_{L^2(\mathbb{R})} (M_q \bar{Q}_q |T_q - \epsilon_F|^{1/2}) dq. \quad (2.44)$$

The weak-* convergence (2.41) is a consequence of the fact that the sequence $\{Q_n\}_{n \geq 1}$ is uniformly bounded in $L^\infty(\mathbb{R}^2; \mathcal{L}(L^2(\mathbb{R})))$, whose pre-dual is $L^1(\mathbb{R}^2; \mathfrak{S}_1)$. The weak convergences (2.42) to (2.44) are a consequence of the inequality

$$\int_{\mathbb{R}^2} \left\| |T_q - \epsilon_F|^{1/2} Q_{n,q} \right\|_{\mathfrak{S}_2}^2 dq \leq \int_{\mathbb{R}^2} \text{Tr}_{L^2(\mathbb{R})} \left(|T_q - \epsilon_F|^{1/2} (Q_{n,q}^{++} - Q_{n,q}^{--}) |T_q - \epsilon_F|^{1/2} \right) dq \leq C, \quad (2.45)$$

which shows that the sequence of operator-valued functions $q \mapsto |T_q - \epsilon_F|^{1/2} Q_{n,q}$ and $q \mapsto Q_{n,q} |T_q - \epsilon_F|^{1/2}$ are uniformly bounded in the Hilbert space $L^2(\mathbb{R}^2; \mathfrak{S}_2)$.

The state \overline{Q} belongs to \mathcal{K} . Note first that the weak convergence of $\left\{ q \mapsto |T_q - \epsilon_F|^{1/2} Q_{n,q} \right\}_{n \geq 1}$ to $q \mapsto |T_q - \epsilon_F|^{1/2} \overline{Q}_q$ in $L^2(\mathbb{R}^2; \mathfrak{S}_2)$ implies

$$\int_{\mathbb{R}^2} \left\| |T_q - \epsilon_F|^{1/2} \overline{Q}_q \right\|_{\mathfrak{S}_2}^2 dq \leq \liminf_{n \rightarrow \infty} \int_{\mathbb{R}^2} \left\| |T_q - \epsilon_F|^{1/2} Q_{n,q} \right\|_{\mathfrak{S}_2}^2 dq.$$

It is therefore sufficient to show that $\text{Tr}((T - \epsilon_F) \overline{Q}) < \infty$ in order to conclude that $\overline{Q} \in \mathcal{K}$. Consider to this end an orthonormal basis $\{\phi_i\}_{i \in \mathbb{N}} \subset H^1(\mathbb{R})$ of $L^2(\mathbb{R})$, and define, for $N \geq 1$ and $R > 0$, the family of operators

$$M_{q,R}^N := |T_q - \epsilon_F|^{1/2} \left(\sum_{i=1}^N |\phi_i\rangle \langle \phi_i| \right) g_R(q),$$

where

$$g_R(q) := \begin{cases} 1 & \text{if } |q|^2 < R \\ \frac{1}{(1 + |q|^2)^2} & \text{if } |q|^2 \geq R. \end{cases}$$

A simple computation shows that $q \mapsto M_{q,R}^N$ is in $L^2(\mathbb{R}^2; \mathfrak{S}_2)$. Using (2.42) with $q \mapsto (1 - \gamma_{0,q}) M_{q,R}^N (1 - \gamma_{0,q})$,

$$\begin{aligned} 0 &\leq \int_{\mathbb{R}^2} \text{Tr}_{L^2(\mathbb{R})} \left(|T_q - \epsilon_F|^{1/2} \overline{Q}_q |T_q - \epsilon_F|^{1/2} (1 - \gamma_{0,q}) M_{q,R}^N (1 - \gamma_{0,q}) \right) dq \\ &= \int_{\mathbb{R}^2} \text{Tr}_{L^2(\mathbb{R})} \left(|T_q - \epsilon_F|^{1/2} \overline{Q}_q^{++} |T_q - \epsilon_F|^{1/2} \left(\sum_{i=1}^N |\phi_i\rangle \langle \phi_i| \right) \right) g_R(q) dq \\ &= \lim_{n \rightarrow \infty} \int_{\mathbb{R}^2} \sum_{i=1}^N \left\langle \phi_i \left| |T_q - \epsilon_F|^{1/2} Q_{n,q}^{++} |T_q - \epsilon_F|^{1/2} \right| \phi_i \right\rangle g_R(q) dq \\ &\leq \liminf_{n \rightarrow \infty} \int_{\mathbb{R}^2} \text{Tr}_{L^2(\mathbb{R})} \left(|T_q - \epsilon_F|^{1/2} Q_{n,q}^{++} |T_q - \epsilon_F|^{1/2} \right) dq \leq C, \end{aligned}$$

where the last inequality is a consequence of the uniform bound (2.40). We can then pass to the limits $R \rightarrow +\infty$ and $N \rightarrow +\infty$ with Fatou's Lemma and get

$$\begin{aligned} 0 &\leq \int_{\mathbb{R}^2} \text{Tr}_{L^2(\mathbb{R})} \left(|T_q - \epsilon_F|^{1/2} \overline{Q}_q^{++} |T_q - \epsilon_F|^{1/2} \right) dq \\ &\leq \liminf_{n \rightarrow +\infty} \int_{\mathbb{R}^2} \text{Tr}_{L^2(\mathbb{R})} \left(|T_q - \epsilon_F|^{1/2} \overline{Q}_{n,q}^{++} |T_q - \epsilon_F|^{1/2} \right) dq. \end{aligned}$$

A similar reasoning shows that

$$\begin{aligned} 0 &\leq - \int_{\mathbb{R}^2} \text{Tr}_{L^2(\mathbb{R})} \left(|T_q - \epsilon_F|^{1/2} \overline{Q}_q^{--} |T_q - \epsilon_F|^{1/2} \right) dq \\ &\leq - \liminf_{n \rightarrow \infty} \int_{\mathbb{R}^2} \text{Tr}_{L^2(\mathbb{R})} \left(|T_q - \epsilon_F|^{1/2} \overline{Q}_{n,q}^{--} |T_q - \epsilon_F|^{1/2} \right) dq. \end{aligned}$$

The combination of the last two inequalities shows that

$$0 \leq \underline{\text{Tr}}((T - \epsilon_F)\overline{Q}) \leq \liminf_{n \rightarrow \infty} \underline{\text{Tr}}((T - \epsilon_F)Q_n) \leq C, \quad (2.46)$$

so that $\overline{Q} \in \mathcal{K}$.

The state \overline{Q} is a minimizer, and its density is uniquely defined. The density $\rho_{\overline{Q}}$ is well defined in view of Proposition 2.2 since $\overline{Q} \in \mathcal{K}$, but it is *a priori* different from $\overline{\rho}_Q$ and $\tilde{\rho}_Q$. The following lemma shows that all these densities actually coincide.

Lemma 2.14. (*Consistency of densities*) *It holds $\rho_{\overline{Q}} - \nu = \overline{\rho}_Q - \nu = \tilde{\rho}_Q - \nu$ in $\mathcal{D}'(\mathbb{R})$. In particular, $\rho_{\overline{Q}} = \overline{\rho}_Q$ as elements of $L^2(\mathbb{R}) + L^p(\mathbb{R})$, and $\rho_{\overline{Q}} - \nu = \tilde{\rho}_Q - \nu$ as elements of $\underline{\mathcal{C}}$.*

We postpone the proof of this result to Section 2.3.4. We use it to obtain that, since $\underline{D}(\cdot, \cdot)$ defines an inner product on $\underline{\mathcal{C}}$,

$$\underline{D}(\rho_{\overline{Q}} - \nu, \rho_{\overline{Q}} - \nu) \leq \liminf_{n \rightarrow \infty} \underline{D}(\rho_{Q_n} - \nu, \rho_{Q_n} - \nu). \quad (2.47)$$

This shows in particular that \overline{Q} is an admissible state (i.e. $\overline{Q} \in \mathcal{F}_\nu$). Moreover, (2.46) and (2.47) imply that the minimizing sequence $\{Q_n\}_{n \geq 1}$ is such that

$$\mathcal{E}_{\nu,0}(\overline{Q}) \leq \liminf_{n \rightarrow \infty} \mathcal{E}_{\nu,0}(Q_n), \quad (2.48)$$

which shows that \overline{Q} is a minimizer of (2.15).

Let us finally prove that all minimizers share the same density. Consider two minimizers \overline{Q}_1 and \overline{Q}_2 . By convexity of \mathcal{F}_ν , it holds $\frac{1}{2}(\overline{Q}_1 + \overline{Q}_2) \in \mathcal{F}_\nu$. Moreover,

$$\mathcal{E}_{\nu,0}\left(\frac{\overline{Q}_1 + \overline{Q}_2}{2}\right) = \frac{1}{2}\mathcal{E}_{\nu,0}(\overline{Q}_1) + \frac{1}{2}\mathcal{E}_{\nu,0}(\overline{Q}_2) - \frac{1}{4}\underline{D}\left(\rho_{\overline{Q}_1} - \rho_{\overline{Q}_2}, \rho_{\overline{Q}_1} - \rho_{\overline{Q}_2}\right),$$

which shows that $\underline{D}\left(\rho_{\overline{Q}_1} - \rho_{\overline{Q}_2}, \rho_{\overline{Q}_1} - \rho_{\overline{Q}_2}\right) = 0$. This implies that all minimizers share the same density.

Proof of Lemma 2.14

We prove the result for Coulomb interactions. The statement of the lemma and its proof for Yukawa interactions are obtained by a straightforward adaptation.

Equality of $\tilde{\rho}_Q$ and $\overline{\rho}_Q$. Let us first show that $\tilde{\rho}_Q - \nu = \overline{\rho}_Q - \nu$ in \mathcal{D}' . Fix $w \in \mathcal{D}(\mathbb{R})$. The weak convergence $\rho_{Q_n} \rightarrow \overline{\rho}_Q$ in $L^2(\mathbb{R}) + L^p(\mathbb{R})$ implies that

$$\langle \rho_{Q_n} - \nu, w \rangle \xrightarrow{n \rightarrow \infty} \langle \overline{\rho}_Q - \nu, w \rangle.$$

Note next that

$$\begin{aligned} \langle \rho_{Q_n} - \nu, w \rangle &= \int_{\mathbb{R}} (\rho_{Q_n} - \nu) w = \int_{\mathbb{R}} \overline{(\widehat{\rho}_{Q_n} - \widehat{\nu})}(k) \widehat{w}(k) dk \\ &= 2 \int_{\mathbb{R}} \frac{\overline{(\widehat{\rho}_{Q_n} - \widehat{\nu})}(k) \widehat{f}(k)}{|k|^2} dk = \underline{D}(\rho_{Q_n} - \nu, f), \end{aligned}$$

where we introduced $f = -w''/2$. Note that $f \in \underline{\mathcal{C}}$ since $\widehat{f} \in L^1_{\text{loc}}(\mathbb{R})$ and $k \mapsto \frac{\widehat{f}(k)}{|k|} = \frac{1}{2}|k|\widehat{w}(k)$ belongs to $L^2(\mathbb{R})$ because $\|k\widehat{w}\|_{L^2(\mathbb{R})}^2 = \|w'\|_{L^2(\mathbb{R})}^2 < +\infty$. The convergence $\underline{D}(\rho_{Q_n} - \nu, f) \xrightarrow{n \rightarrow \infty} \underline{D}(\tilde{\rho}_Q - \nu, f)$ then implies that $\langle \rho_{Q_n} - \nu, w \rangle \xrightarrow{n \rightarrow \infty} \langle \tilde{\rho}_Q - \nu, w \rangle$. The uniqueness of the limit in the sense of distributions finally shows that $\overline{\rho}_Q - \nu = \tilde{\rho}_Q - \nu$ in $\mathcal{D}'(\mathbb{R})$.

Equality of $\rho_{\bar{Q}}$ and $\bar{\rho}_Q$. Fix $w \in \mathcal{D}(\mathbb{R})$. The weak convergence $\rho_{Q_n} \rightharpoonup \bar{\rho}_Q$ in $L^2(\mathbb{R}) + L^p(\mathbb{R})$ implies

$$\langle \rho_{Q_n}, w \rangle \xrightarrow{n \rightarrow \infty} \langle \bar{\rho}_Q, w \rangle.$$

It therefore suffices to prove that the operator-valued function $q \mapsto wQ_{n,q}$ belongs to $L^1(\mathbb{R}^2; \mathfrak{S}_1)$ and that

$$\frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} \text{Tr}_{L^2(\mathbb{R})}(wQ_{n,q}) dq = \underline{\text{Tr}}(wQ_n) = \langle \rho_{Q_n}, w \rangle \xrightarrow{n \rightarrow \infty} \langle \rho_{\bar{Q}}, w \rangle = \underline{\text{Tr}}(w\bar{Q}) = \langle \rho_{\bar{Q}}, w \rangle. \quad (2.49)$$

In order to prove the above convergence, we split the integration domain for $q \in \mathbb{R}^2$ into three parts as $\mathbb{R}^2 = \mathfrak{B}_{\epsilon_F+c} \cup (\mathfrak{B}_R \setminus \bar{\mathfrak{B}}_{\epsilon_F+c}) \cup (\mathbb{R}^2 \setminus \mathfrak{B}_R)$, where $R > 2\epsilon_F$ is large enough and $0 < c < R - \epsilon_F$.

Consider first the case when $q \in \mathbb{R}^2 \setminus \mathfrak{B}_R$. For these values of q , the operator $|T_q - \epsilon_F|^{-1/2}$ is bounded, with operator norm smaller than $\left(\frac{|q|^2}{2} - \epsilon_F\right)^{-1}$. Moreover,

$$\forall q \in \mathbb{R}^2 \setminus \mathfrak{B}_R, \quad \left\| |T_q - \epsilon_F|^{-1/2} w |T_q - \epsilon_F|^{-1/2} \right\| \leq \|w\|_{L^\infty} |R - \epsilon_F|^{-1}.$$

Note also that $|T_q - \epsilon_F|^{1/2} Q_{n,q} |T_q - \epsilon_F|^{1/2} = |T_q - \epsilon_F|^{1/2} Q_{n,q}^{++} |T_q - \epsilon_F|^{1/2} \in \mathfrak{S}_1$ since $|q|^2 > 2\epsilon_F$. Therefore, the operator $wQ_{n,q}$ is trace-class and

$$\begin{aligned} |\text{Tr}_{L^2(\mathbb{R})}(wQ_{n,q})| &= \left| \text{Tr}_{L^2(\mathbb{R})} \left(|T_q - \epsilon_F|^{-1/2} w |T_q - \epsilon_F|^{-1/2} |T_q - \epsilon_F|^{1/2} Q_{n,q} |T_q - \epsilon_F|^{1/2} \right) \right| \\ &\leq \|w\|_{L^\infty} |R - \epsilon_F|^{-1} \left\| |T_q - \epsilon_F|^{1/2} Q_{n,q}^{++} |T_q - \epsilon_F|^{1/2} \right\|_{\mathfrak{S}_1}. \end{aligned}$$

Integrating over $q \in \mathbb{R}^2 \setminus \mathfrak{B}_R$ and relying on the uniform bound (2.40), we finally obtain

$$\left| \int_{\mathbb{R}^2 \setminus \mathfrak{B}_R} \text{Tr}_{L^2(\mathbb{R})}(wQ_{n,q}) dq \right| \leq C \|w\|_{L^\infty} |R - \epsilon_F|^{-1}. \quad (2.50)$$

This term therefore vanishes as $R \rightarrow +\infty$. Note that a similar inequality holds if $Q_{n,q}$ is replaced by $\bar{Q}_{n,q}$.

Consider next the case when $q \in \mathfrak{B}_R \setminus \bar{\mathfrak{B}}_{\epsilon_F+c}$. The Kato–Seiler–Simon inequality (2.37) shows that $w|T_q - \epsilon_F|^{-1/2}$ is Hilbert–Schmidt, and $q \mapsto w|T_q - \epsilon_F|^{-1/2}$ is in $L^2(\mathfrak{B}_R \setminus \bar{\mathfrak{B}}_{\epsilon_F+c}; \mathfrak{S}_2)$. The convergence (2.43) then shows that

$$\begin{aligned} \int_{\mathfrak{B}_R \setminus \bar{\mathfrak{B}}_{\epsilon_F+c}} \text{Tr}_{L^2(\mathbb{R})}(wQ_{n,q}) dq &= \int_{\mathfrak{B}_R \setminus \bar{\mathfrak{B}}_{\epsilon_F+c}} \text{Tr}_{L^2(\mathbb{R})} \left(w |T_q - \epsilon_F|^{-1/2} |T_q - \epsilon_F|^{1/2} Q_{n,q} \right) dq \\ &\xrightarrow{n \rightarrow \infty} \int_{\mathfrak{B}_R \setminus \bar{\mathfrak{B}}_{\epsilon_F+c}} \text{Tr}_{L^2(\mathbb{R})} \left(w |T_q - \epsilon_F|^{-1/2} |T_q - \epsilon_F|^{1/2} \bar{Q}_q \right) dq = \int_{\mathfrak{B}_R \setminus \bar{\mathfrak{B}}_{\epsilon_F+c}} \text{Tr}_{L^2(\mathbb{R})}(w\bar{Q}_q) dq. \end{aligned} \quad (2.51)$$

Consider finally the case when $q \in \bar{\mathfrak{B}}_{\epsilon_F+c}$. Define $\Pi_{1,q} := \mathbf{1}_{(-\infty, 2\epsilon_F]}(T_q)$ and $\Pi_{2,q} := 1 - \Pi_{1,q}$. We decompose the operator $wQ_{n,q}$ as $w\Pi_{2,q}Q_{n,q} + \Pi_{1,q}w\Pi_{1,q}Q_{n,q} + \Pi_{2,q}w\Pi_{1,q}Q_{n,q}$. We show successively that these three operators are trace-class, and characterize their limits as $n \rightarrow +\infty$. Note first that $w\Pi_{2,q}Q_{n,q} = w\Pi_{2,q}|T_q - \epsilon_F|^{-1/2}|T_q - \epsilon_F|^{1/2}Q_{n,q}$ is the product of two Hilbert–Schmidt operators. In fact, a simple computation based on the Kato–Seiler–Simon inequality (2.37) shows that $q \mapsto w\Pi_{2,q}|T_q - \epsilon_F|^{-1/2} \in L^2(\bar{\mathfrak{B}}_{\epsilon_F+c}; \mathfrak{S}_2)$. Therefore, by (2.43),

$$\int_{\bar{\mathfrak{B}}_{\epsilon_F+c}} \text{Tr}_{L^2(\mathbb{R})}(w\Pi_{2,q}Q_{n,q}) dq \xrightarrow{n \rightarrow \infty} \int_{\bar{\mathfrak{B}}_{\epsilon_F+c}} \text{Tr}_{L^2(\mathbb{R})}(w\Pi_{2,q}\bar{Q}_q) dq. \quad (2.52)$$

For the second operator, we denote by w_+ (resp. w_-) the positive (resp. negative) part of w , so that $w = w_+ - w_-$. Since $\Pi_{1,q}\sqrt{w^\pm} \in \mathfrak{S}_2$, it follows that $\Pi_{1,q}w^\pm\Pi_{1,q} \in \mathfrak{S}_1$. A simple computation shows that $q \mapsto \Pi_{1,q}w_\pm\Pi_{1,q} \in L^1(\bar{\mathfrak{B}}_{\epsilon_F+c}; \mathfrak{S}_1)$, so that $q \mapsto \Pi_{1,q}w\Pi_{1,q} \in L^1(\bar{\mathfrak{B}}_{\epsilon_F+c}; \mathfrak{S}_1)$. Therefore, in view of (2.41),

$$\int_{\bar{\mathfrak{B}}_{\epsilon_F+c}} \text{Tr}_{L^2(\mathbb{R})}(\Pi_{1,q}w\Pi_{1,q}Q_{n,q}) dq \xrightarrow{n \rightarrow \infty} \int_{\bar{\mathfrak{B}}_{\epsilon_F+c}} \text{Tr}_{L^2(\mathbb{R})}(\Pi_{1,q}w\Pi_{1,q}\bar{Q}_q) dq. \quad (2.53)$$

For the last operator, we rely on the following lemma.

Lemma 2.15. *The operator-valued function $q \mapsto \Pi_{2,q}w\Pi_{1,q}$ belongs to $L^\infty(\overline{\mathfrak{B}}_{\epsilon_F+c}, \mathfrak{S}_1)$.*

In particular, $q \mapsto \Pi_{2,q}w\Pi_{1,q}$ belongs to $L^1(\overline{\mathfrak{B}}_{\epsilon_F+c}, \mathfrak{S}_1)$, so that, by (2.41),

$$\int_{\overline{\mathfrak{B}}_{\epsilon_F+c}} \text{Tr}_{L^2(\mathbb{R})}(\Pi_{2,q}w\Pi_{1,q}Q_{n,q}) dq \xrightarrow{n \rightarrow \infty} \int_{\overline{\mathfrak{B}}_{\epsilon_F+c}} \text{Tr}_{L^2(\mathbb{R})}(\Pi_{2,q}w\Pi_{1,q}\overline{Q}_q) dq. \quad (2.54)$$

We finally obtain, by summing (2.52), (2.54) and (2.53), that

$$\int_{\overline{\mathfrak{B}}_{\epsilon_F+c}} \text{Tr}_{L^2(\mathbb{R})}(wQ_{n,q}) dq \xrightarrow{n \rightarrow \infty} \int_{\overline{\mathfrak{B}}_{\epsilon_F+c}} \text{Tr}_{L^2(\mathbb{R})}(w\overline{Q}_q) dq. \quad (2.55)$$

The combination of (2.50), (2.51) and (2.55) shows that (2.49) holds, which allows to conclude the proof of the equality $\rho_{\overline{Q}} - \nu = \overline{\rho}_Q - \nu$ in the sense of distributions.

Let us conclude this section by providing the proof of Lemma 2.15.

Proof of Lemma 2.15. Consider $q \in \overline{\mathfrak{B}}_{\epsilon_F+c}$. We decompose the operator $\Pi_{2,q}w\Pi_{1,q}$ as follows:

$$\begin{aligned} \Pi_{2,q}w\Pi_{1,q} &= \Pi_{2,q}(T_q - \epsilon_F)^{-1}(T_q - \epsilon_F)w\Pi_{1,q} \\ &= \Pi_{2,q}(T_q - \epsilon_F)^{-1}w(T_q - \epsilon_F)\Pi_{1,q} - \frac{1}{2}\Pi_{2,q}(T_q - \epsilon_F)^{-1} \left[\frac{d^2}{dz^2}, w \right] \Pi_{1,q}. \end{aligned}$$

By the Kato–Seiler–Simon inequality (2.37), $q \mapsto \Pi_{2,q}(T_q - \epsilon_F)^{-1}\sqrt{w_\pm}$ and $q \mapsto \sqrt{w_\pm}(T_q - \epsilon_F)\Pi_{1,q}$ both belong to $L^\infty(\overline{\mathfrak{B}}_{\epsilon_F+c}, \mathfrak{S}_2)$, so that $q \mapsto \Pi_{2,q}(T_q - \epsilon_F)^{-1}w(T_q - \epsilon_F)\Pi_{1,q}$ is in $L^\infty(\overline{\mathfrak{B}}_{\epsilon_F+c}, \mathfrak{S}_1)$. Moreover,

$$\Pi_{2,q}(T_q - \epsilon_F)^{-1} \left[\frac{d^2}{dz^2}, w \right] \Pi_{1,q} = 2\Pi_{2,q}(T_q - \epsilon_F)^{-1}w' \frac{d}{dz} \Pi_{1,q} + \Pi_{2,q}(T_q - \epsilon_F)^{-1}w'' \Pi_{1,q}.$$

The decomposition

$$\begin{aligned} \Pi_{2,q}(T_q - \epsilon_F)^{-1}w' \frac{d}{dz} \Pi_{1,q} &= \left[\Pi_{2,q}(T_q - \epsilon_F)^{-1}\sqrt{(w')_+} \right] \left[\sqrt{(w')_+} \frac{d}{dz} \Pi_{1,q} \right] \\ &\quad - \left[\Pi_{2,q}(T_q - \epsilon_F)^{-1}\sqrt{(w')_-} \right] \left[\sqrt{(w')_-} \frac{d}{dz} \Pi_{1,q} \right] \end{aligned}$$

shows that $q \mapsto \Pi_{2,q}(T_q - \epsilon_F)^{-1}w' \frac{d}{dz} \Pi_{1,q}$ belongs to $L^\infty(\overline{\mathfrak{B}}_{\epsilon_F+c}, \mathfrak{S}_1)$ as the sum of products of operator-valued functions in $L^\infty(\overline{\mathfrak{B}}_{\epsilon_F+c}, \mathfrak{S}_2)$. It can also similarly be shown that $q \mapsto \Pi_{2,q}(T_q - \epsilon_F)^{-1}w'' \Pi_{1,q}$ is in $L^\infty(\overline{\mathfrak{B}}_{\epsilon_F+c}, \mathfrak{S}_1)$, which proves the statement of the lemma. \square

Step 3. Convergence of Yukawa to Coulomb.

Monotonicity of the ground state. Fix $\nu \in H^{-1}(\mathbb{R})$ and $m_1 \geq m_2 > 0$. Note first that, for any $f \in H^{-1}(\mathbb{R})$,

$$\underline{D}_{m_1}(f, f) \leq \underline{D}_{m_2}(f, f) \leq \underline{D}(f, f), \quad (2.56)$$

with the convention that $\underline{D}(f, f) := +\infty$ if $f \notin \mathcal{C}$. Since $\rho_Q - \nu \in \underline{\mathcal{C}}_m$ for any $m > 0$ when $Q \in \mathcal{K}$ (see Proposition 2.2), it holds $0 \leq \mathcal{E}_{\nu, m_1}(Q) \leq \mathcal{E}_{\nu, m_2}(Q) \leq \mathcal{E}_{\nu, 0}(Q)$ for any $Q \in \mathcal{K}$. This immediately implies that

$$\forall m_1 \geq m_2 \geq 0, \quad 0 \leq I_{\nu, m_1} \leq I_{\nu, m_2} \leq I_{\nu, 0}, \quad (2.57)$$

which proves that $m \mapsto I_{\nu, m}$ is non-increasing on $(0, +\infty)$.

Continuity of the ground state. Fix $m > 0$ and $\delta m > 0$. Denote by \overline{Q}_m (resp. $\overline{Q}_{m+\delta m}$) one of the minimizers of the energy functional $\mathcal{E}_{\nu,m}$ (resp. $\mathcal{E}_{\nu,m+\delta m}$) on \mathcal{K} . Then, in view of the monotonicity property (2.57),

$$\begin{aligned}
0 &\leq I_{\nu,m} - I_{\nu,m+\delta m} = \mathcal{E}_{\nu,m}(\overline{Q}_m) - \mathcal{E}_{\nu,m+\delta m}(\overline{Q}_{m+\delta m}) \\
&\leq \mathcal{E}_{\nu,m}(\overline{Q}_{m+\delta m}) - \mathcal{E}_{\nu,m+\delta m}(\overline{Q}_{m+\delta m}) \\
&= \frac{1}{2} \underline{D}_m(\rho_{\overline{Q}_{m+\delta m}} - \nu, \rho_{\overline{Q}_{m+\delta m}} - \nu) - \underline{D}_{m+\delta m}(\rho_{\overline{Q}_{m+\delta m}} - \nu, \rho_{\overline{Q}_{m+\delta m}} - \nu) \\
&= \int_{\mathbb{R}} \frac{(m + \delta m)^2 - m^2}{k^2 + m^2} \frac{|\widehat{\rho_{\overline{Q}_{m+\delta m}}}(k) - \widehat{\nu}(k)|^2}{k^2 + (m + \delta m)^2} dk \\
&\leq \frac{1}{2} \left[\left(1 + \frac{\delta m}{m}\right)^2 - 1 \right] \underline{D}_{m+\delta m}(\rho_{\overline{Q}_{m+\delta m}} - \nu, \rho_{\overline{Q}_{m+\delta m}} - \nu) \\
&\leq \left[\left(1 + \frac{\delta m}{m}\right)^2 - 1 \right] I_{\nu,m+\delta m} \leq \left[\left(1 + \frac{\delta m}{m}\right)^2 - 1 \right] I_{\nu,m}.
\end{aligned}$$

A similar inequality can be obtained for $\delta m < 0$ sufficiently small. This allows to conclude that $m \mapsto I_{\nu,m}$ is continuous on $(0, +\infty)$.

Limit as $m \rightarrow +\infty$. Fix $\nu \in H^{-1}(\mathbb{R})$. Note that $0 \in \mathcal{K}$, so that

$$0 \leq I_{\nu,m} \leq \mathcal{E}_{\nu,m}(0) = \underline{D}_m(\nu, \nu) = 2 \int_{\mathbb{R}} \frac{|\widehat{\nu}(k)|^2}{k^2 + m^2} dk.$$

The latter integral converges to 0 as $m \rightarrow +\infty$ by dominated convergence. This shows that $I_{\nu,m} \rightarrow 0$ as $m \rightarrow +\infty$.

Limit as $m \rightarrow 0$. Note first that (2.57) implies that $\lim_{m \rightarrow 0} I_{\nu,m} \leq I_{\nu,0}$ for any $\nu \in H^{-1}(\mathbb{R})$. Let us now prove the converse inequality under the conditions $\nu \in L^1(\mathbb{R})$ and $|\cdot|\nu(\cdot) \in L^1(\mathbb{R})$. Denote one of the minimizers of (2.14) by $Q_{\nu,m}$. By (2.57),

$$\forall m > 0, \quad I_{\nu,m} = \underline{\text{Tr}}((T - \epsilon_F)Q_{\nu,m}) + \frac{1}{2} \underline{D}_m(\rho_{Q_{\nu,m}} - \nu, \rho_{Q_{\nu,m}} - \nu) \leq I_{\nu,0}.$$

In particular, $\underline{\text{Tr}}((T - \epsilon_F)Q_{\nu,m})$ is uniformly bounded. By arguments similar to the ones used to establish (2.46) and Lemma 2.14, there exists $Q_{\nu,0} \in \mathcal{K}$ and a subsequence $(Q_{\nu,m_k})_{k \in \mathbb{N}}$ with $m_k \rightarrow 0$ such that (2.16) and (2.17) hold true, $\rho_{Q_{\nu,m_k}} \rightharpoonup \rho_{Q_{\nu,0}}$ weakly in $L^2(\mathbb{R}) + L^p(\mathbb{R})$ (for a fixed $1 < p < 5/3$) and

$$\underline{\text{Tr}}((T - \epsilon_F)Q_{\nu,0}) \leq \lim_{k \rightarrow \infty} \underline{\text{Tr}}((T - \epsilon_F)Q_{\nu,m_k}). \quad (2.58)$$

We prove in the sequel that $Q_{\nu,0}$ is indeed a minimizer of $\mathcal{E}_{\nu,0}$.

In order to do so, we need upper bounds on the Coulomb term $\underline{D}(\rho_{Q_{\nu,0}} - \nu, \rho_{Q_{\nu,0}} - \nu)$. Since $\left\{ \frac{\widehat{\rho_{Q_{\nu,m_k}} - \widehat{\nu}}}{\sqrt{|\cdot|^2 + m_k^2}} \right\}_{k \geq 1}$ is bounded in $L^2(\mathbb{R})$, it is possible to extract a subsequence, still denoted by $\left\{ \frac{\widehat{\rho_{Q_{\nu,m_k}} - \widehat{\nu}}}{\sqrt{|\cdot|^2 + m_k^2}} \right\}_{k \geq 1}$ with some abuse of notation, which weakly converges in $L^2(\mathbb{R})$ to some function \widehat{w} . For a given function $\Phi \in C_c^\infty(\mathbb{R})$, we introduce the sequence $f_{m_k} := (-\Delta + m_k^2)^{1/2} \Phi$ and $f := |\Delta|^{1/2} \Phi$. A simple computation shows that $f_{m_k} \in L^2(\mathbb{R})$ for any $k \geq 1$ and $\|f_{m_k} - f\|_{L^2} \rightarrow 0$ as $k \rightarrow +\infty$. Therefore,

$$\langle \rho_{Q_{\nu,m_k}} - \nu, \Phi \rangle = \left(\frac{\widehat{\rho_{Q_{\nu,m_k}} - \widehat{\nu}}}{\sqrt{|\cdot|^2 + m_k^2}}, \widehat{f_{m_k}} \right)_{L^2(\mathbb{R})} \xrightarrow{k \rightarrow \infty} \left(\widehat{w}, \widehat{f} \right)_{L^2(\mathbb{R})} = \left(\widehat{w}, |\cdot| \widehat{\Phi} \right)_{L^2(\mathbb{R})}. \quad (2.59)$$

Note that $|\cdot|\hat{w} \in H^{-1}(\mathbb{R})$, hence its inverse Fourier transform $\mathcal{F}^{-1}(|\cdot|\hat{w})$ is well defined in $\mathcal{S}'(\mathbb{R})$, and

$$\left(\hat{w}, |\cdot|\hat{\Phi}\right)_{L^2(\mathbb{R})} = \langle \mathcal{F}^{-1}(|\cdot|\hat{w}), \Phi \rangle.$$

The weak convergence $\rho_{Q_{\nu, m_k}} \rightharpoonup \rho_{Q_{\nu, 0}}$ in $L^2(\mathbb{R}) + L^p(\mathbb{R})$ (for a fixed $1 < p < 5/3$) then allows to identify $\rho_{Q_{\nu, 0}} - \nu$ and $\mathcal{F}^{-1}(|\cdot|\hat{w})$ in the sense of distributions. This shows that $\rho_{Q_{\nu, 0}} - \nu \in \underline{\mathcal{C}}$, which together with (2.58) implies that $Q_{\nu, 0} \in \mathcal{F}_\nu$. Moreover, by the properties of weak limits in Hilbert spaces,

$$\underline{D}(\rho_{Q_{\nu, 0}} - \nu, \rho_{Q_{\nu, 0}} - \nu) = 2\|\hat{w}\|_{L^2}^2 \leq 2 \liminf_{k \rightarrow +\infty} \left\| \frac{\hat{\rho}_{Q_{\nu, m_k}} - \hat{\nu}}{\sqrt{|\cdot|^2 + m_k^2}} \right\|_{L^2}.$$

This inequality combined with (2.58) shows that $I_{\nu, 0} \leq \mathcal{E}_{\nu, 0}(Q_{\nu, 0}) \leq \liminf_{m_k \rightarrow 0} I_{m_k}$. We can finally conclude that $Q_{\nu, 0}$ is a minimizer of (2.15), and that $\lim_{m \rightarrow 0} I_{\nu, m} = I_{\nu, 0}$ when $\nu \in L^1(\mathbb{R})$ and $|\cdot|\nu(\cdot) \in L^1(\mathbb{R})$.

2.3.5 Proof of Theorem 2.8

Theorem 2.6 shows that all minimizers of (2.14) share the same density $\rho_{\nu, m}$. To prove Theorem 2.8, we proceed as follows. We first construct a potential $V_{\nu, m}$ from $\rho_{\nu, m} - \nu \in H^{-1}(\mathbb{R})$. We show in Section 2.3.5 that $V_{\nu, m}$ enjoys some regularity property, and that all the minimizers of (2.14) also minimize a linear functional. We next construct a defect state by defining a spectral projector $\bar{\gamma}_m$ associated with the operator $T + V_{\nu, m}$, and show that $\bar{Q}_m := \bar{\gamma}_m - \gamma_0$ is indeed in the kinetic energy space \mathcal{K} (see Section 2.3.5). We finally show in Section 2.3.5 that \bar{Q}_m is the unique minimizer of (2.14) and that it satisfies a self-consistent equation. The proofs of some technical results are postponed until Sections 2.3.6 and 2.3.6.

Step 1. The minimizers of (2.14) also minimize a linear functional.

Given a minimizer $Q_{\nu, m}$ of (2.14), we consider the unique potential $V_{\nu, m} \in H^1(\mathbb{R})$ satisfying the one-dimensional Yukawa equation

$$-V_{\nu, m}'' + m^2 V_{\nu, m} = 2(\rho_{\nu, m} - \nu) \in H^{-1}(\mathbb{R}). \quad (2.60)$$

The potential $V_{\nu, m}$ defined in (2.60) has an explicit expression $V_{\nu, m} = (\rho_{\nu, m} - \nu) \star \frac{e^{-m|\cdot|}}{m}$. Let us first give some properties of the potential $V_{\nu, m}$, which will be useful for the subsequent analysis. Since $H^1(\mathbb{R}) \subset L^\infty(\mathbb{R})$, we have $V_{\nu, m} \in L^\infty(\mathbb{R})$ and that $\lim_{|z| \rightarrow +\infty} V_{\nu, m}(z) = 0$. We denote by $c_{V_{\nu, m}} := \|V_{\nu, m}\|_{L^\infty}$. Note that $V_{\nu, m}$ also belongs to $L^p(\mathbb{R})$ for $p \in [2, +\infty]$ by interpolation. Finally, by the Kato–Seiler–Simon inequality (2.37), it is easy to see that

$$\left\| V_{\nu, m} \left(1 - \frac{d^2}{dz^2}\right)^{-1} \right\|_{\mathfrak{S}_2} \leq \frac{1}{2} \|V_{\nu, m}\|_{L^2(\mathbb{R})}.$$

In particular $V_{\nu, m}$ is $\left(-\frac{d^2}{dz^2}\right)$ -compact.

Let us now show that any minimizer $Q_{\nu, m}$ of (2.14) minimizes a linear functional on \mathcal{K} . Since $Q_{\nu, m}$ minimizes (2.14), it holds, for an arbitrary state $Q \in \mathcal{K}$ and $0 \leq t \leq 1$,

$$\mathcal{E}_m((1-t)Q_{\nu, m} + tQ) - \mathcal{E}_m(Q_{\nu, m}) \geq 0.$$

A simple calculation then shows that $Q_{\nu, m}$ minimizes the following linear functional on \mathcal{K} :

$$F(Q) := \underline{\text{Tr}}((T - \epsilon_F)Q) + \underline{D}_m(\rho_{\nu, m} - \nu, \rho_Q),$$

which can also be written as follows in view of the definition and the regularity of $V_{\nu, m}$:

$$F(Q) = \underline{\text{Tr}}((T - \epsilon_F)Q) + \int_{\mathbb{R}} V_{\nu, m}(z) \rho_Q(z) dz. \quad (2.61)$$

Step 2. Construction of a defect state \overline{Q}_m .

We construct a defect state $\overline{Q}_{\nu,m}$ as follows. First of all, by the Kato-Rellich theorem (see for example [Hel13, Theorem 9.10]), for each $q \in \mathbb{R}^2$, $T_q + V_{\nu,m}$ is a self-adjoint operator on $L^2(\mathbb{R})$ with domain $H^2(\mathbb{R})$ and form domain $H^1(\mathbb{R})$. Let us introduce a spectral projector as follows:

$$\overline{\gamma}_m := \mathbb{1}_{(-\infty, \epsilon_F)}(T + V_{\nu,m}) = \mathcal{U}^{-1} \left(\int_{\mathbb{R}^2}^{\oplus} \overline{\gamma}_{m,q} dq \right) \mathcal{U}, \quad \overline{\gamma}_{m,q} := \mathbb{1}_{(-\infty, \epsilon_F)}(T_q + V_{\nu,m}).$$

By construction, $\overline{\gamma}_{m,q} = 0$ and $\gamma_{0,q} = 0$ when $q \in \mathbb{R}^2 \setminus \overline{\mathfrak{B}}_{\epsilon_F + c_{V_{\nu,m}}}$.

Let us study the spectral structure of $T_q + V_{\nu,m}$ as a function of $|q|$ (See Figure 2.1). It is clear that $T_q + V_{\nu,m}$ depends analytically on $|q|$, and has essential spectrum $[|q|^2/2, +\infty)$ since $V_{\nu,m}$ is T_q -compact. The potential $V_{\nu,m}$ introduces at most countably many eigenvalues below $|q|^2/2$, and $|q|^2/2$ is the only possible accumulation point of these eigenvalues. Denoting by $\sigma_{\text{pp}}(A)$ the set of eigenvalues of an operator A , we

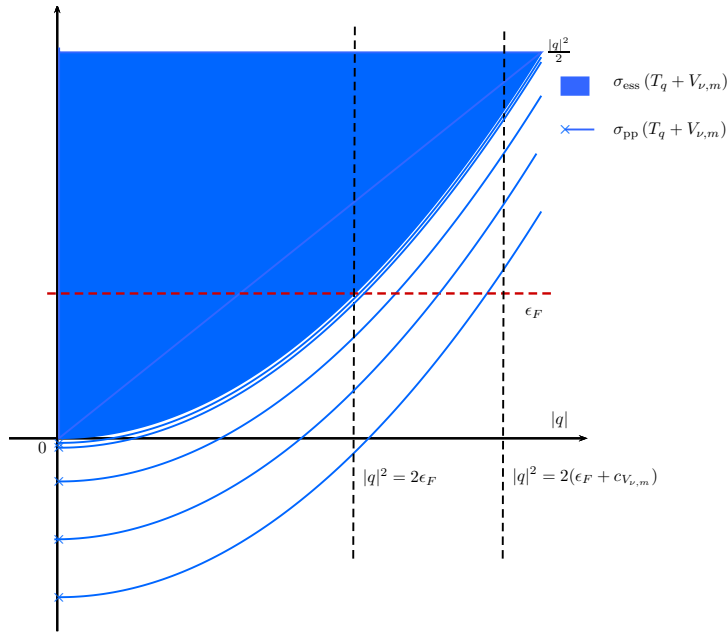


Figure 2.1: The spectrum of $T_q + V_{\nu,m}$ as a function of $|q|$. When $|q|^2 > 2\epsilon_F$, there are at most finitely many states in $\overline{\gamma}_{m,q}$. When $|q|^2 > 2(\epsilon_F + c_{V_{\nu,m}})$, there is no state in $\overline{\gamma}_{m,q}$.

partition the set $\{q \in \mathbb{R}^2\}$ by distinguishing whether the Fermi level ϵ_F is an eigenvalue of $T_q + V_{\nu,m}$ or not:

$$\mathfrak{M}_{\text{pp}} := \{q \in \mathbb{R}^2 \mid \epsilon_F \in \sigma_{\text{pp}}(T_q + V_{\nu,m})\}, \quad \mathfrak{M}_{\text{pp}}^c := \mathbb{R}^2 \setminus \mathfrak{M}_{\text{pp}} := \{q \in \mathbb{R}^2 \mid \epsilon_F \notin \sigma_{\text{pp}}(T_q + V_{\nu,m})\}. \quad (2.62)$$

It is easy to see that \mathfrak{M}_{pp} has Lebesgue measure zero, since $T_0 + V_{\nu,m}$ has at most countably many eigenvalues, and $\epsilon_F \in \sigma_{\text{pp}}(T_q + V_{\nu,m})$ if and only if $\epsilon_F - |q|^2/2 \in \sigma_{\text{pp}}(T_0 + V_{\nu,m})$. The reason for the separation of \mathbb{R}^2 into \mathfrak{M}_{pp} and $\mathfrak{M}_{\text{pp}}^c$ is technical: we will need a regularized operator to approximate the spectral projector $\overline{\gamma}_{m,q}$ for $q \in \overline{\mathfrak{B}}_{\epsilon_F}$. For this reason we need ϵ_F not to be an eigenvalue of $T_q + V_{\nu,m}$ (recall [RS80, Theorem VIII.24]). Remark that when $q \in \overline{\mathfrak{B}}_{\epsilon_F}$, i.e. $|q|^2 \leq 2\epsilon_F$, elements of $\mathfrak{M}_{\text{pp}}^c$ are associated with non-negative eigenvalues of the operator $T_0 + V_{\nu,m} = -\frac{1}{2} \frac{d^2}{dz^2} + V_{\nu,m}$ embedded in its essential spectrum. It can be shown that even in dimension 1 there exist potentials $V \in H^1(\mathbb{R})$ such that $-\frac{1}{2} \frac{d^2}{dz^2} + V$ has positive eigenvalues embedded in the essential spectrum (see [vW29]). In our case, it is highly non trivial to prove the absence of positive eigenvalues of the operator $-\frac{1}{2} \frac{d^2}{dz^2} + V_{\nu,m}$. Standard techniques to this end, such as Mourre estimates [Mou81] or Carleman estimates [KT06], which involve estimating the decay property of $zV'_{\nu,m}(z)$ when $|z| \rightarrow +\infty$, are not immediately applicable as the density $\rho_{\nu,m} - \nu$ is only in $H^{-1}(\mathbb{R})$ a

priori. In order to avoid this difficulty we construct a test defect state by eliminating the points $q \in \mathfrak{M}_{\text{pp}}$:

$$\bar{Q}_m := \mathcal{U}^{-1} \left(\int_{\mathbb{R}^2}^{\oplus} \bar{Q}_{m,q} dq \right) \mathcal{U}, \quad (2.63)$$

where, recalling that $\bar{\gamma}_{m,q} = 0$ when $q \in \mathbb{R}^2 \setminus \bar{\mathfrak{B}}_{\epsilon_F + cV_{\nu,m}}$,

$$\bar{Q}_{m,q} := \bar{\gamma}_{m,q} - \gamma_{0,q}, \quad \text{for } q \in \bar{\mathfrak{B}}_{\epsilon_F + cV_{\nu,m}} \cap \mathfrak{M}_{\text{pp}}^c. \quad (2.64)$$

Denoting by $P^\perp = 1 - P$ for an orthogonal projector P , an easy algebraic calculation shows that

$$- (\bar{Q}_{m,q})^2 = \bar{\gamma}_{m,q}^\perp \bar{Q}_{m,q} \bar{\gamma}_{m,q}^\perp - \bar{\gamma}_{m,q} \bar{Q}_{m,q} \bar{\gamma}_{m,q}, \quad (2.65)$$

and

$$(\bar{Q}_{m,q})^2 = \gamma_{0,q}^\perp \bar{Q}_{m,q} \gamma_{0,q}^\perp - \gamma_{0,q} \bar{Q}_{m,q} \gamma_{0,q} = \bar{Q}_{m,q}^{++} - \bar{Q}_{m,q}^{--}. \quad (2.66)$$

Proposition 2.16. *The defect state \bar{Q}_m defined in (2.63) belongs to the kinetic energy space \mathcal{K} . Moreover, the energy functional $F(\bar{Q}_m)$ can be written as*

$$\begin{aligned} F(\bar{Q}_m) &= \text{Tr} \left((T - \epsilon_F) \bar{Q}_m \right) + \int_{\mathbb{R}} V_{\nu,m} \rho_{\bar{Q}_m} \\ &= \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} \text{Tr}_{L^2(\mathbb{R})} \left(|T_q - \epsilon_F + V_{\nu,m}|^{1/2} (\bar{\gamma}_{m,q}^\perp \bar{Q}_{m,q} \bar{\gamma}_{m,q}^\perp - \bar{\gamma}_{m,q} \bar{Q}_{m,q} \bar{\gamma}_{m,q}) |T_q - \epsilon_F + V_{\nu,m}|^{1/2} \right) dq. \end{aligned}$$

The proof of this proposition, which can be read in Section 2.3.6, is quite technical and constitutes the core of the proof of Theorem 2.8.

Step 3. Form of the minimizers.

We prove that all minimizers satisfy (2.19) by showing that $\bar{Q}_m \in \mathcal{K}$ minimizes $F(Q)$ defined in (2.61). This implies that the only difference between a minimizer $Q_{\nu,m}$ of (2.14) and \bar{Q}_m can be due to bound states at the Fermi level ϵ_F . We show in fact that $Q_{\nu,m} = \bar{Q}_m$.

We first need the following lemma on the density of finite-rank operators in \mathcal{K} .

Lemma 2.17 (Density of direct sums of finite-rank operators in \mathcal{K}). *Every $Q := \mathcal{U}^{-1} \left(\int_{\mathbb{R}^2}^{\oplus} Q_q dq \right) \mathcal{U} \in \mathcal{K}$ can be approximated by a sequence of operators $Q_n := \mathcal{U}^{-1} \left(\int_{\mathbb{R}^2}^{\oplus} Q_{n,q} dq \right) \mathcal{U}$ with the following properties:*

- for all $n \geq 1$ and for almost all $q \in \mathbb{R}^2$, $Q_{n,q} \in \mathcal{K}_q$ is finite-rank, and

$$q \mapsto Q_{n,q} \in L^\infty(\mathbb{R}^2; \mathcal{S}(L^2(\mathbb{R}))), \quad q \mapsto |T_q - \epsilon_F|^{1/2} (Q_{n,q}^{++} - Q_{n,q}^{--}) |T_q - \epsilon_F|^{1/2} \in L^1(\mathbb{R}^2; \mathfrak{S}_1);$$

- the renormalized kinetic energy converges as

$$\begin{aligned} \lim_{n \rightarrow \infty} \int_{\mathbb{R}^2} \text{Tr}_{L^2(\mathbb{R})} \left(|T_q - \epsilon_F|^{1/2} (Q_{n,q}^{++} - Q_{n,q}^{--}) |T_q - \epsilon_F|^{1/2} \right) dq \\ = \int_{\mathbb{R}^2} \text{Tr}_{L^2(\mathbb{R})} \left(|T_q - \epsilon_F|^{1/2} (Q_q^{++} - Q_q^{--}) |T_q - \epsilon_F|^{1/2} \right) dq. \end{aligned} \quad (2.67)$$

Proof. The proof is similar to the proof of Lemma 2.13 and is based on [FLLS13, Lemma 3.2]. First of all, we show that there exists a sequence of operators $\tilde{Q}_n := \mathcal{U}^{-1} \left(\int_{\mathbb{R}^2}^{\oplus} \tilde{Q}_{n,q} dq \right) \mathcal{U} \in \mathcal{K}$ satisfying (2.67) such that $q \mapsto \tilde{Q}_{n,q} \in L^\infty(\mathbb{R}^2; \mathfrak{S}_2)$. Introduce the negligible set $\Omega = \{q \in \mathbb{R}^2 | Q_q \notin \mathcal{K}_q\}$. For $q \in \mathbb{R}^2 \setminus \Omega$

and $n \geq 1$, define $P_{n,q} := \mathbf{1}_{[\frac{1}{n}, n]}(|T_q - \epsilon_F|)$ and $\tilde{Q}_{n,q} := P_{n,q} Q_q P_{n,q}$. It can be checked that $\tilde{Q}_{n,q}$ and $\tilde{Q}_{n,q} |T_q - \epsilon_F|^{1/2}$ are Hilbert–Schmidt by writing

$$\tilde{Q}_{n,q} = P_{n,q} Q_q |T_q - \epsilon_F|^{1/2} \frac{P_{n,q}}{|T_q - \epsilon_F|^{1/2}},$$

and similarly that $\tilde{Q}_{n,q}^{\pm\pm}$ and $|T_q - \epsilon_F|^{1/2} \tilde{Q}_{n,q}^{\pm\pm} |T_q - \epsilon_F|^{1/2}$ are trace-class. Moreover, by the uniform boundedness of $0 \leq P_{n,q} \leq 1$ the fact that P_n commutes with $|T_q - \epsilon_F|^{1/2}$, it is easy to see that $q \mapsto \tilde{Q}_{n,q} \in L^\infty(\mathbb{R}^2; \mathfrak{S}_2)$ and $q \mapsto |T_q - \epsilon_F|^{1/2} (\tilde{Q}_{n,q}^{++} - \tilde{Q}_{n,q}^{--}) |T_q - \epsilon_F|^{1/2} \in L^1(\mathbb{R}^2; \mathfrak{S}_1)$, with

$$0 \leq \pm \operatorname{Tr}_{L^2(\mathbb{R})} \left(|T_q - \epsilon_F|^{1/2} \tilde{Q}_{n,q}^{\pm\pm} |T_q - \epsilon_F|^{1/2} \right) \leq \pm \operatorname{Tr}_{L^2(\mathbb{R})} \left(|T_q - \epsilon_F|^{1/2} Q_q^{\pm\pm} |T_q - \epsilon_F|^{1/2} \right).$$

Let us now turn to the convergence of the relative kinetic energies. First, for all $q \in \mathbb{R}^2 \setminus \Omega$, using that P_n converges strongly to 1 in $L^2(\mathbb{R})$ (which implies that $P_n A P_n$ converges to A in \mathfrak{S}_p for $A \in \mathfrak{S}_p$),

$$\lim_{n \rightarrow +\infty} \left\| |T_q - \epsilon_F|^{1/2} (\tilde{Q}_{n,q}^{\pm\pm} - Q_q^{\pm\pm}) |T_q - \epsilon_F|^{1/2} \right\|_{\mathfrak{S}_1} = 0.$$

Therefore, by the dominated convergence theorem,

$$\begin{aligned} & \lim_{n \rightarrow \infty} \int_{\mathbb{R}^2} \pm \operatorname{Tr}_{L^2(\mathbb{R})} \left(|T_q - \epsilon_F|^{1/2} \tilde{Q}_{n,q}^{\pm\pm} |T_q - \epsilon_F|^{1/2} \right) dq \\ &= \int_{\mathbb{R}^2} \pm \operatorname{Tr}_{L^2(\mathbb{R})} \left(|T_q - \epsilon_F|^{1/2} Q_q^{\pm\pm} |T_q - \epsilon_F|^{1/2} \right) dq. \end{aligned}$$

In order to conclude the proof, it remains to approximate the Hilbert–Schmidt operators $\tilde{Q}_{n,q}$ by finite-rank operators $Q_{n,q} \in \mathcal{K}_q$. This can be done by relying results of [HLS09a, Proposition 2, Theorems 5 and 6], more details can be found in Appendix, Section 2.5.3. \square

Consider $m > 0$ and $\nu \in H^{-1}(\mathbb{R})$, and let us prove that $\mathbf{1}_{(-\infty, \epsilon_F]}(T + V_{\nu, m}) - \gamma_0$ is the unique minimizer of (2.14). For $Q \in \mathcal{K}$ a direct sum of smooth finite-rank operators (*i.e.* as the ones in Lemma 2.17), (2.61) becomes

$$\begin{aligned} F(Q) &= \underline{\operatorname{Tr}}((T - \epsilon_F) Q) + \int_{\mathbb{R}} V_{\nu, m}(x) \rho_Q(x) dx \\ &= \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} \operatorname{Tr}_{L^2(\mathbb{R})} \left((T_q - \epsilon_F + V_{\nu, m}) Q_q \right) dq \\ &= \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} \operatorname{Tr}_{L^2(\mathbb{R})} \left(|T_q - \epsilon_F + V_{\nu, m}|^{1/2} (\bar{\gamma}_{m,q}^\perp Q_q \bar{\gamma}_{m,q}^\perp - \bar{\gamma}_{m,q} Q_q \bar{\gamma}_{m,q}) |T_q - \epsilon_F + V_{\nu, m}|^{1/2} \right) dq. \end{aligned} \tag{2.68}$$

Therefore, by (2.68) and Proposition 2.16,

$$\begin{aligned} F(Q) - F(\bar{Q}_m) &= \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} \operatorname{Tr}_{L^2(\mathbb{R})} \left(|T_q - \epsilon_F + V_{\nu, m}|^{1/2} (\bar{\gamma}_{m,q}^\perp (Q_q - \bar{Q}_{m,q}) \bar{\gamma}_{m,q}^\perp \right. \\ &\quad \left. - \bar{\gamma}_{m,q} (Q_q - \bar{Q}_{m,q}) \bar{\gamma}_{m,q}) |T_q - \epsilon_F + V_{\nu, m}|^{1/2} \right) dq. \end{aligned} \tag{2.69}$$

Remark that, by (2.64), $-\bar{\gamma}_{m,q} \leq Q_q - \bar{Q}_{m,q} \leq 1 - \bar{\gamma}_{m,q}$ for any $q \in \mathbb{R}^2 \setminus \Omega$ with $\Omega = \{q \in \mathbb{R}^2 | Q_q \notin \mathcal{K}_q\}$ negligible, so that

$$\begin{aligned} & \operatorname{Tr}_{L^2(\mathbb{R})} \left(|T_q - \epsilon_F + V_{\nu, m}|^{1/2} (\bar{\gamma}_{m,q}^\perp (Q_q - \bar{Q}_{m,q}) \bar{\gamma}_{m,q}^\perp \right. \\ &\quad \left. - \bar{\gamma}_{m,q} (Q_q - \bar{Q}_{m,q}) \bar{\gamma}_{m,q}) |T_q - \epsilon_F + V_{\nu, m}|^{1/2} \right) \geq 0. \end{aligned}$$

This implies that

$$F(Q) \geq F(\bar{Q}_m).$$

This inequality can be extended to any $Q \in \mathcal{K}$ by (2.67) in Lemma 2.17. This shows that Q is a minimizer of (2.14) if and only if

$$Q = \bar{Q}_m + \delta,$$

where

$$\delta := \mathcal{U}^{-1} \left(\int_{\mathbb{R}^2}^{\oplus} \delta_q dq \right) \mathcal{U},$$

with $0 \leq \delta_q \leq \mathbb{1}_{\{T_q + V_{\nu,m} = \epsilon_F\}}$. Since the set $\mathfrak{M}_{\text{pp}} = \{q \in \mathbb{R}^2 \mid \epsilon_F \in \sigma_{\text{pp}}(T_q + V_{\nu,m})\}$ defined in (2.62) has zero Lebesgue measure as discussed in Section 2.3.5, it follows that $\delta = \mathcal{U}^{-1} \left(\int_{\mathbb{R}^2}^{\oplus} \delta_q dq \right) \mathcal{U} = 0$, and so the unique minimizer of (2.14) is $\mathbb{1}_{(-\infty, \epsilon_F]}(T + V_{\nu,m}) - \gamma_0 = \mathbb{1}_{(-\infty, \epsilon_F]}(T + V_{\nu,m}) - \gamma_0$.

2.3.6 Proof of Proposition 2.16

The statement of the proposition is obtained by a limiting procedure, where we approximate the defect state \bar{Q}_m by a family of regular operators with a spectral gap around ϵ_F , relying on the idea used in [FLLS13, Section 4.2]. Since \bar{Q}_m is defined by a direct integral over $\bar{\mathfrak{B}}_{\epsilon_F + cV_{\nu,m}}$ and \mathfrak{M}_{pp} is negligible, it suffices to construct regularizations of $\bar{Q}_{m,q}$ for $q \in \bar{\mathfrak{B}}_{\epsilon_F + cV_{\nu,m}} \cap \mathfrak{M}_{\text{pp}}^c$.

Construction of a regularized kinetic operator. In order to achieve uniform estimates locally in q , we define a gap-opening function h_q^η which locally does not depend on q for $q \in \bar{\mathfrak{B}}_{\epsilon_F + cV_{\nu,m}} \cap \mathfrak{M}_{\text{pp}}^c$. Let us first define a partition of $|q|$ for $q \in \bar{\mathfrak{B}}_{\epsilon_F + cV_{\nu,m}} \cap \mathfrak{M}_{\text{pp}}^c$. Given $\eta > 0$ small enough, we first note that there exist integers $N_1 \leq N_2$ such that $N_1\eta \leq 2\epsilon_F < (N_1 + 1)\eta$ and $N_2\eta \leq 2(\epsilon_F + cV_{\nu,m}) < (N_2 + 1)\eta$. We then consider the following covering:

$$\left[0, \sqrt{2(\epsilon_F + cV_{\nu,m})}\right] \subset [0, \sqrt{\eta}] \cup [\sqrt{\eta}, \sqrt{2\eta}] \cup \cdots \cup [\sqrt{N_2\eta}, \sqrt{(N_2 + 1)\eta}], \quad (2.70)$$

and an associated gap-opening function:

$$h_q^\eta(k) := \begin{cases} -\eta \mathbb{1} \left(\frac{k^2}{2} \leq \epsilon_F - \frac{n\eta}{2} \right) + \eta \mathbb{1} \left(\frac{k^2}{2} > \epsilon_F - \frac{n\eta}{2} \right), & \text{if } |q| \in [\sqrt{n\eta}, \sqrt{(n+1)\eta}], \\ \text{for } n = 0, 1, 2, \dots, N_1, \\ 0, & \text{if } |q| \in [\sqrt{(N_1 + 1)\eta}, \sqrt{(N_2 + 1)\eta}]. \end{cases}$$

The corresponding approximate kinetic energy operators are defined as

$$K_q^\eta := T_q + h_q^\eta \left(-i \frac{d}{dz} \right) = -\frac{1}{2} \frac{d^2}{dz^2} + \frac{|q|^2}{2} + h_q^\eta \left(-i \frac{d}{dz} \right).$$

Remark that K_q^η has purely absolutely continuous spectrum, and that $\gamma_{0,q} := \mathbb{1}_{(-\infty, \epsilon_F]}(T_q) = \mathbb{1}_{(-\infty, \epsilon_F]}(K_q^\eta)$ for all $q \in \mathbb{R}^2$. Moreover, for $n = 0, 1, \dots, N_1$ and $|q| \in [\sqrt{n\eta}, \sqrt{(n+1)\eta}]$, the operator K_q^η has a spectral gap $\left(\epsilon_F - \eta + \frac{|q|^2 - n\eta}{2}, \epsilon_F + \eta + \frac{|q|^2 - n\eta}{2} \right)$; see Figure 2.2 for a sketch of the spectrum.

The regularized kinetic energy operator is now defined to be $K_q^\eta + V_{\nu,m}$. Since the potential $V_{\nu,m}$ is a compact perturbation of K_q^η (as $(1 + K_q^\eta)^{-1} V_{\nu,m} \in \mathfrak{S}_2$ by the Kato–Seiler–Simon inequality (2.37)), the essential spectrum of $K_q^\eta + V_{\nu,m}$ is the same as for K_q^η , and at most countably many eigenvalues can be introduced in the spectral gap and below $|q|^2/2$, which can only accumulate at the edges $\epsilon_F - \eta + \frac{|q|^2 - n\eta}{2}$ and $\epsilon_F + \eta + \frac{|q|^2 - n\eta}{2}$ of the spectral gap or at $|q|^2/2$. In order to exclude these eigenvalues, we discard the values of q in the set

$$\mathfrak{M}_{\text{pp}}^\eta := \left\{ q \in \bar{\mathfrak{B}}_{\epsilon_F + cV_{\nu,m}} \cap \mathfrak{M}_{\text{pp}}^c \mid \epsilon_F \in \sigma_{\text{disc}}(K_q^\eta + V_{\nu,m}) \right\}.$$

We show next that this set is negligible.

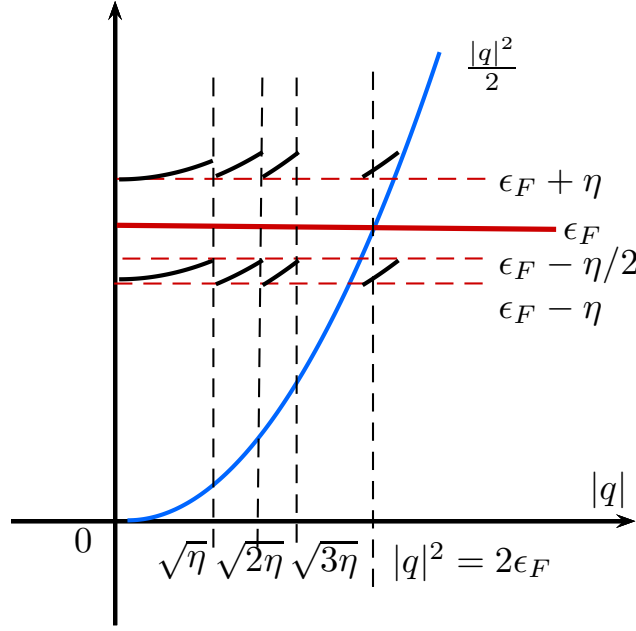


Figure 2.2: Spectrum of K_q^η around ϵ_F . The dark thick lines are the upper/lower bounds of the essential spectrum of K_q^η around ϵ_F .

The set $\mathfrak{M}_{\text{pp}}^\eta$ has Lebesgue measure zero. Let us show that there are only finitely many values of $|q|$ for $q \in \mathfrak{M}_{\text{pp}}^\eta$ for a given $\eta > 0$. We distinguish two cases:

- (i) in the regions $|q| \in [\sqrt{n\eta}, \sqrt{(n+1)\eta})$ for $0 \leq n \leq N_1$, the construction of $K_q^\eta + V_{\nu,m}$ makes sure that there can be at most finitely many values of $|q|$ such that $\epsilon_F \in \sigma_{\text{disc}}(K_q^\eta + V_{\nu,m})$;
- (ii) in the region $|q| \in [\sqrt{(N_1+1)\eta}, \sqrt{(N_2+1)\eta})$, it holds $K_q^\eta = T_q$. The condition $\epsilon_F \in \sigma_{\text{disc}}(K_q^\eta + V_{\nu,m})$ is therefore equivalent to $\epsilon_F - |q|^2/2 \in \sigma_{\text{disc}}(T_0 + V_{\nu,m})$. Since $(N_1+1)\eta > 2\epsilon_F$, there exists $\delta > 0$ such that $\epsilon_F - |q|^2/2 \leq -\delta$ for $|q| \in [\sqrt{(N_1+1)\eta}, \sqrt{(N_2+1)\eta})$. Since $\sigma_{\text{disc}}(T_0 + V_{\nu,m}) \cap (-\infty, -\delta]$ is at most finite, this shows that

$$\mathfrak{M}_{\text{pp}}^\eta \cap \left[\sqrt{(N_1+1)\eta}, \sqrt{(N_2+1)\eta} \right)$$

is at most finite.

Since $\mathfrak{M}_{\text{pp}}^\eta$ is the union of a finite number of circles in \mathbb{R}^2 , it has Lebesgue measure zero.

Construction of a regularized defect state. For $\eta > 0$ small enough, we define a regularized operator in analogy with (2.63) and (2.64) by excluding the set $\mathfrak{M}_{\text{pp}}^\eta$:

$$\overline{Q}_m^\eta := \mathcal{U}^{-1} \left(\int_{\mathbb{R}^2}^\oplus \overline{Q}_{m,q}^\eta dq \right) \mathcal{U}, \quad (2.71)$$

where, with $\Pi_{V,q}^\eta := \mathbb{1}_{(-\infty, \epsilon_F)}(K_q^\eta + V_{\nu,m})$,

$$\overline{Q}_{m,q}^\eta := \begin{cases} \Pi_{V,q}^\eta - \mathbb{1}_{(-\infty, \epsilon_F]}(K_q^\eta) & \text{when } q \in \overline{\mathfrak{B}}_{\epsilon_F + cV_{\nu,m}} \cap \mathfrak{M}_{\text{pp}}^c \cap (\mathfrak{M}_{\text{pp}}^\eta)^c, \\ 0 & \text{when } q \in \left(\mathbb{R}^2 \setminus \overline{\mathfrak{B}}_{\epsilon_F + cV_{\nu,m}} \right) \cup \mathfrak{M}_{\text{pp}} \cup \mathfrak{M}_{\text{pp}}^\eta. \end{cases} \quad (2.72)$$

Moreover, since $\mathbb{1}_{(-\infty, \epsilon_F]}(K_q^\eta) = \gamma_{0,q}$ and similarly to (2.66),

$$(\overline{Q}_{m,q}^\eta)^2 = \overline{Q}_{m,q}^{\eta,++} - \overline{Q}_{m,q}^{\eta,--}. \quad (2.73)$$

A first observation is that, for any $q \in \overline{\mathfrak{B}}_{\epsilon_F + cV_{\nu,m}} \cap \mathfrak{M}_{\text{pp}}^c$,

$$\overline{Q}_{m,q}^\eta \xrightarrow{\eta \rightarrow 0} \overline{Q}_{m,q} \text{ strongly.} \quad (2.74)$$

This follows from the convergence of $K_q^\eta + V_{\nu,m}$ to $T_q + V_{\nu,m}$ in the norm resolvent sense when $\eta \rightarrow 0$ (which comes from the estimate $\|h_q\|_{L^\infty} \leq \eta$), and the result [RS80, Theorem VIII.24] on the convergence of spectral projectors.

The following lemma summarizes some properties of the regularized operator \overline{Q}_m^η .

Lemma 2.18. *For any $\eta > 0$, the regularized operator \overline{Q}_m^η defined in (2.71) belongs to the kinetic energy space \mathcal{K} . Moreover, the following properties hold:*

(1) for all $\eta > 0$ and $q \in \overline{\mathfrak{B}}_{\epsilon_F + cV_{\nu,m}}$,

$$\overline{Q}_{m,q}^\eta \in \mathfrak{S}_2, \quad \left(-\frac{d^2}{dz^2}\right) \overline{Q}_{m,q}^\eta \in \mathfrak{S}_2, \quad (K_q^\eta + V_{\nu,m}) \overline{Q}_{m,q}^\eta \in \mathfrak{S}_2.$$

In particular $\overline{Q}_{m,q}^\eta \in \mathcal{K}_q$.

(2) for any $\eta > 0$ and $q \in \overline{\mathfrak{B}}_{\epsilon_F + cV_{\nu,m}}$,

$$\begin{aligned} & \text{Tr}_{L^2(\mathbb{R})} \left(|T_q - \epsilon_F|^{1/2} \left(\overline{Q}_{m,q}^{\eta,++} - \overline{Q}_{m,q}^{\eta,--} \right) |T_q - \epsilon_F|^{1/2} \right) \\ & + \text{Tr}_{L^2(\mathbb{R})} \left(\left| h_q^\eta \left(-i \frac{d}{dz} \right) \right| \left(\overline{Q}_{m,q}^{\eta,++} - \overline{Q}_{m,q}^{\eta,--} \right) \right) + \int_{\mathbb{R}} V_{\nu,m} \rho_{\overline{Q}_{m,q}^\eta} \\ & = -\text{Tr}_{L^2(\mathbb{R})} \left(|K_q^\eta + V_{\nu,m} - \epsilon_F|^{1/2} \left(\overline{Q}_{m,q}^\eta \right)^2 |K_q^\eta + V_{\nu,m} - \epsilon_F|^{1/2} \right) \leq 0. \end{aligned} \quad (2.75)$$

We postpone the proof of this lemma to Section 2.3.6. Let us however already remark that the terms in the energy functional (2.75) are indeed well defined. In particular,

$$\left| h_q^\eta \left(-i \frac{d}{dz} \right) \right| \left(\overline{Q}_{m,q}^{\eta,++} - \overline{Q}_{m,q}^{\eta,--} \right) \in \mathfrak{S}_1,$$

since $\left| h_q^\eta \left(-i \frac{d}{dz} \right) \right|$ is bounded and $(1 - \gamma_{0,q}) \left(\overline{Q}_{m,q}^\eta \right)^2 = \overline{Q}_{m,q}^{\eta,++} \in \mathfrak{S}_1$ and $\gamma_{0,q} \left(\overline{Q}_{m,q}^\eta \right)^2 = -\overline{Q}_{m,q}^{\eta,--} \in \mathfrak{S}_1$ (relying on $\overline{Q}_{m,q}^\eta \in \mathfrak{S}_2$).

The regularized defect state \overline{Q}_m^η converges to \overline{Q}_m in \mathcal{K} . The remainder of this section is devoted to showing that there exists a sequence $(\eta_i)_{i \geq 1}$ converging to 0 as $i \rightarrow +\infty$ such that $\overline{Q}_m^{\eta_i} \in \mathcal{K}$ converges to the defect state \overline{Q}_m in the sense of (2.17); from which we can conclude that \overline{Q}_m is in \mathcal{K} . The general idea is to use the fact that the total energy of $\overline{Q}_m^{\eta_i}$ is uniformly bounded. By identifying the limit when $\eta_i \rightarrow 0$ with the defect state \overline{Q}_m we obtain the desired result. This can be summarized in the following lemma, which crucially relies on the properties stated in Lemma 2.18.

Lemma 2.19. *There exists a sequence $(\eta_i)_{i \geq 1}$ such that the following convergences hold as $i \rightarrow +\infty$:*

$$\overline{Q}_{m,(\cdot)}^{\eta_i} \left| K_{(\cdot)}^{\eta_i} + V_{\nu,m} - \epsilon_F \right|^{1/2} \xrightarrow{i \rightarrow +\infty} \overline{Q}_{m,(\cdot)} |T_{(\cdot)} + V_{\nu,m} - \epsilon_F|^{1/2} \text{ weakly in } L^2 \left(\overline{\mathfrak{B}}_{\epsilon_F + cV_{\nu,m}}; \mathfrak{S}_2 \right), \quad (2.76)$$

$$\overline{Q}_{m,(\cdot)}^{\eta_i} |T_{(\cdot)} - \epsilon_F|^{1/2} \xrightarrow{i \rightarrow +\infty} \overline{Q}_{m,(\cdot)} |T_{(\cdot)} - \epsilon_F|^{1/2} \text{ weakly in } L^2 \left(\overline{\mathfrak{B}}_{\epsilon_F + cV_{\nu,m}}; \mathfrak{S}_2 \right). \quad (2.77)$$

Moreover, the defect state \overline{Q}_m belongs to \mathcal{K} and

$$\underline{\text{Tr}} \left((T - \epsilon_F) \overline{Q}_m \right) = \frac{1}{(2\pi)^2} \int_{\overline{\mathfrak{B}}_{\epsilon_F + cV_{\nu,m}}} \text{Tr}_{L^2(\mathbb{R})} \left(|T_q - \epsilon_F|^{1/2} \left(\overline{Q}_{m,q}^{++} - \overline{Q}_{m,q}^{--} \right) |T_q - \epsilon_F|^{1/2} \right) dq < \infty. \quad (2.78)$$

The proof of this result can be read in Section 2.3.6. In order to conclude the proof of Proposition 2.16, it suffices to obtain the claimed expression for $F(\overline{Q}_m)$. This is a consequence of (2.65) and (2.78), combined with arguments similar to the ones used to establish (2.75) in Section 2.3.6.

Proof of Lemma 2.18

We start by stating a useful lemma.

Lemma 2.20. *Fix $\eta > 0$ and an integer $0 \leq n \leq N_2$ (appearing in the covering (2.70)). There exist positive constants $a_1(n, \eta), a_2(n, \eta), b_1(n, \eta), b_2(n, \eta)$ and $c(n, \eta)$ such that, for any $q \in \overline{\mathfrak{B}}_{\epsilon_F + cV_{\nu, m}} \cap \mathfrak{M}_{\text{pp}}^c \cap (\mathfrak{M}_{\text{pp}}^\eta)^\complement$ with $|q| \in \left[\sqrt{n\eta}, \sqrt{(n+1)\eta} \right)$, there is a smoothed closed contour $\mathcal{C}_q \subset \mathbb{C}$ enclosing the spectra of K_q^η and $K_q^\eta + V_{\nu, m}$ below the Fermi level ϵ_F without intersecting them, for which*

$$\forall \zeta \in \mathcal{C}_q, \quad |K_q^\eta + V_{\nu, m} - \zeta| \geq c(n, \eta) > 0, \quad (2.79)$$

and

$$\forall \zeta \in \mathcal{C}_q, \quad a_1(n, \eta) \left(1 + \frac{|q|^2}{2} - \frac{1}{2} \frac{d^2}{dz^2} \right) \leq |K_q^\eta + V_{\nu, m} - \zeta| \leq a_2(n, \eta) \left(1 + \frac{|q|^2}{2} - \frac{1}{2} \frac{d^2}{dz^2} \right), \quad (2.80)$$

$$\forall \zeta \in \mathcal{C}_q, \quad b_1(n, \eta) \left(1 + \frac{|q|^2}{2} - \frac{1}{2} \frac{d^2}{dz^2} \right) \leq |K_q^\eta - \zeta| \leq b_2(n, \eta) \left(1 + \frac{|q|^2}{2} - \frac{1}{2} \frac{d^2}{dz^2} \right). \quad (2.81)$$

We postpone the proof of this result to Section 2.3.6. Let us first prove the statement (1) of Lemma 2.18. Given $q \in \overline{\mathfrak{B}}_{\epsilon_F + cV_{\nu, m}} \cap \mathfrak{M}_{\text{pp}}^c \cap (\mathfrak{M}_{\text{pp}}^\eta)^\complement$, and with the curve \mathcal{C}_q introduced in Lemma 2.20, Cauchy's formula gives

$$\overline{Q}_{m, q}^\eta = -\frac{1}{2i\pi} \oint_{\mathcal{C}_q} \left(\frac{1}{K_q^\eta + V_{\nu, m} - \zeta} - \frac{1}{K_q^\eta - \zeta} \right) d\zeta = \frac{1}{2i\pi} \oint_{\mathcal{C}_q} \frac{1}{K_q^\eta + V_{\nu, m} - \zeta} V_{\nu, m} \frac{1}{K_q^\eta - \zeta} d\zeta.$$

Since the function $k \mapsto f_q(k) := \left(\frac{k^2}{2} + \frac{|q|^2}{2} + 1 \right)^{-1}$ belongs to $L^2(\mathbb{R})$ with $\|f_q\|_{L^2} \leq \|f_0\|_{L^2}$, the Kato–Seiler–Simon inequality (2.37) together with (2.80) and (2.81) implies that, for $|q| \in \left[\sqrt{n\eta}, \sqrt{(n+1)\eta} \right)$, there exists $C(n, \eta) \in \mathbb{R}_+$ such that

$$\begin{aligned} & \left\| \left(1 + \frac{|q|^2}{2} - \frac{1}{2} \frac{d^2}{dz^2} \right) \overline{Q}_{m, q}^\eta \right\|_{\mathfrak{S}_2} \\ &= \left\| \frac{1}{2i\pi} \left(1 + \frac{|q|^2}{2} - \frac{1}{2} \frac{d^2}{dz^2} \right) \oint_{\mathcal{C}_q} \left(\frac{1}{K_q^\eta + V_{\nu, m} - \zeta} V_{\nu, m} \frac{1}{K_q^\eta - \zeta} \right) d\zeta \right\|_{\mathfrak{S}_2} \\ &\leq C(n, \eta) \left\| V_{\nu, m} \left(1 + \frac{|q|^2}{2} - \frac{1}{2} \frac{d^2}{dz^2} \right)^{-1} \right\|_{\mathfrak{S}_2} \leq \frac{C(n, \eta)}{\sqrt{2\pi}} \|V_{\nu, m}\|_{L^2} \|f_q\|_{L^2}. \end{aligned}$$

Similar computations show that $\overline{Q}_{m, q}^\eta$, $\left(-\frac{d^2}{dz^2} \right) \overline{Q}_{m, q}^\eta$, $(K_q^\eta + V_{\nu, m}) \overline{Q}_{m, q}^\eta$ and $|T_q - \epsilon_F|^{1/2} \overline{Q}_{m, q}^\eta$ all belong to \mathfrak{S}_2 , while $|T_q - \epsilon_F|^{1/2} \overline{Q}_{m, q}^{\eta, \pm\pm} |T_q - \epsilon_F|^{1/2}$ is in \mathfrak{S}_1 . This implies that $\overline{Q}_{m, q}^\eta \in \mathcal{K}_q$.

The proof of (2.75) in the statement (2) is obtained by an easy adaptation of [FLLS13, Lemma 4.2]. We approximate $\overline{Q}_{m, q}^\eta \in \mathcal{K}_q$ by finite-rank operators for which we prove the equality, and then rely on a density argument based on Lemma 2.13 to conclude.

Let us finally prove that $\overline{Q}_m^\eta \in \mathcal{K}$. It remains to show that

$$\int_{\overline{\mathfrak{B}}_{\epsilon_F + cV_{\nu, m}}} \text{Tr}_{L^2(\mathbb{R})} \left(|T_q - \epsilon_F|^{1/2} \left(\overline{Q}_{m, q}^{\eta, ++} - \overline{Q}_{m, q}^{\eta, --} \right) |T_q - \epsilon_F|^{1/2} \right) dq < \infty.$$

Consider $q \in \overline{\mathfrak{B}}_{\epsilon_F + cV_{\nu, m}} \cap \mathfrak{M}_{\text{pp}}^c \cap (\mathfrak{M}_{\text{pp}}^\eta)^\complement$ and an associated integer $0 \leq n \leq N_2$ such that $|q| \in \left[\sqrt{n\eta}, \sqrt{(n+1)\eta} \right)$ for the covering (2.70). In view of (2.73), (2.80) and (2.81), there exists $R(n, \eta) \in \mathbb{R}_+$

such that

$$\begin{aligned}
\mathrm{Tr}_{L^2(\mathbb{R})} \left(|T_q - \epsilon_F|^{1/2} \left(\overline{Q}_{m,q}^{\eta,++} - \overline{Q}_{m,q}^{\eta,--} \right) |T_q - \epsilon_F|^{1/2} \right) &= \left\| \overline{Q}_{m,q}^\eta |T_q - \epsilon_F|^{1/2} \right\|_{\mathfrak{S}_2}^2 \\
&= \left\| \frac{1}{2i\pi} \oint_{\mathcal{C}_q} \left(\frac{1}{K_q^\eta + V_{\nu,m} - \zeta} V_{\nu,m} \frac{1}{K_q^\eta - \zeta} |T_q - \epsilon_F|^{1/2} \right) d\zeta \right\|_{\mathfrak{S}_2}^2 \\
&\leq R(n, \eta) \left\| \left(1 + \frac{|q|^2}{2} - \frac{1}{2} \frac{d^2}{dz^2} \right)^{-1} V_{\nu,m} \right\|_{\mathfrak{S}_2}^2 \leq \frac{R(n, \eta)}{\sqrt{2\pi}} \|V_{\nu,m}\|_{L^2}^2 \|f_q\|_{L^2}^2.
\end{aligned}$$

Therefore, since $\mathfrak{M}_{\mathrm{pp}}$ and $\mathfrak{M}_{\mathrm{pp}}^\eta$ are negligible, and $\|f_q\|_{L^2} \leq \|f_0\|_{L^2}$,

$$\begin{aligned}
&\int_{\mathfrak{B}_{\epsilon_F + cV_{\nu,m}}} \mathrm{Tr}_{L^2(\mathbb{R})} \left(|T_q - \epsilon_F|^{1/2} \left(\overline{Q}_{m,q}^{\eta,++} - \overline{Q}_{m,q}^{\eta,--} \right) |T_q - \epsilon_F|^{1/2} \right) dq \\
&= \int_{\mathfrak{B}_{\epsilon_F + cV_{\nu,m}} \cap \mathfrak{M}_{\mathrm{pp}}^c \cap (\mathfrak{M}_{\mathrm{pp}}^\eta)^c} \mathrm{Tr}_{L^2(\mathbb{R})} \left(|T_q - \epsilon_F|^{1/2} \left(\overline{Q}_{m,q}^{\eta,++} - \overline{Q}_{m,q}^{\eta,--} \right) |T_q - \epsilon_F|^{1/2} \right) dq \\
&\leq \max_{n=0,1,\dots,N_2+1} \frac{R(n, \eta)}{\sqrt{2\pi}} \|V_{\nu,m}\|_{L^2}^2 \int_{\mathfrak{B}_{\epsilon_F + cV_{\nu,m}}} \|f_q\|_{L^2}^2 dq < +\infty,
\end{aligned}$$

which allows to conclude.

Proof of Lemma 2.19

Let us prove (2.76) by showing that

$$\int_{\mathfrak{B}_{\epsilon_F + cV_{\nu,m}}} \left\| \overline{Q}_{m,q}^\eta |K_q^\eta + V_{\nu,m} - \epsilon_F|^{1/2} \right\|_{\mathfrak{S}_2}^2 dq \geq 0$$

is upper bounded uniformly with respect to $\eta \in [0, 1]$. Remark that the state \overline{Q}_m^η belongs to \mathcal{K} for all $\eta > 0$ by Lemma 2.18. Since $Q_{\nu,m}$ minimizes the functional (2.61),

$$\begin{aligned}
F(\overline{Q}_m^\eta) &= \mathrm{Tr} \left((T - \epsilon_F) \overline{Q}_m^\eta \right) + \int_{\mathbb{R}} V_{\nu,m}(z) \rho_{\overline{Q}_m^\eta}(z) dz \\
&= \frac{1}{(2\pi)^2} \int_{\mathfrak{B}_{\epsilon_F + cV_{\nu,m}}} \left(\left\| \overline{Q}_{m,q}^\eta |T_q - \epsilon_F|^{1/2} \right\|_{\mathfrak{S}_2}^2 + \int_{\mathbb{R}} V_{\nu,m}(z) \rho_{\overline{Q}_{m,q}^\eta}(z) dz \right) dq \geq F(Q_{\nu,m}).
\end{aligned} \tag{2.82}$$

In addition,

$$\begin{aligned}
&\mathrm{Tr}_{L^2(\mathbb{R})} \left(\left| h_q^\eta \left(-i \frac{d}{dz} \right) \right| \left(\overline{Q}_{m,q}^{\eta,++} - \overline{Q}_{m,q}^{\eta,--} \right) \right) \\
&= \mathrm{Tr}_{L^2(\mathbb{R})} \left(\left| h_q^\eta \left(-i \frac{d}{dz} \right) \right|^{1/2} \left(\overline{Q}_{m,q}^\eta \right)^2 \left| h_q^\eta \left(-i \frac{d}{dz} \right) \right|^{1/2} \right) \geq 0.
\end{aligned}$$

Combining this inequality with (2.75) and (2.82) leads to the uniform bound

$$\begin{aligned}
(2\pi)^2 F(Q_{\nu,m}) &\leq \int_{\mathfrak{B}_{\epsilon_F + cV_{\nu,m}}} \left(\left\| \overline{Q}_{m,q}^\eta |T_q - \epsilon_F|^{1/2} \right\|_{\mathfrak{S}_2}^2 + \int_{\mathbb{R}} V_{\nu,m}(z) \rho_{\overline{Q}_{m,q}^\eta}(z) dz \right) dq \\
&\leq - \int_{\mathfrak{B}_{\epsilon_F + cV_{\nu,m}}} \left\| \overline{Q}_{m,q}^\eta |K_q^\eta + V_{\nu,m} - \epsilon_F|^{1/2} \right\|_{\mathfrak{S}_2}^2 dq \leq 0.
\end{aligned} \tag{2.83}$$

It is therefore possible to extract a sequence $\{\eta_i\}_{i \geq 1}$ such that $\overline{Q}_{m,(\cdot)}^{\eta_i} \left| K_{(\cdot)}^{\eta_i} + V_m - \epsilon_F \right|^{1/2}$ converges weakly in $L^2(\overline{\mathfrak{B}}_{\epsilon_F + cV_{\nu,m}}; \mathfrak{S}_2)$ to some operator $S_{(\cdot)} \in L^2(\overline{\mathfrak{B}}_{\epsilon_F + cV_{\nu,m}}; \mathfrak{S}_2)$. We next show that for all $q \in \overline{\mathfrak{B}}_{\epsilon_F + cV_{\nu,m}}$, $S_q = \overline{Q}_{m,q} |T_q + V_{\nu,m} - \epsilon_F|^{1/2}$. By the same reasoning as in [FLLS13, Section 4.2], it can be shown that, for all $q \in \overline{\mathfrak{B}}_{\epsilon_F + cV_{\nu,m}}$, the following strong convergence holds in $L^2(\mathbb{R})$: for any $\varphi \in H^2(\mathbb{R})$,

$$\overline{Q}_{m,q}^{\eta_i} |K_q^{\eta_i} + V_{\nu,m} - \epsilon_F|^{1/2} \varphi \xrightarrow{i \rightarrow +\infty} \overline{Q}_{m,q} |T_q + V_{\nu,m} - \epsilon_F|^{1/2} \varphi \quad \text{in } L^2(\mathbb{R}). \quad (2.84)$$

Now, consider $\phi \in H^2(\mathbb{R})$ and the associated rank-1 operator $K := |\phi\rangle\langle\phi| \in \mathfrak{S}_1$. In particular K can be seen as a constant function of $L^2(\overline{\mathfrak{B}}_{\epsilon_F + cV_{\nu,m}}; \mathfrak{S}_2)$. On the one hand, by the weak convergence of $\overline{Q}_{m,(\cdot)}^{\eta_i} \left| K_{(\cdot)}^{\eta_i} + V_{\nu,m} - \epsilon_F \right|^{1/2}$ to $S_{(\cdot)}$ in $L^2(\overline{\mathfrak{B}}_{\epsilon_F + cV_{\nu,m}}; \mathfrak{S}_2)$,

$$\begin{aligned} & \int_{\overline{\mathfrak{B}}_{\epsilon_F + cV_{\nu,m}}} \left\langle \phi \left| \overline{Q}_{m,q}^{\eta_i} \left| K_q^{\eta_i} + V_{\nu,m} - \epsilon_F \right|^{1/2} \right| \phi \right\rangle dq \\ &= \int_{\overline{\mathfrak{B}}_{\epsilon_F + cV_{\nu,m}}} \text{Tr}_{L^2(\mathbb{R})} \left(\overline{Q}_{m,q}^{\eta_i} \left| K_q^{\eta_i} + V_{\nu,m} - \epsilon_F \right|^{1/2} K \right) dq \\ & \xrightarrow{i \rightarrow +\infty} \int_{\overline{\mathfrak{B}}_{\epsilon_F + cV_{\nu,m}}} \text{Tr}_{L^2(\mathbb{R})} (S_q K) dq = \int_{\overline{\mathfrak{B}}_{\epsilon_F + cV_{\nu,m}}} \langle \phi | S_q | \phi \rangle dq. \end{aligned} \quad (2.85)$$

On the other hand, by the strong convergence (2.84), it holds, for all $q \in \overline{\mathfrak{B}}_{\epsilon_F + cV_{\nu,m}}$,

$$\left\langle \phi \left| \overline{Q}_{m,q}^{\eta_i} \left| K_q^{\eta_i} + V_{\nu,m} - \epsilon_F \right|^{1/2} \right| \phi \right\rangle \xrightarrow{i \rightarrow +\infty} \left\langle \phi \left| \overline{Q}_{m,q} |T_q + V_{\nu,m} - \epsilon_F|^{1/2} \right| \phi \right\rangle.$$

A simple computation shows that there exists $C_\phi \in \mathbb{R}_+$ such that

$$\left| \left\langle \phi \left| \overline{Q}_{m,q}^{\eta_i} \left| K_q^{\eta_i} + V_{\nu,m} - \epsilon_F \right|^{1/2} \right| \phi \right\rangle \right| \leq C_\phi$$

for all $i \geq 1$ and $q \in \overline{\mathfrak{B}}_{\epsilon_F + cV_{\nu,m}}$. By the dominated convergence theorem,

$$\begin{aligned} & \int_{\overline{\mathfrak{B}}_{\epsilon_F + cV_{\nu,m}}} \left\langle \phi \left| \overline{Q}_{m,q}^{\eta_i} \left| K_q^{\eta_i} + V_{\nu,m} - \epsilon_F \right|^{1/2} \right| \phi \right\rangle dq \\ & \xrightarrow{i \rightarrow +\infty} \int_{\overline{\mathfrak{B}}_{\epsilon_F + cV_{\nu,m}}} \left\langle \phi \left| \overline{Q}_{m,q} |T_q + V_{\nu,m} - \epsilon_F|^{1/2} \right| \phi \right\rangle dq. \end{aligned}$$

The comparison of the previous limit and (2.85) implies that

$$\overline{Q}_{m,(\cdot)} |T_{(\cdot)} + V_{\nu,m} - \epsilon_F|^{1/2} = S_{(\cdot)} \in L^2(\overline{\mathfrak{B}}_{\epsilon_F + cV_{\nu,m}}; \mathfrak{S}_2).$$

We next prove (2.77) by showing that

$$\int_{\overline{\mathfrak{B}}_{\epsilon_F + cV_{\nu,m}}} \left\| |T_q - \epsilon_F|^{1/2} \overline{Q}_{m,q}^\eta \right\|_{\mathfrak{S}_2}^2 dq \geq 0$$

is upper bounded uniformly with respect to $\eta \in [0, 1]$. Introduce

$$\rho_{\overline{Q}_m^\eta}(z) = \int_{\mathbb{R}^2} \rho_{\overline{Q}_{m,q}^\eta}(z) dq = \int_{\overline{\mathfrak{B}}_{\epsilon_F + cV_{\nu,m}}} \rho_{\overline{Q}_{m,q}^\eta}(z) dq,$$

which is well defined by Proposition 2.2 since $\overline{Q}_m^\eta \in \mathcal{K}$. Moreover, in view of (2.8) with $c = c_{V_{\nu,m}}$, there exists a constant $R \in \mathbb{R}_+$ such that

$$\left\| \rho_{\overline{Q}_m^\eta} \right\|_{L^2}^2 \leq R \int_{\mathfrak{B}_{\epsilon_F + c_{V_{\nu,m}}}} \left\| |T_q - \epsilon_F|^{1/2} \overline{Q}_{m,q}^\eta \right\|_{\mathfrak{S}_2}^2 dq.$$

In view of (2.83),

$$\int_{\mathfrak{B}_{\epsilon_F + c_{V_{\nu,m}}}} \left\| |T_q - \epsilon_F|^{1/2} \overline{Q}_{m,q}^\eta \right\|_{\mathfrak{S}_2}^2 dq \leq - \int_{\mathbb{R}} V_{\nu,m} \rho_{\overline{Q}_m^\eta},$$

so that a Cauchy–Schwarz inequality leads to

$$0 \leq \int_{\mathfrak{B}_{\epsilon_F + c_{V_{\nu,m}}}} \left\| |T_q - \epsilon_F|^{1/2} \overline{Q}_{m,q}^\eta \right\|_{\mathfrak{S}_2}^2 dq \leq R \|V_{\nu,m}\|_{L^2}^2.$$

By arguments similar to the ones used above, we deduce that it is possible to further extract a subsequence (still denoted by $(\eta_i)_{i \geq 1}$ with some abuse of notation) such that $\overline{Q}_{m,(\cdot)}^{\eta_i} |T_{(\cdot)} - \epsilon_F|^{1/2} \xrightarrow{i \rightarrow +\infty} \overline{Q}_{m,(\cdot)} |T_{(\cdot)} - \epsilon_F|^{1/2}$ weakly in $L^2(\mathfrak{B}_{\epsilon_F + c_{V_{\nu,m}}}; \mathfrak{S}_2)$ and

$$0 \leq \int_{\mathfrak{B}_{\epsilon_F + c_{V_{\nu,m}}}} \left\| \overline{Q}_{m,q} |T_q - \epsilon_F|^{1/2} \right\|_{\mathfrak{S}_2}^2 dq \leq \liminf_{i \rightarrow +\infty} \int_{\mathfrak{B}_{\epsilon_F + c_{V_{\nu,m}}}} \left\| \overline{Q}_{m,q}^{\eta_i} |T_q - \epsilon_F|^{1/2} \right\|_{\mathfrak{S}_2}^2 dq < \infty.$$

This allows us to conclude that $\overline{Q}_m \in \mathcal{K}$ using (2.66), and shows that (2.78) holds.

Proof of Lemma 2.20

Since $V_{\nu,m}$ is a compact perturbation of K_q^η for any $q \in \mathbb{R}^2$, the only possible accumulation points of the discrete spectrum of $K_q^\eta + V_{\nu,m}$ are $|q|^2/2, \epsilon_F - \eta + \frac{|q|^2 - n\eta}{2}$ and $\epsilon_F + \eta + \frac{|q|^2 - n\eta}{2}$, where $0 \leq n \leq N_2$ is such that $\sqrt{n\eta} \leq |q| < \sqrt{(n+1)\eta}$. For the remainder of the proof, we fix an integer $0 \leq n \leq N_2$ and an element $q_0 \in \mathbb{R}^2$ with $|q_0| = \sqrt{n\eta}$. The objects we introduce are depicted in Figure 2.3. First of all remark that the gap-opening function h_q^η is independent of $|q|$ in each interval $[\sqrt{n\eta}, \sqrt{(n+1)\eta})$. Introduce the integer $M \geq 0$ such that

$$\sigma_{\text{disc}}(K_{q_0}^\eta + V_{\nu,m}) \cap \left[\epsilon_F - \frac{3\eta}{4}, \epsilon_F + \frac{\eta}{4} \right] = \{\varepsilon_i\}_{0 \leq i \leq M}, \quad \epsilon_F - \frac{3\eta}{4} \leq \varepsilon_0 < \dots < \varepsilon_M \leq \epsilon_F + \frac{\eta}{4}.$$

Note that we restrict the spectral window around ϵ_F in order to discard the possible accumulation points of the discrete spectrum. We assume that $q_0 \notin \mathfrak{M}_{\text{pp}}$; the case when $q_0 \in \mathfrak{M}_{\text{pp}}$ can however be handled by a simple modification of our arguments. Note that, since $K_q^\eta = K_{q_0}^\eta + \frac{|q|^2 - |q_0|^2}{2}$,

$$\sigma_{\text{disc}}(K_q^\eta + V_{\nu,m}) \cap \left[\epsilon_F - \frac{\eta}{4}, \epsilon_F + \frac{\eta}{4} \right] \subset \frac{|q|^2 - |q_0|^2}{2} + \sigma_{\text{disc}}(K_{q_0}^\eta + V_{\nu,m}) \cap \left[\epsilon_F - \frac{3\eta}{4}, \epsilon_F + \frac{\eta}{4} \right],$$

and the distances between the eigenvalues of $K_q^\eta + V_{\nu,m}$ in the spectral region $[\epsilon_F - \eta/4, \epsilon_F + \eta/4]$ are independent of q .

Note next that we eliminated the values of q for which $\epsilon_F \in \sigma_{\text{disc}}(K_q^\eta + V_{\nu,m})$ by the definition of the set $\mathfrak{M}_{\text{pp}}^\eta$. The number of the corresponding values of $|q|$ is at most equal to M , which corresponds to a further partition of the interval $[\sqrt{n\eta}, \sqrt{(n+1)\eta})$ into finitely many subintervals $[\alpha_i, \alpha_{i+1})$ with $\alpha_0 := |q_0| = \sqrt{n\eta}$.

Let us concentrate on the region $\mathcal{R} = \{q \in \mathbb{R}^2, n\eta \leq |q| < \alpha_1\}$. As $\sigma_{\text{disc}}(K_q^\eta + V_{\nu,m})$ intersects the Fermi level ϵ_F at $|q| = \alpha_1$, there exists a unique integer $0 \leq j \leq M$ such that $\varepsilon_j + \frac{|\alpha_1|^2 - |q_0|^2}{2} = \epsilon_F$. We now consider curves $\mathcal{C}_q \subset \mathbb{C}$ for $q \in \mathcal{R}$ satisfying the following properties:

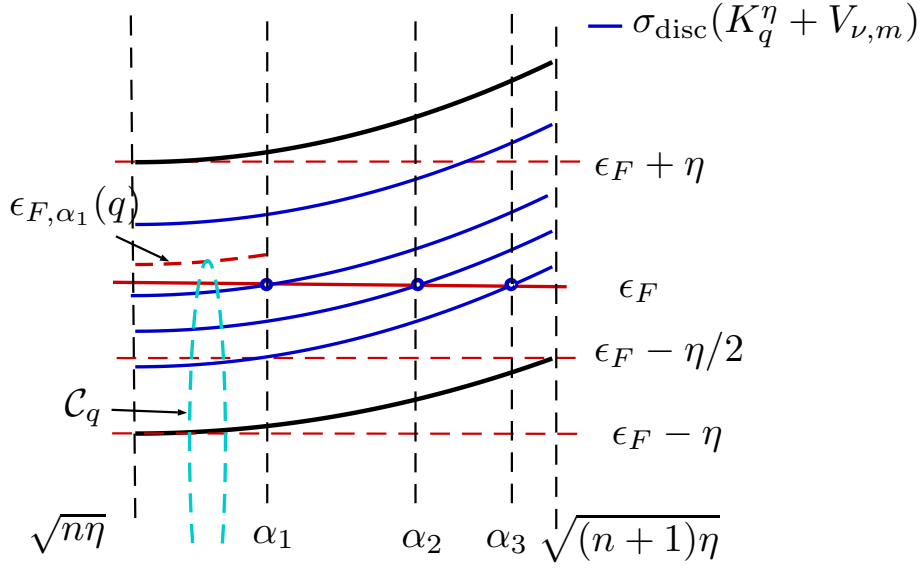


Figure 2.3: Spectral structure of $K_q^\eta + V_m$ around the Fermi level ϵ_F for $|q| \in [\sqrt{n\eta}, \sqrt{(n+1)\eta}]$. The dark blue lines correspond to elements of $\sigma_{\text{disc}}(K_q^\eta + V_{\nu, m})$ which are obtained from those at q_0 such that $|q_0| = \sqrt{n\eta}$ by adding $(|q|^2 - |q_0|^2)/2$. The points q such that $|q| = \alpha_i$ are removed. The curve \mathcal{C}_q (dashed light blue line) is defined to pass through $\epsilon_{F, \alpha_1}(q)$ for $|q| \in [\sqrt{n\eta}, \alpha_1)$.

- the top of the curve passes through

$$\epsilon_{F, \alpha_1}(q) := \frac{\epsilon_{j+1} + \epsilon_j}{2} + \frac{|q|^2 - |q_0|^2}{2}, \quad |q| \in [\sqrt{n\eta}, \alpha_1),$$

with $\epsilon_{M+1} := \epsilon_F + \eta/4$. Note that, when $j = M$, it holds $\epsilon_M \leq \epsilon_F$, so that the above definition makes sense since there is no other eigenvalue in the spectral region $(\epsilon_M, \epsilon_F + \eta/4]$. Note also that the distance between $\epsilon_{F, \alpha_1}(q)$ and $\sigma_{\text{disc}}(K_q^\eta + V_{\nu, m}) \cap [\epsilon_F - \eta/2, \epsilon_F]$ is independent of $|q|$, and that $\mathbb{1}_{(-\infty, \epsilon_{F, \alpha_1}(q)]}(K_q^\eta + V_{\nu, m}) = \mathbb{1}_{(-\infty, \epsilon_F]}(K_q^\eta + V_{\nu, m})$, i.e. the states below the Fermi level have not been changed.

- the curve encloses the spectrum of $K_q^\eta + V_{\nu, m}$ below ϵ_F without intersecting it.

It is then easy to see that there exists a positive constant $c_1(n, \eta)$ such that $|K_q^\eta + V_{\nu, m} - \zeta| \geq c_1(n, \eta) > 0$ uniformly for $|q| \in [\sqrt{n\eta}, \alpha_1)$ and $\zeta \in \mathcal{C}_q$.

The same procedure can be applied to other intervals. As the number of intervals is finite, there exists a constant $c(n, \eta)$ (which depends only on the properties of the discrete spectrum of $K_{q_0}^\eta + V_{\nu, m}$ in the spectral region $[\epsilon_F - 3\eta/4, \epsilon_F + \eta/4]$) such that, for any $q \in \mathbb{R}^2$ with $\sqrt{n\eta} \leq |q| < \sqrt{(n+1)\eta}$, there is a curve $\mathcal{C}_q \subset \mathbb{C}$ such that $|K_q^\eta + V_{\nu, m} - \zeta| \geq c(n, \eta) > 0$ for any $\zeta \in \mathcal{C}_q$. The proof of inequalities (2.80) and (2.81) is then easily obtained by replacing $-\frac{1}{2} \frac{d^2}{dz^2}$ with $-\frac{1}{2} \frac{d^2}{dz^2} + \frac{|q|^2}{2}$ in [CDL08a, Lemma 1].

2.4 Numerical simulation of slab-like defects

We present in this section some numerical simulations where we compute an approximation of the minimal energy states for (2.14). The approximation first consists in restricting the physical space to a supercell with periodic boundary conditions in the z direction, the problem being still invariant by translation in the (x, y) -directions. As made precise in Section 2.4.1, it is then possible to formulate the counterpart of the minimization problem (2.14) in this setting, see (2.87) below. In particular, solutions of the supercell minimization problem are characterized by a nonlinear Euler–Lagrange equation. We discuss in Section 2.4.2

how to numerically solve the latter equation. We finally present some results of numerical simulations for defects corresponding to sharp trenches in Section 2.4.3. In particular, we observe Friedel oscillations. These results are obtained for Yukawa interactions only since the convergence of our numerical method is poor for Coulomb interactions, and most likely would deserve a dedicated mathematical analysis.

2.4.1 Supercell model

Supercell models consider states periodic in the z -direction, and invariant by translation in the (x, y) -directions. We first make precise the set of admissible states in Section 2.4.1, then present the reduced Hartree–Fock model in this setting in Section 2.4.1, and finally write the Euler–Lagrange equations characterizing the ground state in this framework (see Section 2.4.1).

Admissible states for supercell models

Supercell models are obtained by restricting the z -variable to the unit cell $\Lambda_L = [-L/2, L/2)$ of the physical space \mathbb{R} . This unit cell is seen as a periodic domain of spatial periodicity $L > 0$. More precisely, denoting by $\mathcal{R}_L := L\mathbb{Z}$, we consider all operators to be defined on the functional space

$$L^2_{\text{per},z}(\mathbb{R}^2 \times \Lambda_L) = \left\{ u \in L^2_{\text{loc}}(\mathbb{R}^3) \mid u(r, \cdot) \text{ is } \mathcal{R}_L\text{-periodic for a.e. } r \in \mathbb{R}^2, \int_{\mathbb{R}^2} \int_{\Lambda_L} |u(r, z)|^2 dr dz < +\infty \right\}.$$

It is possible to introduce a supercell unitary transform \mathcal{U}_L which is the counterpart of (2.1): for $q, r \in \mathbb{R}^2$ and $z \in \mathbb{R}$, we can first define, for functions $\Phi \in L^2_{\text{per},z}(\mathbb{R}^2 \times \Lambda_L)$ which are smooth and with compact support in $\mathbb{R}^2 \times \Lambda_L$,

$$(\mathcal{U}_L \Phi)_q(z) := \frac{1}{2\pi} \int_{\mathbb{R}^2} e^{-iq \cdot r} \Phi(r, z) dr,$$

and extend this formula as an isometric isomorphism from $L^2_{\text{per},z}(\mathbb{R}^2 \times \Lambda_L)$ to $L^2(\mathbb{R}^2, L^2_{\text{per}}(\Lambda_L))$, where $L^2_{\text{per}}(\Lambda_L) = \{ \phi \in L^2_{\text{loc}}(\mathbb{R}) \mid \phi \text{ is } \mathcal{R}_L\text{-periodic} \}$. The inverse of the unitary transform \mathcal{U}_L^{-1} reads, for $\Psi = (\Psi_q)_{q \in \mathbb{R}^2} \in L^2(\mathbb{R}^2, L^2_{\text{per}}(\Lambda_L))$,

$$(\mathcal{U}_L^{-1} \Psi)_q(r, z) := \frac{1}{2\pi} \int_{\mathbb{R}^2} e^{iq \cdot r} \Psi_q(z) dq.$$

In order to introduce the set of admissible states, we define the kinetic energy operator on $L^2_{\text{per},z}(\mathbb{R}^2 \times \Lambda_L)$ as

$$T_L = \mathcal{U}_L^{-1} \left(\int_{\mathbb{R}^2}^{\oplus} T_{q,L} dq \right) \mathcal{U}_L, \quad T_{q,L} = T_{\text{per},z,L} + \frac{|q|^2}{2},$$

where $T_{\text{per},z,L} = -\frac{1}{2} \frac{d^2}{dz^2}$ is considered as an operator on $L^2_{\text{per}}(\Lambda_L)$. The corresponding supercell free Fermi state operator reads

$$\gamma_0^L = \mathcal{U}_L^{-1} \left(\int_{\mathbb{R}^2}^{\oplus} \gamma_{0,q}^L dq \right) \mathcal{U}_L, \quad (2.86)$$

where $\{\gamma_{0,q}^L\}_{q \in \mathbb{R}^2}$ is the following family of orthogonal projectors acting on $L^2_{\text{per}}(\Lambda_L)$:

$$\gamma_{0,q}^L := \begin{cases} \mathbb{1}_{(-\infty, \epsilon_F]}(T_{q,L}) & \text{if } q \in \overline{\mathfrak{B}}_{\epsilon_F}, \\ 0 & \text{if } q \in \mathbb{R}^2 \setminus \overline{\mathfrak{B}}_{\epsilon_F}. \end{cases}$$

We can finally define admissible defect states for the supercell model by mimicking the construction in Section 2.2.2: for any $q \in \mathbb{R}^2$, we introduce

$$\mathcal{X}_q^{\Lambda_L} := \left\{ Q_q^L \in \mathcal{S}(L^2_{\text{per}}(\Lambda_L)) \mid |T_{q,L} - \epsilon_F|^{1/2} Q_q^L \in \mathfrak{S}_2(L^2_{\text{per}}(\Lambda_L)), \right. \\ \left. |T_{q,L} - \epsilon_F|^{1/2} Q_q^{L, \pm \pm} |T_{q,L} - \epsilon_F|^{1/2} \in \mathfrak{S}_1(L^2_{\text{per}}(\Lambda_L)) \right\},$$

equipped with the norm

$$\begin{aligned} \|Q_q^L\|_{\mathcal{X}_q^{\Lambda_L}} := & \|Q_q^L\|_{\mathcal{L}(L_{\text{per}}^2(\Lambda_L))} + \left\| |T_{q,L} - \epsilon_F|^{1/2} Q_q^L \right\|_{\mathfrak{S}_2(L_{\text{per}}^2(\Lambda_L))} \\ & + \sum_{\alpha \in \{+, -\}} \left\| |T_{q,L} - \epsilon_F|^{1/2} Q_q^{L, \alpha \alpha} |T_{q,L} - \epsilon_F|^{1/2} \right\|_{\mathfrak{S}_1(L_{\text{per}}^2(\Lambda_L))}, \end{aligned}$$

as well as the convex set $\mathcal{K}_q^{\Lambda_L} := \{Q_q^L \in \mathcal{X}_q^{\Lambda_L} \mid -\gamma_{0,q}^L \leq Q_q^L \leq 1 - \gamma_{0,q}^L\}$. Admissible states Q^L with finite renormalized kinetic free energy per unit area in the supercell model are elements of

$$\begin{aligned} \mathcal{K}^{\Lambda_L} := & \left\{ Q^L = \mathcal{U}_L^{-1} \left(\int_{\mathbb{R}^2}^{\oplus} Q_q^L dq \right) \mathcal{U}_L \mid q \mapsto Q_q^L \in L^\infty(\mathbb{R}^2; \mathcal{S}(L_{\text{per}}^2(\Lambda_L))), Q_q^L \in \mathcal{K}_q^{\Lambda_L} \text{ a.e.}, \right. \\ & \left. \underline{\text{Tr}}_L((T_L - \epsilon_F)Q^L) < \infty \right\}, \end{aligned}$$

where

$$\underline{\text{Tr}}_L((T_L - \epsilon_F)Q^L) := \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} \text{Tr}_{L_{\text{per}}^2(\Lambda_L)} \left(|T_{q,L} - \epsilon_F|^{1/2} (Q_q^{L,++} - Q_q^{L,--}) |T_{q,L} - \epsilon_F|^{1/2} \right) dq.$$

Reduced Hartree–Fock model for supercells

Before we construct the reduced Hartree–Fock energy functional, we need to define Yukawa interactions for models periodic in the z -variable. We rely to this end on a Fourier series decomposition (instead of a Fourier transform as in Section 2.2.2), obtained with the orthonormal basis $\{e_k\}_{k \in \mathbb{Z}}$ of $L_{\text{per}}^2(\Lambda_L)$ composed of the Fourier modes $e_k(z) := \frac{1}{\sqrt{L}} e^{2i\pi k z/L}$. Any function $u \in L_{\text{per}}^2(\Lambda_L)$ can be decomposed as

$$u = \sum_{k \in \mathbb{Z}} c_k(u) e_k, \quad c_k(u) := (e_k, u)_{L_{\text{per}}^2}.$$

The Yukawa space for the supercell model is then defined as the following subset of periodic distributions:

$$\underline{\mathcal{C}}_{m, \Lambda_L} := \left\{ \rho = \sum_{k \in \mathbb{Z}} c_k(\rho) e_k \mid \sum_{k \in \mathbb{Z}} \frac{|c_k(\rho)|^2}{m^2 + |\frac{2\pi k}{L}|^2} < \infty \right\},$$

and for $\rho_1, \rho_2 \in \underline{\mathcal{C}}_{m, \Lambda_L}$, the supercell Yukawa interaction is given by

$$\underline{D}_{m, \Lambda_L}(\rho_1, \rho_2) := 2 \sum_{k \in \mathbb{Z}} \frac{\overline{c_k(\rho_1)} c_k(\rho_2)}{m^2 + |\frac{2\pi k}{L}|^2}.$$

Consider now a periodized defect obtain from the reference perturbation ν :

$$\nu_{\text{per}, L} := \sum_{n \in \mathbb{Z}} (\mathbf{1}_{\Lambda_L} \nu)(\cdot - nL).$$

The density $\nu_{\text{per}, L}$ belongs to $\underline{\mathcal{C}}_{m, \Lambda_L}$ when

$$\sum_{k \in \mathbb{Z}} \frac{1}{m^2 + |\frac{2\pi k}{L}|^2} \left| \int_{\Lambda_L} \nu(z) \overline{e_k(z)} dz \right|^2 < \infty,$$

which we assume in the sequel. The supercell energy functional is then defined as

$$\mathcal{E}_{m, \Lambda_L}(Q^L) = \underline{\text{Tr}}_L((T_L - \epsilon_F)Q^L) + \frac{1}{2} \underline{D}_{m, \Lambda_L}(\rho_{Q^L} - \nu_{\text{per}, L}, \rho_{Q^L} - \nu_{\text{per}, L}),$$

on the admissible set $\mathcal{F}_{m, \Lambda_L} := \{Q^L \in \mathcal{K}^{\Lambda_L} \mid \rho_{Q^L} - \nu_{\text{per}} \in \underline{\mathcal{C}}_{m, \Lambda_L}\}$. The counterpart of the minimization problem (2.14) in the supercell framework finally is:

$$\boxed{I_{m, \Lambda_L} = \inf \{ \mathcal{E}_{m, \Lambda_L}(Q^L), Q^L \in \mathcal{F}_{m, \Lambda_L} \}.} \quad (2.87)$$

Euler–Lagrange equations

Since the energy functional $\mathcal{E}_{m,\Lambda_L}$ is convex, standard techniques from calculus of variation can be used to prove that (2.87) admits minimizers. Moreover, using the compactness of the domain Λ_L (and hence the fact that $T_{q,L}$ has compact resolvent for any $q \in \mathbb{R}^2$), minimizers are characterized by the following Euler-Lagrange equations (where for clarity we do not indicate the dependence on L in all quantities):

$$\left\{ \begin{array}{l} (T_{q,L} + V) \phi_i^q = \varepsilon_i^q \phi_i^q, \quad \forall q \in \mathbb{R}^2, \quad \phi_i^q \in L^2_{\text{per}}(\Lambda_L), \quad (\phi_i^q, \phi_j^q)_{L^2_{\text{per}}} = \delta_{ij}, \quad \varepsilon_1^q \leq \varepsilon_2^q \leq \dots \\ -V'' + m^2 V = 2(\rho_{\overline{Q}} - \nu_{\text{per},L}), \\ \rho_{\overline{Q}} = \rho_\gamma - \rho_0, \\ \gamma := \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} \mathbb{1}_{(-\infty, \varepsilon_F]}(T_{q,L} + V) dq = \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} \left(\sum_{i=1}^{+\infty} \mathbb{1}_{(-\infty, \varepsilon_F]}(\varepsilon_i^q) |\phi_i^q\rangle \langle \phi_i^q| \right) dq, \end{array} \right. \quad (2.88)$$

with $\rho_0 = (2\varepsilon_F)^{3/2}/(6\pi^2)$ and

$$\rho_\gamma(z) = \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} \left(\sum_{i=1}^{+\infty} \mathbb{1}_{(-\infty, \varepsilon_F]}(\varepsilon_i^q) |\phi_i^q(z)|^2 \right) dq.$$

In fact, solving the family of eigenproblems in the first line of (2.88) requires only solving a single eigenvalue problem for $q = 0$ since $T_{q,L} = T_{\text{per},z,L} + |q|^2/2$. More precisely, (2.88) can be rewritten as

$$\left\{ \begin{array}{l} (T_{\text{per},z,L} + V) \phi_i = \varepsilon_i \phi_i, \quad \phi_i \in L^2_{\text{per}}(\Lambda_L), \quad (\phi_i, \phi_j)_{L^2_{\text{per}}} = \delta_{ij}, \quad \varepsilon_1 \leq \varepsilon_2 \leq \dots \\ -V'' + m^2 V = 2(\rho_\gamma - (\rho_0 + \nu_{\text{per}})), \\ \rho_\gamma(z) = \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} \left(\sum_{i=1}^{+\infty} \mathbb{1}_{(\varepsilon_i \leq \varepsilon_F - |q|^2/2)} |\phi_i(z)|^2 \right) dq = \frac{1}{2\pi} \sum_{i=1}^{+\infty} \max(0, \varepsilon_F - \varepsilon_i) |\phi_i(z)|^2. \end{array} \right. \quad (2.89)$$

Therefore, in order to solve (2.87), we look for a solution to (2.89). We discuss in the next section how to do this in practice.

2.4.2 Discretization of the supercell model

We explain in this section how to solve (2.89). The method is based on two ingredients: discretizing the variational formula associated with the first equation in (2.89) using a spectral Galerkin basis of Fourier modes, as studied in [CCM12]; and relying on a fixed-point strategy (with appropriate mixing) in order to find a solution to the nonlinear problem (2.89).

Discretization of the variational formulation of the Euler–Lagrange equations

We assume in this section that the potential V is fixed, and discuss how to construct a density from a given potential. We consider to this end the following finite-dimensional subspace of $H^1_{\text{per}}(\Lambda_L)$ (for $N \geq 1$)

$$X_N(\Lambda_L) := \text{Span} \{e_k \mid k \in \mathbb{Z}, |k| \leq N\}. \quad (2.90)$$

For $\psi(x) \in X_N(\Lambda_L)$, we have the following representation:

$$\psi(x) = \sum_{k=-N}^N c_k(\psi) e_k(x), \quad c_k(\psi) := \frac{L}{2N+1} \sum_{x \in \frac{L}{2N+1}\mathbb{Z} \cap \Lambda_L} \psi(x) e_{-k}(x). \quad (2.91)$$

Let us verify that the normalization is correct. First of all

$$\begin{aligned}
\psi(x) &= \sum_{k=-N}^N c_k(\psi) e_k(x) = \sum_{k=-N}^N \left(\frac{L}{2N+1} \sum_{x' \in \mathcal{G}_N \cap \Lambda_L} \psi(x') e_{-k}(x') \right) e_k(x) \\
&= \frac{L}{2N+1} \sum_{x' \in \frac{L}{2N+1} \mathbb{Z} \cap \Lambda_L} \psi(x') \left(\frac{1}{L} \sum_{k=-N}^N e^{i \frac{2\pi}{L} k(x-x')} \right) \\
&\stackrel{\tilde{k}=k+N}{=} \frac{L}{2N+1} \sum_{x' \in \frac{L}{2N+1} \mathbb{Z} \cap \Lambda_L} \psi(x') \left(\frac{1}{L} \sum_{\tilde{k}=0}^{2N} e^{i \frac{2\pi}{L} (\tilde{k}-N)(x-x')} \right).
\end{aligned} \tag{2.92}$$

For $x, x' \in \frac{L}{2N+1} \mathbb{Z} \cap \Lambda_L$, there exists $0 \leq m, n \leq 2N$ such that $x = -\frac{L}{2} + \frac{L}{2N+1} n$ and $x' = -\frac{L}{2} + \frac{L}{2N+1} m$. Therefore (2.92) becomes

$$\begin{aligned}
\psi(x) &= \frac{L}{2N+1} \sum_{x' \in \frac{L}{2N+1} \mathbb{Z} \cap \Lambda_L} \psi(x') \left(\frac{1}{L} \sum_{\tilde{k}=0}^{2N} e^{i \frac{2\pi}{L} (\tilde{k}-N)(x-x')} \right) \\
&= \frac{1}{2N+1} \sum_{0 \leq m \leq 2N} \psi(x') \left(\sum_{\tilde{k}=0}^{2N} e^{i 2\pi (\tilde{k}-N) \frac{n-m}{2N+1}} \right) \\
&= \frac{1}{2N+1} \sum_{0 \leq m \leq 2N} \psi(x') \left(\sum_{\tilde{k}=0}^{2N} e^{i 2\pi \frac{n-m}{2N+1} \tilde{k}} \right) e^{-i 2\pi \frac{n-m}{2N+1} N} \\
&= \frac{1}{2N+1} \sum_{0 \leq m \leq 2N} \psi(x') ((2N+1) \delta_{m,n}) e^{-i 2\pi \frac{n-m}{2N+1} N} \\
&= \psi(x).
\end{aligned}$$

Introduce the variational problem on $X_N(\Lambda_L)$: find $\phi_{0,N}, \phi_{1,N}, \dots \in X_N(\Lambda_L)$ and $\varepsilon_{0,N} \leq \varepsilon_{1,N} \leq \dots$ such that

$$\begin{cases} \forall \varphi_N \in X_N(\Lambda_L), \quad \frac{1}{2} \int_{\Lambda_L} \overline{\phi'_{i,N}(z)} \varphi'_N(z) dz + \int_{\Lambda_L} \Pi_N(\overline{V \phi_{i,N}})(z) \varphi_N(z) dz = \varepsilon_{i,N} \int_{\Lambda_L} \overline{\phi_{i,N}(z)} \varphi_N(z) dz, \\ \int_{\Lambda_L} \overline{\phi_{j,N}(z)} \phi_{i,N}(z) dz = \delta_{i,j}, \end{cases} \tag{2.93}$$

where Π_N is the projection onto $X_N(\Lambda_L)$. The problem (2.93) can be recasted as

$$\begin{cases} \text{For } -N \leq k \leq N, \quad 1 \leq i \leq 2N+1 : \\ \frac{1}{2} \int_{\Lambda_L} \sum_{j=-N}^N \overline{c_j(\phi_{i,N})} e'_j e'_k + \int_{\Lambda_L} \left(\sum_{\ell=-2N}^{2N} c_\ell(\tilde{V}_N) e_\ell \right) \left(\sum_{j=-N}^N \overline{c_j(\phi_{i,N})} e_j e_k \right) \\ = \varepsilon_i \int_{\Lambda_L} \sum_{j=-N_e}^{N_e} \overline{c_j(\phi_{i,N_e})} e_j e_k, \\ \int_{\Lambda_L} \left(\sum_{j=-N}^N \overline{c_j(\phi_{i,N})} e_j \right) \left(\sum_{\ell=-N}^N c_\ell(\phi_{k,N}) e_\ell \right) = \delta_{i,k}, \end{cases} \tag{2.94}$$

which can be simplified as:

$$\begin{cases} \text{For } -N \leq k \leq N, \quad 1 \leq i \leq 2N+1 : \\ \frac{1}{2} \left| \frac{2\pi k}{L} \right|^2 c_k(\phi_{i,N}) + \frac{1}{\sqrt{L}} \sum_{j=-N}^N c_j(\phi_{i,N}) c_{k-j}(\tilde{V}_N) = \varepsilon_i c_k(\phi_{i,N}). \end{cases} \tag{2.95}$$

In order to write (2.95) in matrix form, we define a $(2N + 1) \times (2N + 1)$ matrix

$$A_{2N+1} := \begin{pmatrix} \frac{1}{2} \left| \frac{2\pi N}{L} \right|^2 + \frac{1}{\sqrt{L}} c_0(\tilde{V}_N) & \frac{1}{\sqrt{L}} c_{-1}(\tilde{V}_N) & \cdots & \frac{1}{\sqrt{L}} c_{-2N}(\tilde{V}_N) \\ \frac{1}{\sqrt{L}} c_1(\tilde{V}_N) & \frac{1}{2} \left| \frac{2\pi(N-1)}{L} \right|^2 + \frac{1}{\sqrt{L}} c_0(\tilde{V}_N) & \cdots & \frac{1}{\sqrt{L}} c_{-2N+1}(\tilde{V}_N) \\ \vdots & \ddots & \ddots & \vdots \\ \frac{1}{\sqrt{L}} c_{2N}(\tilde{V}_N) & \frac{1}{\sqrt{L}} c_{2N-1}(\tilde{V}_N) & \cdots & \frac{1}{2} \left| \frac{2\pi N}{L} \right|^2 + \frac{1}{\sqrt{L}} c_0(\tilde{V}_N) \end{pmatrix}$$

Hence (2.95) can be represented as a spectral problem of A_{2N+1} :

$$A_{2N+1} \begin{pmatrix} c_{-N}(\phi_{i,N}) \\ c_{-N+1}(\phi_{i,N}) \\ \vdots \\ c_N(\phi_{i,N}) \end{pmatrix} = \varepsilon_i \begin{pmatrix} c_{-N}(\phi_{i,N}) \\ c_{-N+1}(\phi_{i,N}) \\ \vdots \\ c_N(\phi_{i,N}) \end{pmatrix}. \quad (2.96)$$

Remark that A_{2N+1} is a Hermitian matrix, which only has real eigenvalues. Once the wavefunctions $\phi_{i,N}$ are obtained, the density follows from the last equation in (2.89):

$$\begin{aligned} \rho_{\gamma,N}(x) &= \sum_{k=-2N}^{2N} c_k(\rho_{\gamma,N}) e_k(x) = \frac{1}{2\pi} \sum_{\varepsilon_i \leq \varepsilon_F} (\varepsilon_F - \varepsilon_i) |\phi_{i,N}(x)|^2 \\ &= \frac{1}{2\pi} \frac{1}{L} \sum_{\varepsilon_i \leq \varepsilon_F} \sum_{j=-N}^N \sum_{\ell=-N}^N (\varepsilon_F - \varepsilon_i) \overline{c_j(\phi_{i,N})} c_\ell(\phi_{i,N}) e^{i \frac{2\pi}{L}(\ell-j)x} \\ &\stackrel{\ell-j=k}{=} \frac{1}{2\pi} \sum_{k=-2N}^{2N} \left(\frac{1}{\sqrt{L}} \sum_{\varepsilon_i \leq \varepsilon_F} \left((\varepsilon_F - \varepsilon_i) \sum_{j=\max(-N, -N-k)}^{\min(N, N-k)} \overline{c_j(\phi_{i,N})} c_{j+k}(\phi_{i,N}) \right) \right) e_k(x). \end{aligned} \quad (2.97)$$

Hence

$$c_k(\rho_{\gamma,N}) := \frac{1}{2\pi} \frac{1}{\sqrt{L}} \sum_{\varepsilon_i \leq \varepsilon_F} \left((\varepsilon_F - \varepsilon_i) \sum_{j=\max(-N, -N-k)}^{\min(N, N-k)} \overline{c_j(\phi_{i,N})} c_{j+k}(\phi_{i,N}) \right), \quad -2N \leq k \leq 2N. \quad (2.98)$$

Note that the density is represented in $X_{2N}(\Lambda_L)$ since it involves squares of functions in $X_N(\Lambda_L)$. Finally, it is possible to associate a potential $\tilde{V}_N \in X_{2N}(\Lambda_L)$ to $\rho_{\gamma,N} \in X_{2N}(\Lambda_L)$ with the second equation in (2.89). The Fourier coefficients of \tilde{V}_N read From (2.89), the coefficient of the approximated potential can be written as:

$$\begin{aligned} \forall -2N \leq k \leq 2N : \\ c_k(\tilde{V}_N) &= 2 \frac{c_k(\rho_{\gamma,N}) - \sqrt{L} \rho_0 \delta_{k,0} - c_k(\nu_{\text{per},L})}{m^2 + |2\pi k/L|^2} \\ &= \frac{1}{\pi} \frac{\frac{1}{\sqrt{L}} \sum_{\varepsilon_i \leq \varepsilon_F} ((\varepsilon_F - \varepsilon_i) \cdot \sum_{j=\max(-N, -N-k)}^{\min(N, N-k)} \overline{c_j(\phi_{i,N})} c_{j+k}(\phi_{i,N})) - \sqrt{L} \rho_0 \delta_{k,0} - c_k(\nu_{\text{per},L})}{m^2 + |2\pi k/L|^2}, \end{aligned} \quad (2.99)$$

where $\delta_{k,\ell}$ is the Kronecker symbol.

Iterative resolution of the problem

We rely on an iterative procedure to solve the nonlinear fixed-point problem (2.89). The integer N is related to the dimension of the Galerkin space (2.90), while the integer n indexes the iterations in the fixed-point loop. Take a positive constant η small enough as convergence rate parameter (Step (4) below). Starting from the potential $V_N^0 = 0$ so that $\gamma_N^0 = \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2}^{\oplus} \mathbb{1}_{(-\infty, \varepsilon_F]}(T_{q,L}) dq$ and

$$\mathcal{E}_{m,\Lambda_L}(\gamma_N^0) = \frac{1}{(2\pi)^2} \text{Tr}_L((T_L - \varepsilon_F) \gamma_N^0) = -\frac{1}{2} \sum_i \mathbb{1}(\varepsilon_i^1 \leq \varepsilon_F) (\varepsilon_F - \varepsilon_i^1)^2.$$

the procedure is the following: For $n \geq 0$,

- (1) Compute the wavefunctions $\{\phi_{i,N}^n\}_{i \geq 1}$ and eigenvalues $\{\varepsilon_{i,N}^n\}_{i \geq 1}$ obtained from (2.96) with V replaced by V_N^n , and construct the corresponding density matrix as

$$\tilde{\gamma}_N^{n+1} = \frac{1}{2\pi} \sum_{i=1}^{2N+1} \max(0, \epsilon_F - \varepsilon_{i,N}^n) |\phi_{i,N}^n\rangle \langle \phi_{i,N}^n|;$$

- (2) Use the optimal damping algorithm (ODA) to obtain the new density matrix γ_N^{n+1} from γ_N^n and $\tilde{\gamma}_N^{n+1}$ (see below);
- (3) Construct the potential V_N^{n+1} using (2.99) from the new density $\rho_{\gamma_N^{n+1}}(z) = \gamma_N^{n+1}(z, z)$ obtained by (2.98);
- (4) Check whether some termination criterion is met (e.g. $\|\rho_{\gamma_N^{n+1}} - \rho_{\gamma_N^n}\|_{L^2_{\text{per}}(\Lambda_L)} \leq \eta \|\rho_{\gamma_N^n}\|_{L^2_{\text{per}}(\Lambda_L)}$ for some small tolerance η); otherwise increment n and go back to (1).

Let us now make precise how Step (2) is performed. The idea of ODA [Can00] is to write γ_N^{n+1} as a convex combination of γ_N^n and $\tilde{\gamma}_N^{n+1}$, and optimize upon the parameter determining the combination in order to minimize the energy. More precisely, we introduce a mixing parameter $\alpha \in [0, 1]$ and the objective function

$$f_N^{n+1}(\alpha) := \mathcal{E}_{m,\Lambda_L}((1-\alpha)\gamma_N^n + \alpha\tilde{\gamma}_N^{n+1}).$$

Denoting by $\alpha_{\text{opt}}^{n+1} = \text{argmin}\{f_N^{n+1}(\alpha), \alpha \in [0, 1]\}$ the optimal mixing parameter, the new density matrix is then defined as $(1 - \alpha_{\text{opt}}^{n+1})\gamma_N^n + \alpha_{\text{opt}}^{n+1}\tilde{\gamma}_N^{n+1}$. For the rHF model, determining this parameter amounts to finding the roots of a second order polynomial. More details can be found in Section 2.5.1.

2.4.3 Numerical results

We finally present results of numerical simulations to illustrate the behavior of the perturbation of the electronic density induced by sharp trenches modeling a capacitor. More precisely, we consider $\nu(z) = -\rho_0 \mathbb{1}_{|z| \leq w}$ for $w > 0$. The physical parameters are chosen as $\epsilon_F = 2.0$, $w = 4$, while the computational parameters are set to $L = 300$, $N = 1500$ and $\eta = 10^{-8}$.

We plot in Figures 2.4 and 2.5 the total electronic density $\rho_0 + \nu + \rho_{\nu,m}$ for two values of the Yukawa parameter $m > 0$. We can observe Friedel oscillations [Fri52] in the densities, which can be fitted away from the defect as

$$\rho_{\nu,m}(z) = \rho_0 + a \frac{\cos(2\epsilon z + \delta)}{|z|^3};$$

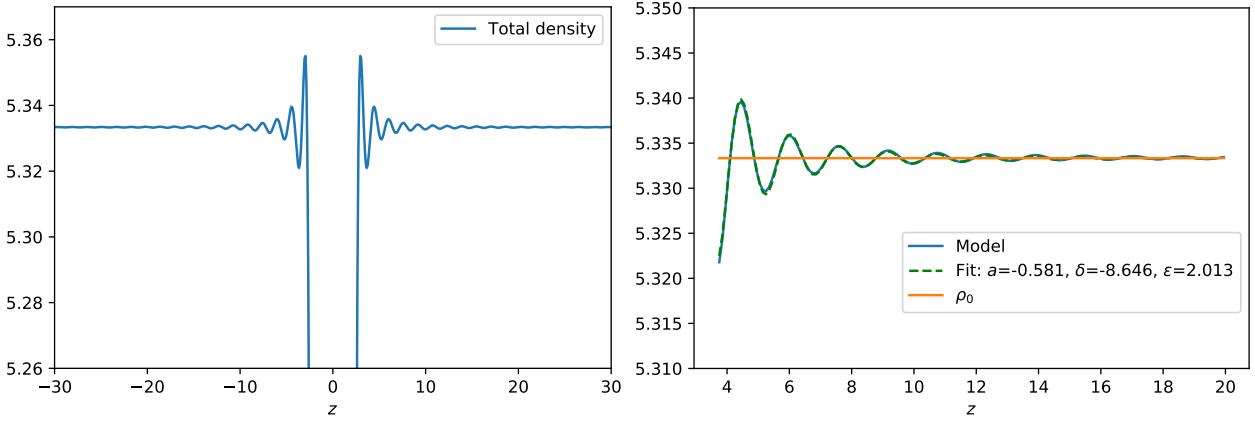
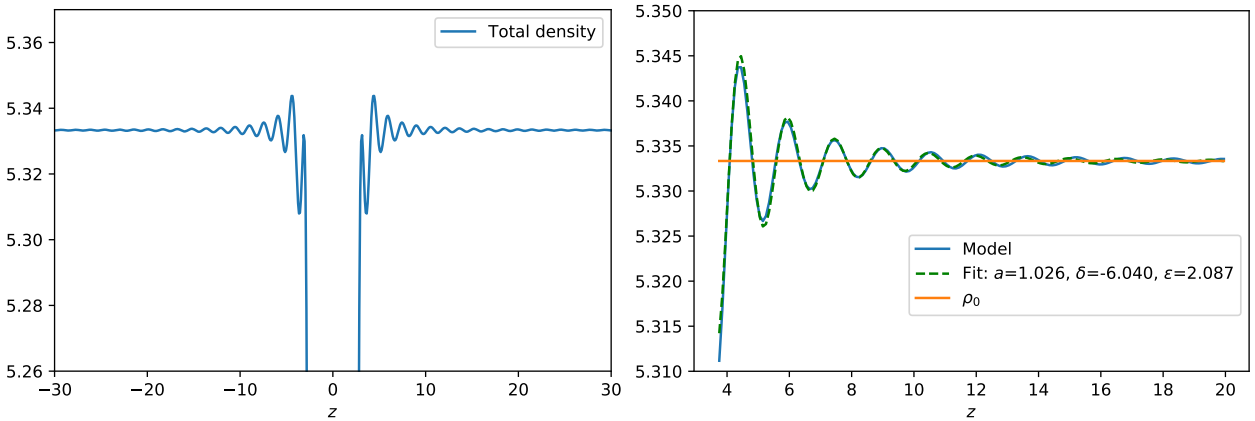
see the values of a, δ, ϵ obtained by our fit in the captions of the figures. Remark that the fitted value of ϵ is close to the Fermi level, as predicted by [Fri52].

2.5 Appendix

2.5.1 Optimal damping algorithm

In this section we give more details of the ODA used for the iterative solutions of (2.96), (2.98) and (2.99). It consists in finding an optimal mixing parameter to construct the density matrix at step $n+1$ from step n . At iteration step n , denote by γ_N^n the density matrix with density $\rho_{\gamma_N^n}(x) := \gamma_N^n(x, x)$. Denote by V_N^n the potential. Denote by $\tilde{\gamma}_N^{n+1}$ the solution of Euler-Lagrange equation (2.88) at iteration step $n+1$, we then have

$$\tilde{\gamma}_N^{n+1} := \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2}^{\oplus} \mathbb{1}_{(-\infty, \epsilon_F]}(T_{q,L} + V_N^n) dq = \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2}^{\oplus} \left(\sum_{i=0}^{+\infty} \mathbb{1}_{(\varepsilon_i^{q,n+1} \leq \epsilon_F)} |\phi_i^q\rangle \langle \phi_i^q| \right) dq. \quad (2.100)$$

Figure 2.4: Electronic density $\rho_{\nu,m}$ for $m = 4$.Figure 2.5: Electronic density $\rho_{\nu,m}$ for $m = 2$.

with density $\tilde{\rho}_{\gamma,N}^{n+1}(x) := \tilde{\gamma}_N^{n+1}(x, x)$. Remark that we do not need to calculate explicitly γ_N^n and $\tilde{\gamma}_N^{n+1}$. The ODA algorithm consists in finding the minimizer of total energy $\mathcal{E}_{m,\Lambda_L}(\gamma)$ in the segment $[\gamma_N^n, \tilde{\gamma}_N^{n+1}]$ as density matrix γ_N^{n+1} at step $n + 1$. In order to do so, we introduce a mixing parameter $\alpha \in [0, 1]$, and an objective function

$$f^{n+1}(\alpha) := \mathcal{E}_{m,\Lambda_L}((1 - \alpha)\gamma_N^n + \alpha\tilde{\gamma}_N^{n+1}).$$

We look for the optimal α to minimize $f^{n+1}(\alpha)$, that is

$$\alpha_{\text{opt}}^{n+1} = \operatorname{argmin} \{f^{n+1}(\alpha), \alpha \in [0, 1]\}. \quad (2.101)$$

Moreover,

$$\mathcal{E}_{m,\Lambda_L}(\gamma_N^{n+1}) \equiv f^{n+1}(\alpha_{\text{opt}}^{n+1}). \quad (2.102)$$

Denote the kinetic energy by

$$\tilde{K}^{n+1} := \underline{\operatorname{Tr}}_L((T_L - \epsilon_F)\tilde{\gamma}_N^{n+1}), K^n := \underline{\operatorname{Tr}}_L((T_L - \epsilon_F)\gamma_N^n).$$

An explicit calculation of f^{n+1} gives:

$$\begin{aligned} f^{n+1}(\alpha) &= \mathcal{E}_{m,\Lambda_L}((1 - \alpha)\gamma_N^n + \alpha\tilde{\gamma}_N^{n+1}) = \underline{\operatorname{Tr}}_L((T_L - \epsilon_F)((1 - \alpha)\gamma_N^n + \alpha\tilde{\gamma}_N^{n+1})) \\ &\quad + \frac{1}{2} \underline{D}_{m,\Lambda_L} \left(\left((1 - \alpha)\rho_{\gamma,N}^n + \alpha\tilde{\rho}_{\gamma,N}^{n+1} \right) - \nu_{\text{per}}, \left((1 - \alpha)\rho_{\gamma,N}^n + \alpha\tilde{\rho}_{\gamma,N}^{n+1} \right) - \nu_{\text{per}} \right) \\ &= a^{n+1}\alpha^2 + b^{n+1}\alpha + c^{n+1}, \end{aligned}$$

where

$$\begin{aligned}
a^{n+1} &= \frac{1}{2} \underline{D}_{m, \Lambda_L} \left(\tilde{\rho}_{\gamma, N}^{n+1} - \rho_{\gamma, N}^n, \tilde{\rho}_{\gamma, N}^{n+1} - \rho_{\gamma, N}^n \right) \\
&= \frac{1}{2} \sum_{-2N \leq k \leq 2N} \left(c_k \left(\tilde{V}_N^{n+1} \right) - c_k \left(V_N^n \right) \right) \left(c_k \left(\tilde{\rho}_N^{n+1} \right) - c_k \left(\rho_N^n \right) \right), \\
b^{n+1} &= \underline{\text{Tr}}_L \left((T_L - \epsilon_F) \left(\tilde{\gamma}_N^{n+1} - \gamma_N^n \right) \right) + \underline{D}_{m, \Lambda_L} \left(\rho_{\gamma, N}^n - \nu_{\text{per}}, \tilde{\rho}_{\gamma, N}^{n+1} - \rho_{\gamma, N}^n \right) \\
&= \underline{\text{Tr}}_L \left((T_L + V_N^n - \epsilon_F) \left(\tilde{\gamma}_N^{n+1} - \gamma_N^n \right) \right) \\
&= -\pi \sum_i \mathbf{1} \left(\epsilon_i^{n+1} \leq \epsilon_F \right) \left(\epsilon_F - \epsilon_i^{n+1} \right)^2 - K^n - \sum_{-2N \leq k \leq 2N} c_k \left(V_N^n \right) c_k \left(\rho_N^n \right), \\
c^{n+1} &= \underline{\text{Tr}}_L \left((T_L - \epsilon_F) \gamma_N^n \right) + \frac{1}{2} \underline{D}_{m, \Lambda_L} \left(\rho_{\gamma, N}^n - \nu_{\text{per}}, \rho_{\gamma, N}^n - \nu_{\text{per}} \right) = \mathcal{E}_{m, \Lambda_L} \left(\gamma_N^n \right) \\
&= K^n + \frac{1}{2} \sum_{-2N \leq k \leq 2N} c_k \left(V_N^n \right) \left(c_k \left(\rho_N^n \right) - c_k \left(\nu \right) \right).
\end{aligned}$$

We now give more details for the calculations of a^{n+1} , b^{n+1} and c^{n+1} . Since $\tilde{\rho}_{\gamma, N}^{n+1}$ verifies the Poisson equation $-\widetilde{V}_N^{n+1}'' + m^2 \widetilde{V}_N^{n+1} = 2(\tilde{\rho}_{\gamma, N}^{n+1} - \rho_0 - \nu_{\text{per}})$, and $\{c_k(V_N^n)\}_{-2N \leq k \leq 2N}$ are obtained by (2.99) from the Fourier coefficients $\{c_k(\rho_N^n)\}_{-2N \leq k \leq 2N}$ of $\rho_{\gamma, N}^n$, thus verifying the numerical Poisson equation $-(V_N^n)'' + m^2 V_N^n = 2(\rho_{\gamma, N}^n - \rho_0 - \nu_{\text{per}})$. Therefore

$$\begin{aligned}
a^{n+1} &= \frac{1}{2} \underline{D}_{m, \Lambda_L} \left(\tilde{\rho}_{\gamma, N}^{n+1} - \rho_{\gamma, N}^n, \tilde{\rho}_{\gamma, N}^{n+1} - \rho_{\gamma, N}^n \right) \\
&= \frac{1}{2} \sum_{-2N \leq k \leq 2N} \left(c_k \left(\tilde{V}_N^{n+1} \right) - c_k \left(V_N^n \right) \right) \left(c_k \left(\tilde{\rho}_N^{n+1} \right) - c_k \left(\rho_N^n \right) \right)
\end{aligned}$$

Let us now turn to b^{n+1} and c^{n+1} . Remark that

$$\left(\left(-\frac{1}{2} \frac{d^2}{dz^2} \right)_L + V_N^n \right) \phi_i^{n+1} = \epsilon_i^{n+1} \phi_i^{n+1}, \quad \epsilon_i^{n+1} \leq \epsilon_F.$$

Together with (2.100) we get $\epsilon_i^{n+1} = \epsilon_i^{q, n+1} + \epsilon_F - \frac{|q|^2}{2}$ and

$$\begin{aligned}
\tilde{K}^{n+1} + \sum_{-N \leq k \leq N} c_k \left(V_N^n \right) c_k \left(\tilde{\rho}_N^{n+1} \right) &= \underline{\text{Tr}}_L \left((T_L + V_N^n - \epsilon_F) \tilde{\gamma}_N^{n+1} \right) \\
&= \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} \text{Tr}_{L_{\text{per}}^2(\Lambda_L)} \left(\left(\left(-\frac{1}{2} \frac{d^2}{dz^2} \right)_L + \frac{|q|^2}{2} + V_N^n - \epsilon_F \right) \tilde{\gamma}_N^{n+1} \right) dq \\
&= \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} \sum_i \left(\epsilon_i^{q, n+1} \mathbf{1}_{\epsilon_i^{q, n+1} \leq 0} \right) dq \\
&= \frac{1}{(2\pi)^2} \sum_i \left(\int_{\mathbb{R}^2} \left(\epsilon_i^{n+1} - \epsilon_F + \frac{|q|^2}{2} \right) \mathbf{1}_{\epsilon_i^{n+1} - \epsilon_F + \frac{|q|^2}{2} \leq 0} dq \right) \\
&= \frac{1}{2\pi} \sum_i \mathbf{1} \left(\epsilon_i^{n+1} \leq \epsilon_F \right) \left(\int_0^{\sqrt{2(\epsilon_F - \epsilon_i^{n+1})}} \left(\epsilon_i^{n+1} - \epsilon_F + \frac{r^2}{2} \right) r dr \right) \\
&= \frac{1}{2\pi} \sum_i \mathbf{1} \left(\epsilon_i^{n+1} \leq \epsilon_F \right) \left(\left(\epsilon_i^{n+1} - \epsilon_F \right) \frac{r^2}{2} + \frac{r^4}{8} \right) \Big|_0^{\sqrt{2(\epsilon_F - \epsilon_i^{n+1})}} \\
&= -\frac{1}{2} \sum_i \mathbf{1} \left(\epsilon_i^{n+1} \leq \epsilon_F \right) \left(\epsilon_F - \epsilon_i^{n+1} \right)^2.
\end{aligned} \tag{2.103}$$

This allows us to give the results of b^{n+1} and c^{n+1} .

2.5.2 Expressions of $\gamma_{0,q}$ and ρ_0

By density of $\mathcal{S}(\mathbb{R}^3)$ in $L^2(\mathbb{R}^3)$, it is sufficient to prove that, for any $\phi \in \mathcal{S}(\mathbb{R}^3)$, it holds

$$(\mathcal{U}(\gamma_0\phi))_q(z) = \left(\gamma_{0,q}(\mathcal{U}\phi)_q\right)(z) = (\gamma_{0,q}\phi_q)(z), \quad (2.104)$$

where $(q, z) \mapsto \phi_q(z) := (\mathcal{U}\phi)_q(z) \in \mathcal{S}(\mathbb{R}^3)$. Now, by pseudo-differential calculus,

$$\begin{aligned} (\gamma_{0,q}(\mathcal{U}\phi)_q)(z) &= \frac{1}{\sqrt{2\pi}} \int_{k \in \mathbb{R}} \mathbb{1}\left(\frac{k^2}{2} + \frac{|q|^2}{2} \leq \epsilon_F\right) e^{ikz} \widehat{\phi}_q(k) dk \\ &= \frac{1}{2\pi} \int_{k \in \mathbb{R}} \int_{z' \in \mathbb{R}} \mathbb{1}\left(\frac{k^2}{2} + \frac{|q|^2}{2} \leq \epsilon_F\right) e^{ik(z-z')} \phi_q(z') dz' dk \\ &= \frac{1}{(2\pi)^2} \int_{z' \in \mathbb{R}} \int_{r' \in \mathbb{R}^2} \int_{k \in \mathbb{R}} \mathbb{1}\left(\frac{k^2}{2} + \frac{|q|^2}{2} \leq \epsilon_F\right) e^{ik(z-z')} e^{-iq \cdot r'} \phi(r', z') dk dr' dz'. \end{aligned}$$

On the other hand, for $r \in \mathbb{R}^2$ and $z \in \mathbb{R}$,

$$\begin{aligned} (\gamma_0\phi)(r, z) &= \frac{1}{(2\pi)^{3/2}} \int_{\xi \in \mathbb{R}^3} \mathbb{1}\left(\frac{|\xi|^2}{2} \leq \epsilon_F\right) e^{i\xi \cdot (r, z)} \widehat{\phi}(\xi) d\xi \\ &= \frac{1}{(2\pi)^3} \int_{\xi \in \mathbb{R}^3} \int_{r' \in \mathbb{R}^2, z' \in \mathbb{R}} \mathbb{1}\left(\frac{|\xi|^2}{2} \leq \epsilon_F\right) e^{i\xi \cdot (r-r', z-z')} \phi(r', z') d\xi dr' dz'. \end{aligned}$$

Writing $\xi = (q', k)$, it holds

$$\begin{aligned} (\mathcal{U}(\gamma_0\phi))_q(z) &= \frac{1}{2\pi} \int_{r \in \mathbb{R}^2} e^{-iq \cdot r} (\gamma_0\phi)(r, z) dr \\ &= \frac{1}{(2\pi)^2} \int_{k \in \mathbb{R}} \int_{r' \in \mathbb{R}^2, z' \in \mathbb{R}} \mathbb{1}\left(\frac{|q|^2}{2} + \frac{k^2}{2} \leq \epsilon_F\right) e^{ik(z-z')} e^{-iq \cdot r'} \phi(r', z') dk dr' dz' \\ &= \gamma_{0,q}(\mathcal{U}\phi)_q(z), \end{aligned}$$

which shows that (2.104) is satisfied.

Remark 2.21. *The integral kernel of $\gamma_{0,q}$ reads*

$$\gamma_{0,q}(z, z') = \frac{1}{2\pi} \int_{k \in \mathbb{R}} \mathbb{1}\left(\frac{k^2}{2} + \frac{|q|^2}{2} \leq \epsilon_F\right) e^{ik(z-z')} dk.$$

Therefore,

$$\rho_{0,q}(z) := \gamma_{0,q}(z, z) = \frac{1}{\pi} \sqrt{2\epsilon_F - |q|^2}, \quad (2.105)$$

which is independent of z . The total electronic density is then

$$\begin{aligned} \rho_0 &:= \frac{1}{(2\pi)^2} \int_{|q|^2 \leq 2\epsilon_F} \rho_{0,q}(z) dq = \frac{1}{(2\pi)^2} \int_0^{\sqrt{2\epsilon_F}} 2r \sqrt{2\epsilon_F - r^2} dr, \\ &= \frac{1}{(2\pi)^2} \left[-\frac{2}{3} (2\epsilon_F - r^2)^{3/2} \right]_0^{\sqrt{2\epsilon_F}} = \frac{1}{(2\pi)^2} \frac{2}{3} (2\epsilon_F)^{3/2}, \end{aligned}$$

which provides the expression of ϵ_F in (2.3).

2.5.3 More details for the proof of Lemma 2.17

In this section we show that for $q \in \mathbb{R}^2$, a Hilbert–Schmidt operator with finite kinetic energies in \mathcal{K}_q can be approximated by finite-rank operators in \mathcal{K}_q . Moreover, the convergence (2.67) holds. To this end, let us prove that for a fixed $N \in \mathbb{N}^*$ and $q \in \mathbb{R}^2$ such that $P_{N,q} Q_q P_{N,q}$ with $Q_q \in \tilde{\mathcal{Q}}_{\gamma_{0,q}}$ can be approximated by finite-rank operators in \mathcal{K}_q , where recall that $P_{N,q} := \mathbb{1}_{[\frac{1}{N}, N]}(|T_q - \epsilon_F|)$ and

$$\tilde{\mathcal{Q}}_{\gamma_{0,q}} := \{Q_q \in \mathfrak{S}_2 \mid Q_q = Q_q^*, Q_q^{\pm\pm} \in \mathfrak{S}_1, -\gamma_{0,q} \leq Q_q \leq 1 - \gamma_{0,q}\}.$$

We first show that for all $q \in \mathbb{R}^2$ any Hilbert-Schmidt operator $Q_q \in \tilde{\mathcal{Q}}_{\gamma_{0,q}}$ can be approximated by finite-rank operators $(Q_{n,q})_{n \in \mathbb{N}^*} \in \tilde{\mathcal{Q}}_{\gamma_{0,q}}$. The proof relies on the results in [HLS09a, Proposition 2, Theorem 5 and 6], which consist in characterizing mathematical properties for two general orthogonal projectors P and Π on a Hilbert space \mathfrak{H} such that $P - \Pi \in \mathfrak{S}_2(\mathfrak{H})$. See also [Lew09, Appendix A] for a detailed and pedagogic summary for the properties of these orthogonal projectors.

Lemma 2.22 ([HLS09a, Theorem 5] Projectors and BDF-states in the Fock space). *Let Ξ, Θ be orthogonal projectors on \mathfrak{H} . Denote by $\mathfrak{H}_+ := (1 - \Theta)\mathfrak{H}$ and $\mathfrak{H}_- := \Theta\mathfrak{H}$. Assume also that $\Xi - \Theta \in \mathfrak{S}_2(\mathfrak{H})$. Denote by $(f_1, \dots, f_L) \in (\mathfrak{H}_+)^L$ an orthonormal basis of $E_1 = \text{Ker}(\Xi - \Theta - 1) = \text{Ker}(\Theta) \cap \text{Ker}(1 - \Xi)$ and by $(g_1, \dots, g_M) \in (\mathfrak{H}_-)^M$ an orthonormal basis of $E_{-1} = \text{Ker}(\Xi - \Theta + 1) = \text{Ker}(1 - \Theta) \cap \text{Ker}(\Xi)$. Then there exists an orthonormal basis $(v_i)_{i \geq 1} \subset \mathfrak{H}_+$ of E_1^\perp in \mathfrak{H}_+ , and an orthonormal basis $(u_i)_{i \geq 1} \subset \mathfrak{H}_-$ of E_{-1}^\perp in \mathfrak{H}_- , and a sequence $(\lambda_i)_{i \geq 1} \in \ell^2(\mathbb{R}^+)$ such that*

$$\Theta = \sum_{m=1}^M |g_m\rangle\langle g_m| + \sum_{i \geq 1} |u_i\rangle\langle u_i|, \quad (2.106)$$

and

$$\begin{aligned} \Xi - \Theta &= \sum_{n=1}^L |f_n\rangle\langle f_n| - \sum_{m=1}^M |g_m\rangle\langle g_m| + \sum_{i \geq 1} \frac{\lambda_i^2}{1 + \lambda_i^2} (|v_i\rangle\langle v_i| - |u_i\rangle\langle u_i|) \\ &\quad + \sum_{i \geq 1} \frac{\lambda_i}{1 + \lambda_i^2} (|u_i\rangle\langle v_i| + |v_i\rangle\langle u_i|). \end{aligned} \quad (2.107)$$

Remark that

$$\begin{aligned} \|\Xi - \Theta\|_{\mathfrak{S}_2}^2 &= \text{Tr}_{\mathfrak{H}} \left((\Xi - \Theta)^2 \right) = \text{Tr}_{\mathfrak{H}} \left(\Theta^\perp (\Xi - \Theta) \Theta^\perp - \Theta (\Xi - \Theta) \Theta \right) \\ &= L + M + 2 \sum_{i \geq 1} \frac{\lambda_i^2}{1 + \lambda_i^2}. \end{aligned}$$

Relying on Lemma 2.22, let us now give the structure of operators belonging to $\tilde{\mathcal{Q}}_{\gamma_{0,q}}$ for any $q \in \mathbb{R}^2$.

Lemma 2.23 (The structure of $\tilde{\mathcal{Q}}_{\gamma_{0,q}}$ [HLS09a, Theorem 6]). *For any $q \in \mathbb{R}^2$, the operators in $\tilde{\mathcal{Q}}_{\gamma_{0,q}}$ are of the form*

$$Q_q = U_{D_q} (\gamma_{0,q} + \Pi_q) U_{-D_q} - \gamma_{0,q}, \quad U_{D_q} := \exp(D_q - D_q^*), \quad (2.108)$$

where

1. $D_q \in \mathfrak{S}_2(\mathfrak{H})$ such that $\text{Ker}(\gamma_{0,q}) \subseteq \text{Ker}(D_q)$ and $\text{Ker}(1 - \gamma_{0,q}) \subseteq \text{Ker}(D_q^*)$;
2. $\Pi_q \in \mathfrak{S}_1(\mathfrak{H})$ is a self-adjoint and trace-class operator such that

$$[\gamma_{0,q}, \Pi_q] = 0, \quad -\gamma_{0,q} \leq \Pi_q^{--} \leq 0, \quad 0 \leq \Pi_q^{++} \leq 1 - \gamma_{0,q}.$$

Proof. We give here a brief description as elements used in the proof will be used in the sequel. Fixing $q \in \mathbb{R}^2$, one first show that [HLS09a, Lemma 15] any $Q_q \in \tilde{\mathcal{Q}}_{\gamma_{0,q}}$ can be written as

$$Q_q = \Xi_q - \gamma_{0,q} + \Pi'_q, \quad (2.109)$$

with Ξ_q an orthogonal projector and Π'_q a trace-class operator such that $[\Xi_q, \Pi'_q] = 0$ and

$$\mathrm{Tr}_{L^2(\mathbb{R})} ((\Xi_q - \gamma_{0,q})^{++} + (\Xi_q - \gamma_{0,q})^{--}) = \mathrm{Tr}_{L^2(\mathbb{R})} (\gamma_{0,q}^\perp (\Xi_q - \gamma_{0,q}) \gamma_{0,q}^\perp + \gamma_{0,q} (\Xi_q - \gamma_{0,q}) \gamma_{0,q}) = 0. \quad (2.110)$$

By taking $\mathfrak{H} = L^2(\mathbb{R}^2)$, $\Theta = \gamma_{0,q}$, as well as orthonormal basis indexed by $q \in \mathbb{R}^2$ (with a slight abuse of notation) in Lemma 2.22, in view of (2.107), there exists $L_q \in \mathbb{N}^*$ such that

$$\begin{aligned} Q_q = \Xi_q - \gamma_{0,q} + \Pi'_q &= \sum_{n=1}^{L_q} |f_{n,q}\rangle\langle f_{n,q}| - \sum_{m=1}^{L_q} |g_{m,q}\rangle\langle g_{m,q}| + \sum_{i \geq 1} \frac{\lambda_{i,q}^2}{1 + \lambda_{i,q}^2} (|v_{i,q}\rangle\langle v_{i,q}| - |u_{i,q}\rangle\langle u_{i,q}|) \\ &+ \sum_{i \geq 1} \frac{\lambda_{i,q}}{1 + \lambda_{i,q}^2} (|u_{i,q}\rangle\langle v_{i,q}| + |v_{i,q}\rangle\langle u_{i,q}|) + \Pi'_q, \end{aligned}$$

with

$$\Xi_q = \sum_{n=1}^{L_q} |f_{n,q}\rangle\langle f_{n,q}| + \sum_{i \geq 1} \frac{|u_{i,q} + \lambda_{i,q} v_{i,q}\rangle\langle u_{i,q} + \lambda_{i,q} v_{i,q}|}{1 + \lambda_{i,q}^2}, \quad (2.111)$$

and

$$\gamma_{0,q} = \sum_{m=1}^{L_q} |g_{m,q}\rangle\langle g_{m,q}| + \sum_{i \geq 1} |u_{i,q}\rangle\langle u_{i,q}|. \quad (2.112)$$

Remark that because of (2.110),

$$\dim(\mathrm{Ker}(\Xi_q - \gamma_{0,q} - 1)) = \dim(\mathrm{Ker}(\Xi_q - \gamma_{0,q} + 1)) = L_q.$$

With these ingredients, the following lemma gives the structure of $\tilde{\mathcal{Q}}_{\gamma_{0,q}}$. Define

$$D_q = \sum_{k=1}^{L_q} \frac{\pi}{2} |g_{k,q}\rangle\langle f_{k,q}| + \sum_{i \geq 1} \arccos\left(\frac{1}{\sqrt{1 + \lambda_{i,q}^2}}\right) |u_{i,q}\rangle\langle v_{i,q}|.$$

Then the following *Bogoliubov transformation* holds¹

$$\Xi_q = U_{D_q} \gamma_{0,q} U_{-D_q}. \quad (2.113)$$

The inequality (2.108) holds by defining $\Pi_q := U_{-D_q} \Pi'_q U_{D_q}$. □

Following the ideas in the proof of [HLS09a, Proposition 2], one can always find a sequence of finite-rank operators

$$(D_{\ell,q})_{\ell \in \mathbb{N}^*} := \sum_{k=1}^{L_q} \frac{\pi}{2} |g_{k,q}\rangle\langle f_{k,q}| + \sum_{i=1}^{\ell} \arccos\left(\frac{1}{\sqrt{1 + \lambda_{i,q}^2}}\right) |u_{i,q}\rangle\langle v_{i,q}| \quad (2.114)$$

such that

$$D_{\ell,q} \xrightarrow[\ell \rightarrow \infty]{\mathfrak{S}_2} D_q. \quad (2.115)$$

¹We refer the reader to the end of this section for the proof of the Bogoliubov transform (2.113) of $\gamma_{0,q}$ by U_{D_q} .

In view of the decomposition (2.112) of $\gamma_{0,q}$, it holds

$$U_{D_{\ell,q}} \gamma_{0,q} U_{-D_{\ell,q}} = \sum_{n=1}^{L_q} |f_{n,q}\rangle \langle f_{n,q}| + \sum_{i=1}^{\ell} \frac{|u_{i,q} + \lambda_{i,q} v_{i,q}\rangle \langle u_{i,q} + \lambda_{i,q} v_{i,q}|}{1 + \lambda_{i,q}^2} + \sum_{i \geq \ell+1} |u_{i,q}\rangle \langle u_{i,q}|.$$

Therefore

$$\begin{aligned} U_{D_{\ell,q}} \gamma_{0,q} U_{-D_{\ell,q}} - \gamma_{0,q} &= \sum_{n=1}^{L_q} |f_{n,q}\rangle \langle f_{n,q}| - \sum_{m=1}^{L_q} |g_{m,q}\rangle \langle g_{m,q}| + \sum_{i=1}^{\ell} \frac{\lambda_{i,q}^2}{1 + \lambda_{i,q}^2} (|v_{i,q}\rangle \langle v_{i,q}| - |u_{i,q}\rangle \langle u_{i,q}|) \\ &\quad + \sum_{i=1}^{\ell} \frac{\lambda_{i,q}}{1 + \lambda_{i,q}^2} (|u_{i,q}\rangle \langle v_{i,q}| + |v_{i,q}\rangle \langle u_{i,q}|) \\ &\xrightarrow{\ell \rightarrow \infty} \sum_{n=1}^{L_q} |f_{n,q}\rangle \langle f_{n,q}| - \sum_{m=1}^{L_q} |g_{m,q}\rangle \langle g_{m,q}| + \sum_{i \geq 1} \frac{\lambda_{i,q}^2}{1 + \lambda_{i,q}^2} (|v_{i,q}\rangle \langle v_{i,q}| - |u_{i,q}\rangle \langle u_{i,q}|) \\ &\quad + \sum_{i \geq 1} \frac{\lambda_{i,q}}{1 + \lambda_{i,q}^2} (|u_{i,q}\rangle \langle v_{i,q}| + |v_{i,q}\rangle \langle u_{i,q}|) \\ &= U_{D_q} \gamma_{0,q} U_{-D_q} - \gamma_{0,q} \text{ in } \mathfrak{S}_2. \end{aligned} \tag{2.116}$$

Moreover, there exists an orthonormal basis $(e_{n,q})_{n \in \mathbb{N}^*}$ of $L^2(\mathbb{R})$ and sequences of real numbers $0 \leq (\lambda_{\Pi,n,q}^{\pm\pm})_{n \in \mathbb{N}^*} \leq 1$ tending to 0 when $n \rightarrow \infty$, such that

$$(\Pi'_q)^{\pm\pm} = \pm \sum_{n \geq 1} \lambda_{\Pi,n,q}^{\pm\pm} |e_{n,q}\rangle \langle e_{n,q}|.$$

Define, for all $\ell \in \mathbb{N}^*$, $(\Pi'_{\ell,q})^{\pm\pm} := \pm \sum_{n=1}^{\ell} \lambda_{\Pi,n,q}^{\pm\pm} |e_{n,q}\rangle \langle e_{n,q}|$. Hence a result of [RS80, Corollary VI.21 and Theorem VI.22] gives

$$(\Pi'_{\ell,q})^{\pm\pm} \xrightarrow[\ell \rightarrow \infty]{\mathfrak{S}_1} (\Pi'_q)^{\pm\pm}. \tag{2.117}$$

Therefore in view of (2.116) and (2.117),

$$Q_{\ell,q} := U_{D_{\ell,q}} \gamma_{0,q} U_{-D_{\ell,q}} - \gamma_{0,q} + \Pi'_{\ell,q} \xrightarrow[\ell \rightarrow \infty]{} U_{D_q} \gamma_{0,q} U_{-D_q} - \gamma_{0,q} + \Pi'_q = Q_q \text{ in } \tilde{\mathcal{Q}}_{\gamma_{0,q}}.$$

This shows that $Q_q \in \tilde{\mathcal{Q}}_{\gamma_{0,q}}$ can be approximated by finite-rank operators $(Q_{\ell,q})_{\ell \in \mathbb{N}^*}$ in $\tilde{\mathcal{Q}}_{\gamma_{0,q}}$. Let us prove that for any $N \in \mathbb{N}^*$, the operator $P_{N,q} Q_q P_{N,q}$ can be approximated by finite-rank operators $(P_{N,q} Q_{\ell,q} P_{N,q})_{\ell \in \mathbb{N}^*}$ in \mathcal{K}_q . By definition,

$$\left\| |T_q - \epsilon_F|^{1/2} P_{N,q} (Q_{\ell,q} - Q_q) P_{N,q} \right\|_{\mathfrak{S}_2} \leq \left\| |T_q - \epsilon_F|^{1/2} P_{N,q} \right\| \left\| Q_{\ell,q} - Q_q \right\|_{\mathfrak{S}_2} \xrightarrow[\ell \rightarrow \infty]{} 0.$$

Similarly, for any $q \in \mathbb{R}^2$

$$\begin{aligned} &\left\| |T_q - \epsilon_F|^{1/2} P_{N,q} (Q_{\ell,q}^{\pm\pm} - Q_q^{\pm\pm}) P_{N,q} |T_q - \epsilon_F|^{1/2} \right\|_{\mathfrak{S}_1} \\ &\leq \left\| |T_q - \epsilon_F|^{1/2} P_{N,q} \right\|^2 \left\| Q_{\ell,q}^{\pm\pm} - Q_q^{\pm\pm} \right\|_{\mathfrak{S}_1} \xrightarrow[\ell \rightarrow \infty]{} 0. \end{aligned} \tag{2.118}$$

Therefore $Q_{\ell,q}$ can be approximated by finite-rank operators $(P_{N,q} Q_{\ell,q} P_{N,q})_{n \in \mathbb{N}^*}$ in \mathcal{K}_q . Let us finally prove that

$$q \mapsto |T_q - \epsilon_F|^{1/2} P_{N,q} (Q_q^{++} - Q_q^{--}) P_{N,q} |T_q - \epsilon_F|^{1/2} \in L^1(\mathbb{R}^2; \mathfrak{S}_1)$$

can be approximated by

$$q \mapsto |T_q - \epsilon_F|^{1/2} P_{N,q} (Q_{\ell,q}^{++} - Q_{\ell,q}^{--}) P_{N,q} |T_q - \epsilon_F|^{1/2} \text{ in } L^1(\mathbb{R}^2, \mathfrak{S}_1).$$

The following lemma allows us to conclude.

Lemma 2.24. *The following uniform bound holds: for any $q \in \mathbb{R}^2$,*

$$\begin{aligned} \forall \ell \in \mathbb{N}^*, \quad 0 &\leq \text{Tr}_{L^2(\mathbb{R})} \left(|T_q - \epsilon_F|^{1/2} P_{N,q} (Q_{\ell,q}^{++} - Q_{\ell,q}^{--}) P_{N,q} |T_q - \epsilon_F|^{1/2} \right) \\ &\leq \left\| |T_q - \epsilon_F|^{1/2} P_{N,q} \right\|^2 \|Q_{\ell,q}^{++} - Q_{\ell,q}^{--}\|_{\mathfrak{S}_1} \\ &\leq \left\| |T_q - \epsilon_F|^{1/2} P_{N,q} \right\|^2 \|Q_q^{++} - Q_q^{--}\|_{\mathfrak{S}_1} \leq N^2 \|Q_q^{++} - Q_q^{--}\|_{\mathfrak{S}_1}. \end{aligned} \quad (2.119)$$

Moreover,

$$q \mapsto Q_q^{++} - Q_q^{--} \text{ also belongs to } L^1(\mathbb{R}^2, \mathfrak{S}_1). \quad (2.120)$$

Furthermore,

$$\begin{aligned} \lim_{n \rightarrow \infty} \int_{\mathbb{R}^2} \text{Tr}_{L^2(\mathbb{R})} \left(|T_q - \epsilon_F|^{1/2} P_{N,q} (Q_{\ell,q}^{++} - Q_{\ell,q}^{--}) P_{N,q} |T_q - \epsilon_F|^{1/2} \right) dq \\ = \int_{\mathbb{R}^2} \text{Tr}_{L^2(\mathbb{R})} \left(|T_q - \epsilon_F|^{1/2} P_{N,q} (Q_q^{++} - Q_q^{--}) P_{N,q} |T_q - \epsilon_F|^{1/2} \right) dq. \end{aligned} \quad (2.121)$$

Proof. First of all, remark that for any $q \in \mathbb{R}^2$ and ℓ large enough, from the proof of [HLS09a, Proposition 2] (see also [JRB94, Theorem 4.1]) we know that

$$\begin{aligned} \text{Tr}_{L^2(\mathbb{R})} \left((U_{D_{\ell,q}} \gamma_{0,q} U_{-D_{\ell,q}} - \gamma_{0,q})^{++} + (U_{D_{\ell,q}} \gamma_{0,q} U_{-D_{\ell,q}} - \gamma_{0,q})^{--} \right) \\ = \text{Tr}_{L^2(\mathbb{R})} \left((U_{D_q} \gamma_{0,q} U_{-D_q} - \gamma_{0,q})^{++} + (U_{D_q} \gamma_{0,q} U_{-D_q} - \gamma_{0,q})^{--} \right). \end{aligned}$$

In view of (2.114), the above approximation implies that finitely many particle-holes have been created from the Fermi sea and when ℓ is large enough, and that the total charge is conserved by the approximation. See [Lew09, Appendix A.2.3] for more details. This also implies that the particle number is uniformly bounded. Together with (2.116) we deduce that

$$\begin{aligned} \text{Tr}_{L^2(\mathbb{R})} \left((U_{D_{\ell,q}} \gamma_{0,q} U_{-D_{\ell,q}} - \gamma_{0,q})^{++} - (U_{D_{\ell,q}} \gamma_{0,q} U_{-D_{\ell,q}} - \gamma_{0,q})^{--} \right) \\ = 2L_q + 2 \sum_{i=1}^{\ell} \frac{\lambda_{i,q}^2}{1 + \lambda_{i,q}^2} \leq 2L_q + 2 \sum_{i=1}^{+\infty} \frac{\lambda_{i,q}^2}{1 + \lambda_{i,q}^2} \\ = \text{Tr}_{L^2(\mathbb{R})} \left((U_{D_q} \gamma_{0,q} U_{-D_q} - \gamma_{0,q})^{++} - (U_{D_q} \gamma_{0,q} U_{-D_q} - \gamma_{0,q})^{--} \right). \end{aligned}$$

The approximation (2.117) together with the fact that $-\gamma_{0,q} \leq (\Pi'_{\ell,q})^{--} \leq 0$, and $0 \leq (\Pi'_{\ell,q})^{++} \leq 1 - \gamma_{0,q}$ implies that

$$\text{Tr}_{L^2(\mathbb{R})} \left((\Pi'_{\ell,q})^{++} - (\Pi'_{\ell,q})^{--} \right) = \sum_{n=1}^{\ell} \lambda_{\Pi,n,q}^{\pm\pm} \leq \sum_{n=1}^{+\infty} \lambda_{\Pi,n,q}^{\pm\pm} = \text{Tr}_{L^2(\mathbb{R})} \left((\Pi'_q)^{++} - (\Pi'_q)^{--} \right).$$

Hence

$$\begin{aligned} \|Q_{\ell,q}^{++} - Q_{\ell,q}^{--}\|_{\mathfrak{S}_1} &= \text{Tr}_{L^2(\mathbb{R})} (Q_{\ell,q}^{++} - Q_{\ell,q}^{--}) \\ &= \text{Tr}_{L^2(\mathbb{R})} \left((U_{D_{\ell,q}} \gamma_{0,q} U_{-D_{\ell,q}} - \gamma_{0,q})^{++} - (U_{D_{\ell,q}} \gamma_{0,q} U_{-D_{\ell,q}} - \gamma_{0,q})^{--} \right) + \text{Tr}_{L^2(\mathbb{R})} \left((\Pi'_{\ell,q})^{++} - (\Pi'_{\ell,q})^{--} \right) \\ &\leq \text{Tr}_{L^2(\mathbb{R})} \left((U_{D_q} \gamma_{0,q} U_{-D_q} - \gamma_{0,q})^{++} - (U_{D_q} \gamma_{0,q} U_{-D_q} - \gamma_{0,q})^{--} \right) + \text{Tr}_{L^2(\mathbb{R})} \left((\Pi'_q)^{++} - (\Pi'_q)^{--} \right) \\ &= \text{Tr}_{L^2(\mathbb{R})} (Q_q^{++} - Q_q^{--}) = \|Q_q^{++} - Q_q^{--}\|_{\mathfrak{S}_1}. \end{aligned}$$

Therefore (2.119) holds by the fact that $\frac{1}{N^2} \leq \| |T_q - \epsilon_F|^{1/2} P_{N,q} \|^2 \leq N^2$. Use again this fact it is easy to see that $q \mapsto |T_q - \epsilon_F|^{1/2} P_{N,q}$ belongs to $L^\infty(\mathbb{R}^2; \mathcal{L}(L^2(\mathbb{R})))$. With this result, by writing

$$\begin{aligned} (Q_q^{++} - Q_q^{--}) \\ = \left(|T_q - \epsilon_F|^{1/2} P_{N,q} \right)^{-1/2} \left(|T_q - \epsilon_F|^{1/2} P_{N,q} (Q_q^{++} - Q_q^{--}) P_{N,q} |T_q - \epsilon_F|^{1/2} \right) \left(|T_q - \epsilon_F|^{1/2} P_{N,q} \right)^{-1/2}, \end{aligned}$$

and use the fact that $|T_q - \epsilon_F|^{1/2} P_{N,q} (Q_q^{++} - Q_q^{--}) P_{N,q} |T_q - \epsilon_F|^{1/2}$ belongs to $L^1(\mathbb{R}^2; \mathfrak{S}_1)$, we deduce that (2.120) holds. In view of (2.118), (2.119) and (2.120), by the dominated convergence theorem we can conclude (2.121). \square

Proof of Bogoliubov transformation (2.113) of $\gamma_{0,q}$ by D_q .

In order to simplify the notation, we discard for convenience the indexes $q \in \mathbb{R}^2$ to prove (2.113). First of all, as $\langle f_i | g_j \rangle = 0$, $\langle f_i | f_j \rangle = \delta_{ij}$, and $\langle g_i | g_j \rangle = \delta_{ij}$ for all $1 \leq i, j \leq L$, for $(\theta_i)_{1 \leq i \leq L} \in \mathbb{R}^L$, it holds

$$\exp \left(\sum_i^L \theta_i (|g_i\rangle\langle f_i| - |f_i\rangle\langle g_i|) \right) = \prod_i^L \exp(\theta_i (|g_i\rangle\langle f_i| - |f_i\rangle\langle g_i|)). \quad (2.122)$$

Similar relationship holds for orthonormal basis $(u_i)_{i \geq 1}$ and $(v_i)_{i \geq 1}$. In view of this, we first consider a rank-1 Bogoliubov transformation.

Step 1. Rank-1 Bogoliubov transformation.

For $\langle f | g \rangle = 0$ and $\langle f | f \rangle = 1$ and $\langle g | g \rangle = 1$, we consider the unitary transform $U_\theta := e^{\theta(|g\rangle\langle f| - |f\rangle\langle g|)}$ of the rank-1 projector $\gamma_\theta := |f\rangle\langle f|$ for $\theta \in \mathbb{R}_+$, where $\langle f | g \rangle = 0$. Denote by $T := |g\rangle\langle f| - |f\rangle\langle g|$, note that $T^2 = -|f\rangle\langle f| - |g\rangle\langle g|$ and $T^3 = -T$, therefore

$$\begin{aligned} U_\theta &= e^{\theta(|g\rangle\langle f| - |f\rangle\langle g|)} = e^{\theta T} = \sum_{n=1}^{+\infty} \frac{\theta^n T^n}{n!} = 1 + \sum_{m=0}^{\infty} \frac{(-1)^m}{(2m+1)!} \theta^{2m+1} T - \sum_{j=1}^{\infty} \frac{(-1)^j}{(2j)!} \theta^{2j} T^2 \\ &= 1 + \sin(\theta) T + (1 - \cos(\theta)) T^2. \end{aligned} \quad (2.123)$$

In view of this, the Bogoliubov transformation of γ_θ is

$$\begin{aligned} U_\theta \gamma_\theta U_{-\theta} &= (1 + \sin(\theta) T + (1 - \cos(\theta)) T^2) \gamma_\theta (1 - \sin(\theta) T + (1 - \cos(\theta)) T^2) \\ &= (\sin(\theta) |g\rangle\langle f| + \cos(\theta) |f\rangle\langle f|) (1 - \sin(\theta) |g\rangle\langle f| + \sin(\theta) |f\rangle\langle g| - (1 - \cos(\theta)) (|f\rangle\langle f| + |g\rangle\langle g|)) \\ &= \sin^2(\theta) |g\rangle\langle g| + \cos^2(\theta) |f\rangle\langle f| + \sin(\theta) \cos(\theta) (|f\rangle\langle g| + |g\rangle\langle f|). \end{aligned} \quad (2.124)$$

By taking $\theta = \frac{\pi}{2}$,

$$U_\theta \gamma_\theta U_{-\theta} = |g\rangle\langle g|. \quad (2.125)$$

By taking $\theta = \arccos\left(\frac{1}{\sqrt{1+\lambda^2}}\right)$ for some $\lambda > 0$, (2.124) gives

$$\begin{aligned} U_\theta \gamma_\theta U_{-\theta} &= \frac{\lambda^2}{1+\lambda^2} |g\rangle\langle g| + \frac{1}{1+\lambda^2} |f\rangle\langle f| + \frac{\lambda}{1+\lambda^2} (|f\rangle\langle g| + |g\rangle\langle f|) \\ &= \frac{|f + \lambda g\rangle\langle f + \lambda g|}{1+\lambda^2}. \end{aligned} \quad (2.126)$$

Remark also that in view of (2.123), for u orthogonal to both g and f , that is $\langle u | g \rangle = 0$ and $\langle u | f \rangle = 0$, it holds

$$U_\theta (|u\rangle\langle u|) U_{-\theta} = 0. \quad (2.127)$$

Step 2. Bogoliubov transformation of $\gamma_{0,q}$ by D_q .

In view of (2.122), (2.125) and (2.126), by using the orthogonality (2.127), it holds

$$\begin{aligned}
& U_{D_q} \gamma_{0,q} U_{-D_q} \\
&= \prod_{k=1}^{L_q} \exp\left(\frac{\pi}{2} (|g_{k,q}\rangle\langle f_{k,q}| - |f_{k,q}\rangle\langle g_{k,q}|)\right) \prod_{i \geq 1} \exp\left(\arccos\left(\frac{1}{\sqrt{1+\lambda_{i,q}^2}}\right) (|u_{i,q}\rangle\langle v_{i,q}| - |v_{i,q}\rangle\langle u_{i,q}|)\right) \\
&\quad \left(\sum_{m=1}^{L_q} |g_{m,q}\rangle\langle g_{m,q}| + \sum_{i \geq 1} |u_{i,q}\rangle\langle u_{i,q}|\right) \prod_{k=1}^{L_q} \exp\left(-\frac{\pi}{2} (|g_{k,q}\rangle\langle f_{k,q}| - |f_{k,q}\rangle\langle g_{k,q}|)\right) \\
&\quad \prod_{i \geq 1} \exp\left(-\arccos\left(\frac{1}{\sqrt{1+\lambda_{i,q}^2}}\right) (|u_{i,q}\rangle\langle v_{i,q}| - |v_{i,q}\rangle\langle u_{i,q}|)\right) \\
&= \sum_{n=1}^{L_q} |f_{n,q}\rangle\langle f_{n,q}| + \sum_{i \geq 1} \frac{|u_{i,q} + \lambda_{i,q} v_{i,q}\rangle\langle u_{i,q} + \lambda_{i,q} v_{i,q}|}{1 + \lambda_{i,q}^2}.
\end{aligned}$$

Therefore we can conclude (2.113).

CHAPTER 3

JUNCTION OF QUASI 1D SYSTEMS WITH COULOMB INTERACTIONS

This chapter describes results obtained in [Cao19].

Abstract. Junctions appear naturally when one studies surface states or transport properties of quasi one dimensional materials such as carbon nanotubes, polymers and quantum wires. These materials can be seen as 1D systems embedded in the 3D space. We first establish a mean-field description of reduced Hartree-Fock type for a 1D periodic system in the 3D space (a quasi 1D system), the unit cell of which is unbounded. With mild summability condition, we next show that a quasi 1D system in its ground state can be described by a mean-field Hamiltonian. We also prove that the Fermi level of this system is always negative. A junction system is described by two different infinitely extended quasi 1D systems occupying separately half spaces in 3D, where Coulombic electron-electron interactions are taken into account and without any assumption on the commensurability of the periods. We prove the existence of the ground state for a junction system, the ground state is a spectral projector of a mean-field Hamiltonian, and the ground state density is unique.

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3.1 Introduction

We consider a junction of two different quasi 1D periodic systems without any assumption on the commensurability of the periods. Generally speaking, there are two regimes for the junction of two different periodic systems: when the chemical potentials of the underlying periodic systems are separated by some occupied bands (non-equilibrium regime, see Fig. 3.1), and when the chemical potential are in a common spectral gap (equilibrium regime, see Fig. 3.2). The non-equilibrium regime models a persistent (non-perturbative) current in the junction system [BJLP15, BJLP16a, BJLP16b, CDP12], while the equilibrium regime can model either the ground state of the junction material or the presence of perturbative current in the linear response regime [CDNP08]. In this article we consider the equilibrium regime, and only briefly comment on the non-equilibrium regime in Section 3.3.2, as the study of this situation requires different techniques.

We establish a mean-field model to describe the junction of two different quasi 1D periodic systems (see Fig. 1.7) in the 3D space with Coulomb interactions in the rHF description. This non-linear model can be employed to describe the junction of two nanotubes, or a more realistic model of junction of two quasi 1D crystals for electronic structure calculations. It can be further explored to study the linear response with respect to different Fermi levels between two semi-infinite chains: recall that the famous Landauer–Büttiker [Lan70, BILP85] formalism for electronic (thermal) transport which is based on the lead-device-lead description, can be seen as the junction of two different quasi 1D systems (leads) with different chemical (thermal) potentials, and the device as a perturbation of this junction. Remark also that p-n junctions of carbon nanotubes without external battery [LT99, LGH04] correspond to the equilibrium regime, and can thus be described by the model we consider. Furthermore, our model can also be adapted to describe some 1D dislocation problems in the 3D space, while the linear 1D dislocation problems have been studied in [Kor00, Kor03] and some generalizations have been provided for higher dimensional systems [DPR11, HK11, HKS15].

3.2 A reduced Hartree–Fock description of quasi 1D periodic systems

In this section, we give a mathematical description of a quasi 1D periodic system in the framework of the reduced Hartree-Fock (rHF) approach. In Section 3.2.1, we introduce some mathematical preliminaries. In Section 3.2.2 we construct a periodic rHF energy functional for a quasi 1D system.

Unless otherwise specified, the functions on \mathbb{R}^d considered in this article are complex-valued. Elements of \mathbb{R}^3 are denoted by $\mathbf{x} = (x, \mathbf{r})$, where $x \in \mathbb{R}$.

3.2.1 Mathematical preliminaries

We first introduce a decomposition of the operator which is \mathbb{Z} -translation invariant in the x -direction based on the partial Bloch transform. In order to describe the 1D periodic system in the 3D space, we next introduce a mixed Fourier transform. We also introduce a Green’s function which is periodic only in the x -direction. Finally we introduce the kinetic energy space of density matrices and Coulomb interactions for quasi 1D systems.

Bloch transform in the x -direction. For $k \in \mathbb{Z}$, we denote by τ_k^x the translation operator in the x -direction acting on $L_{\text{loc}}^2(\mathbb{R}^3)$:

$$\forall u \in L_{\text{loc}}^2(\mathbb{R}^3), \quad (\tau_k^x u)(\cdot, \mathbf{r}) = u(\cdot - k, \mathbf{r}) \quad \text{for a.a. } \mathbf{r} \in \mathbb{R}^2.$$

An operator A on $L^2(\mathbb{R}^3)$ is called \mathbb{Z} -translation invariant in the x -direction if it commutes with τ_k^x for all $k \in \mathbb{Z}$. In order to decompose operators which are \mathbb{Z} -translation invariant in the x -direction, let us without loss of generality choose a unit cell $\Gamma := [-1/2, 1/2) \times \mathbb{R}^2$, and introduce the L^p spaces and H^1 spaces of functions which are 1-periodic in the x -direction: for $1 \leq p \leq +\infty$,

$$\begin{aligned} L_{\text{per},x}^p(\Gamma) &:= \left\{ u \in L_{\text{loc}}^p(\mathbb{R}^3) \mid \|u\|_{L^p(\Gamma)} < +\infty, \tau_k^x u = u, \forall k \in \mathbb{Z} \right\}, \\ H_{\text{per},x}^1(\Gamma) &:= \left\{ u \in L_{\text{per},x}^2(\Gamma) \mid \nabla u \in (L_{\text{per},x}^2(\Gamma))^3 \right\}. \end{aligned}$$

Let us also introduce the following constant fiber direct integral of Hilbert spaces [RS78]:

$$L^2(\Gamma^*; L_{\text{per},x}^2(\Gamma)) := \int_{\Gamma^*}^{\oplus} L_{\text{per},x}^2(\Gamma) \frac{d\xi}{2\pi},$$

with the base $\Gamma^* := [-\pi, \pi) \times \{0\}^2 \equiv [-\pi, \pi)$. The partial Bloch transform \mathcal{B} is a unitary operator from $L^2(\mathbb{R}^3)$ to $L^2(\Gamma^*; L_{\text{per},x}^2(\Gamma))$, defined on the dense subspace of $C_c^\infty(\mathbb{R}^3)$ of $L^2(\mathbb{R}^3)$:

$$\forall (x, \mathbf{r}) \in \Gamma, \forall \xi \in \Gamma^*, \quad (\mathcal{B}\phi)_\xi(x, \mathbf{r}) := \sum_{k \in \mathbb{Z}} e^{-i(x+k)\xi} \phi(x+k, \mathbf{r}).$$

Its inverse is given, for $f_\bullet = (f_\xi)_{\xi \in \Gamma^*}$ by

$$\forall k \in \mathbb{Z}, \text{ for a.a. } (x, \mathbf{r}) \in \Gamma, \quad (\mathcal{B}^{-1}f_\bullet)(x+k, \mathbf{r}) := \int_{\Gamma^*} e^{i(k+x)\xi} f_\xi(x, \mathbf{r}) \frac{d\xi}{2\pi}.$$

The partial Bloch transform has the property that any operator A on $L^2(\mathbb{R}^3)$ which commutes with τ_k^x for $k \in \mathbb{Z}$ is decomposed by \mathcal{B} : for any $A \in \mathcal{L}(L^2(\mathbb{R}^3))$ such that $\tau_k^x A = A \tau_k^x$, there exists $A_\bullet \in L^\infty(\Gamma^*; \mathcal{L}(L_{\text{per},x}^2(\Gamma)))$ such that for all $u \in L^2(\mathbb{R}^3)$,

$$(\mathcal{B}(Au))_\xi = A_\xi(\mathcal{B}u)_\xi \quad \text{for a.a. } \xi \in \Gamma^*.$$

We hence use the following notation for the decomposition of an operator A which is \mathbb{Z} -translation invariant in the x -direction:

$$A = \mathcal{B}^{-1} \left(\int_{\Gamma^*}^{\oplus} A_\xi \frac{d\xi}{2\pi} \right) \mathcal{B}.$$

In addition, $\|A\|_{\mathcal{L}(L^2(\mathbb{R}^3))} = \|\|A_\bullet\|_{\mathcal{L}(L_{\text{per},x}^2(\Gamma))}\|_{L^\infty(\Gamma^*)}$. In particular, if A is positive and locally trace-class, then for almost all $\xi \in \Gamma^*$, A_ξ is locally trace-class. The densities of these operators are related by the formula

$$\rho_A(\mathbf{x}) = \frac{1}{2\pi} \int_{\Gamma^*} \rho_{A_\xi}(\mathbf{x}) d\xi. \quad (3.1)$$

If A is a (not necessarily bounded) self-adjoint operator such that $\tau_k^x(A+i)^{-1} = (A+i)^{-1}\tau_k^x$ for all $k \in \mathbb{Z}$, then A is decomposed by \mathcal{U} (see [RS78, Theorems XIII.84 and XIII.85]). In particular, denoting by Δ the Laplace operator acting on $L^2(\mathbb{R}^3)$, the kinetic energy operator $-\frac{1}{2}\Delta$ on $L^2(\mathbb{R}^3)$ is decomposed by \mathcal{B} as follows:

$$-\frac{1}{2}\Delta = \mathcal{B}^{-1} \left(\int_{\Gamma^*} -\frac{1}{2}\Delta_\xi \frac{d\xi}{2\pi} \right) \mathcal{B}, \quad -\Delta_\xi = (-i\nabla_\xi)^2 = (i\partial_x - \xi)^2 - \Delta_{\mathbf{r}}, \quad (3.2)$$

where $\Delta_{\mathbf{r}}$ is the Laplace operator acting on $L^2(\mathbb{R}^2)$.

Mixed Fourier transform. The mixed Fourier transform consists of a Fourier series transform in the x -direction and an integral Fourier transform in the \mathbf{r} -direction. Denote by $\mathcal{S}_{\text{per},x}(\Gamma)$ the space of functions that are C^∞ on \mathbb{R}^3 and Γ -periodic, decaying faster than any power of $|\mathbf{r}|$ when $|\mathbf{r}|$ tends to infinity, as well as their derivatives. Denote by $\mathcal{S}'_{\text{per},x}(\Gamma)$ the dual space of $\mathcal{S}_{\text{per},x}(\Gamma)$. The mixed Fourier transform is the

unitary transform $\mathcal{F} : L^2_{\text{per},x}(\Gamma) \rightarrow \ell^2(\mathbb{Z}, L^2(\mathbb{R}^2))$ defined on the dense subspace $\mathcal{S}_{\text{per},x}(\Gamma)$ of $L^2_{\text{per},x}(\Gamma)$ by:

$$\forall \phi \in \mathcal{S}_{\text{per},x}(\Gamma), \forall (n, \mathbf{k}) \in \mathbb{Z} \times \mathbb{R}^2, \quad \mathcal{F}\phi(n, \mathbf{k}) := \frac{1}{2\pi} \int_{\Gamma} \phi(x, \mathbf{r}) e^{-i(2\pi n x + \mathbf{k} \cdot \mathbf{r})} dx d\mathbf{r}. \quad (3.3)$$

Its inverse is given by,

$$\forall (\psi_n(\mathbf{k}))_{n \in \mathbb{Z}, \mathbf{k} \in \mathbb{R}^2} \in \ell^2(\mathbb{Z}; L^2(\mathbb{R}^2)), \quad \mathcal{F}^{-1}\psi(x, \mathbf{r}) := \frac{1}{2\pi} \sum_{n \in \mathbb{Z}} \int_{\mathbb{R}^2} \psi_n(\mathbf{k}) e^{i(2\pi n x + \mathbf{k} \cdot \mathbf{r})} d\mathbf{k}.$$

Note that \mathcal{F} can be extended from $\mathcal{S}'_{\text{per},x}(\Gamma)$ to $\mathcal{S}'(\mathbb{R}^3)$. One can easily see that \mathcal{F} is an isometry from $L^2_{\text{per},x}(\Gamma)$ to $\ell^2(\mathbb{Z}, L^2(\mathbb{R}^2))$ in the following sense:

$$\forall f, g \in L^2_{\text{per},x}(\Gamma), \quad \int_{\Gamma} \overline{f(x, \mathbf{r})} g(x, \mathbf{r}) dx d\mathbf{r} = \sum_{n \in \mathbb{Z}} \int_{\mathbb{R}^2} \overline{\mathcal{F}f(n, \mathbf{k})} \mathcal{F}g(n, \mathbf{k}) d\mathbf{k}. \quad (3.4)$$

Moreover, it is easy to verify that for $f, g \in L^2_{\text{per},x}(\Gamma)$,

$$\mathcal{F}(f \star_{\Gamma} g) = 2\pi (\mathcal{F}f)(\mathcal{F}g), \quad (3.5)$$

where $(f \star_{\Gamma} g)(x) := \int_{\Gamma} f(x - x')g(x') dx'$. As an application of the mixed Fourier transform, let us introduce a Kato–Seiler–Simon type inequality [SS75] for the operator $-i\nabla_{\xi} = (-i\partial_x + \xi, -i\partial_{\mathbf{r}})$ for all $\xi \in \Gamma^*$, which will be repeatedly used in the proofs.

Lemma 3.1. Fix $\xi \in \Gamma^*$. Let $2 \leq p \leq +\infty$ and $f, g \in L^p_{\text{per},x}(\Gamma)$. Then

$$\|f(-i\nabla_{\xi})g\|_{\mathfrak{S}_p(L^2_{\text{per},x}(\Gamma))} \leq (2\pi)^{-2/p} \|g\|_{L^p_{\text{per},x}(\Gamma)} \left(\sum_{n \in \mathbb{Z}} \|f(2\pi n + \xi, \cdot)\|_{L^p(\mathbb{R}^2)}^p \right)^{1/p}, \quad (3.6)$$

for any $2 \leq p < \infty$ and

$$\|f(-i\nabla_{\xi})g\| \leq \|g\|_{L^{\infty}_{\text{per},x}(\Gamma)} \sup_{n \in \mathbb{Z}} \|f(2\pi n + \xi, \cdot)\|_{L^{\infty}(\mathbb{R}^2)},$$

when $p = +\infty$.

The proof of this lemma can be read in Section 3.4.1.

Periodic Green's function. We introduce a 3D Green's function which is 1-periodic in the x -direction in the same spirit as in [BLB00, LIE].

Definition 3.2 (Periodic Green's function). For $(x, \mathbf{r}) \in \mathbb{R}^3$, the periodic Green's function is defined as

$$G(x, \mathbf{r}) = -2 \log(|\mathbf{r}|) + \tilde{G}(x, \mathbf{r}), \quad \tilde{G}(x, \mathbf{r}) := 4 \sum_{n \geq 1} K_0(2\pi n |\mathbf{r}|) \cos(2\pi n x), \quad (3.7)$$

where $K_0(\alpha) := \int_0^{+\infty} e^{-\alpha \cosh(t)} dt$ is the modified Bessel function of the second kind.

The following lemma summarizes the properties of the periodic Green's function defined in (3.7).

Lemma 3.3. 1. The Green's function $G(x, \mathbf{r})$ defined in (3.7) satisfies the following Poisson's equation:

$$-\Delta G(x, \mathbf{r}) = 4\pi \sum_{n \in \mathbb{Z}} \delta_{(x, \mathbf{r})=(n, 0)} \in \mathcal{S}'(\mathbb{R}^3),$$

where $\delta_a \in \mathcal{S}'(\mathbb{R}^d)$ is the Dirac distribution at $a \in \mathbb{R}^d$. Moreover $G \in \mathcal{S}'_{\text{per},x}(\Gamma)$ and

$$\mathcal{F}(G)(n, \mathbf{k}) = \frac{2}{4\pi^2 n^2 + |\mathbf{k}|^2} \in \mathcal{S}'(\mathbb{R}^3). \quad (3.8)$$

2. The function \tilde{G} defined in (3.7) belongs to $L^p_{\text{per},x}(\Gamma)$ for $1 \leq p < 2$ and satisfies $\int_{\Gamma} \tilde{G} \equiv 0$. Moreover, there exist positive constants d_1 and d_2 such that $|\tilde{G}(\cdot, \mathbf{r})| \leq d_1 \frac{e^{-2\pi|\mathbf{r}|}}{\sqrt{|\mathbf{r}|}}$ when $|\mathbf{r}| \rightarrow +\infty$, and $|\tilde{G}(\cdot, \mathbf{r})| \leq \frac{d_2}{|\mathbf{r}|}$ when $|\mathbf{r}| \rightarrow 0$, uniformly with respect to x . Finally, the function $\tilde{G}(x, \mathbf{r})$ can also be written as

$$\tilde{G}(x, \mathbf{r}) = \sum_{n \in \mathbb{Z}} \left(\frac{1}{\sqrt{(x-n)^2 + |\mathbf{r}|^2}} - \int_{-1/2}^{1/2} \frac{1}{\sqrt{(x-y-n)^2 + |\mathbf{r}|^2}} dy \right). \quad (3.9)$$

The proof of this lemma can be read in Section 3.4.2.

One-body density matrices and kinetic energy space. In mean-field models, electronic states can be described by one-body density matrices (see e.g. [CDL08a, FLLS13]). Recall that for a finite system with N electrons, a density matrix is a trace-class self-adjoint operator $\gamma \in \mathcal{S}(L^2(\mathbb{R}^3)) \cap \mathfrak{S}_1(L^2(\mathbb{R}^3))$ satisfying the Pauli principle $0 \leq \gamma \leq 1$ and the normalization condition $\text{Tr}(\gamma) = \int_{\mathbb{R}^3} \rho_{\gamma} = N$. The kinetic energy of γ is given by $\text{Tr}(-\frac{1}{2}\Delta\gamma) := \frac{1}{2}\text{Tr}(|\nabla|\gamma|\nabla|)$ (see [CLBL01, CDL08a, CS12]).

Consider a 1D periodic system in the 3D space, where atoms are arranged periodically in the x -direction with unit cell Γ and first Brillouin zone Γ^* . Since the rHF model is strictly convex in the density [Sol91], we do not expect any spontaneous symmetry breaking. Therefore the electronic state of this quasi 1D system will be described by a one-body density matrix which commutes with the translations $\{\tau_k^x\}_{k \in \mathbb{Z}}$, hence is decomposed by the partial Bloch transform \mathcal{B} . In view of the decomposition (3.2), we define the following admissible set of one-body density matrices, which guarantees that the number of electrons per unit cell and the kinetic energy per unit cell are finite:

$$\mathcal{P}_{\text{per},x} := \left\{ \gamma \in \mathcal{S}(L^2(\mathbb{R}^3)) \mid 0 \leq \gamma \leq 1, \forall k \in \mathbb{Z}, \tau_k^x \gamma = \gamma \tau_k^x, \int_{\Gamma^*} \text{Tr}_{L^2_{\text{per},x}}(\sqrt{1-\Delta_{\xi}} \gamma_{\xi} \sqrt{1-\Delta_{\xi}}) d\xi < \infty \right\}, \quad (3.10)$$

where

$$\gamma = \mathcal{B}^{-1} \left(\int_{\Gamma^*} \gamma_{\xi} \frac{d\xi}{2\pi} \right) \mathcal{B}. \quad (3.11)$$

For any $\gamma \in \mathcal{P}_{\text{per},x}$, it is easy to see that $\rho_{\gamma} \in L^1_{\text{per},x}(\Gamma)$. Moreover, a Hoffmann-Ostenhof type inequality [HOHO77] can also be deduced from [CLBL01, Equation (4.42)]:

$$\int_{\Gamma} |\nabla \sqrt{\rho_{\gamma}}|^2 \leq \int_{\Gamma^*} \text{Tr}_{L^2_{\text{per},x}}(-\Delta_{\xi} \gamma_{\xi}) \frac{d\xi}{2\pi}. \quad (3.12)$$

Therefore $\sqrt{\rho_{\gamma}}$ is in $H^1_{\text{per},x}(\Gamma)$ hence in $L^6_{\text{per},x}(\Gamma)$ by Sobolev embeddings, so that $\rho_{\gamma} \in L^p_{\text{per},x}(\Gamma)$ for $1 \leq p \leq 3$ by an interpolation argument.

Coulomb interactions. Recall that the Coulomb interaction energy of charge densities f and g belonging to $L^{6/5}(\mathbb{R}^3)$ can be written in real and reciprocal space as:

$$D(f, g) := \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{f(\mathbf{x})g(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|} d\mathbf{x} d\mathbf{x}' = 4\pi \int_{\mathbb{R}^3} \frac{\widehat{f}(\mathbf{k})\widehat{g}(\mathbf{k})}{|\mathbf{k}|^2}.$$

In order to describe Coulomb interactions in the reciprocal space for a quasi 1D periodic system, we gather the results obtained in (3.4), (3.5) and (3.8), and define the Coulomb interaction energy per unit cell for charge densities f, g belonging to $\mathcal{S}_{\text{per},x}(\Gamma)$ as:

$$D_{\Gamma}(f, g) := 4\pi \sum_{n \in \mathbb{Z}} \int_{\mathbb{R}^2} \frac{\widehat{\mathcal{F}}(f)(n, \mathbf{k})\widehat{\mathcal{F}}(g)(n, \mathbf{k})}{|\mathbf{k}|^2 + 4\pi^2 n^2} d\mathbf{k}. \quad (3.13)$$

It is easy to see that $D_\Gamma(\cdot, \cdot)$ is a positive definite bilinear form on $\mathcal{S}_{\text{per},x}(\Gamma)$. Let us introduce the Coulomb space for the 1D periodic system in the 3D space as

$$\mathcal{C}_\Gamma := \left\{ f \in \mathcal{S}'_{\text{per},x}(\Gamma) \mid \forall n \in \mathbb{Z}, \mathcal{F}(f)(n, \cdot) \in L^1_{\text{loc}}(\mathbb{R}^2), D_\Gamma(f, f) < +\infty \right\}, \quad (3.14)$$

which is a Hilbert space endowed with the inner product $D_\Gamma(\cdot, \cdot)$.

Remark 3.4. *Remark that charge densities in \mathcal{C}_Γ are neutral in some weak sense. Indeed, for $f \in \mathcal{C}_\Gamma \cap L^1_{\text{per},x}(\Gamma)$, the condition $\int_{\mathbb{R}^2} \frac{|\mathcal{F}(f)(0, \mathbf{k})|^2}{|\mathbf{k}|^2} d\mathbf{k} < +\infty$ implies that $\mathcal{F}(f)(0, \mathbf{0}) = \int_\Gamma f(x, \mathbf{r}) dx d\mathbf{r} = 0$.*

3.2.2 Reduced Hartree–Fock description for a quasi 1D periodic system

Based on the kinetic energy space and Coulomb interactions defined in the previous section, we construct here a rHF energy functional for a quasi 1D periodic system which is 1-periodic only in the x -direction. Actually the previous situation is perturbed by adding positive charges spread periodically along the x -axis and we want to study the new nonlinear equilibrium. We show that its ground state is given by the solution of some minimization problem. Denote by $Z \in \mathbb{N}^*$ the total nuclear charge in each unit cell. For the sake of technical reasons we model the nuclear density of a quasi 1D system by a smooth function (smeared nuclei) which is 1-periodic in the x -direction

$$\mu_{\text{per}}(x, \mathbf{r}) = \sum_{n \in \mathbb{Z}} Z m(x - n, \mathbf{r}),$$

where $m(x, \mathbf{r})$ is a non-negative $C_c^\infty(\Gamma)$ function such that $\int_{\mathbb{R}^3} m = 1$. In particular $\int_\Gamma \mu_{\text{per}} = Z$.

For any trial density matrix γ which commutes with the translations τ_k^x in the x -direction, the periodic rHF energy functional for a quasi 1D system associated with the nuclear density μ_{per} is defined as:

$$\mathcal{E}_{\text{per},x}(\gamma) := \frac{1}{2\pi} \int_{\Gamma^*} \text{Tr}_{L^2_{\text{per},x}(\Gamma)} \left(-\frac{1}{2} \Delta_\xi \gamma \xi \right) d\xi + \frac{1}{2} D_\Gamma(\rho_\gamma - \mu_{\text{per}}, \rho_\gamma - \mu_{\text{per}}). \quad (3.15)$$

Let us introduce the following set of admissible density matrices for this rHF energy functional, which guarantees that the kinetic energy and Coulomb interaction energy per-unit cell are finite:

$$\mathcal{F}_\Gamma := \left\{ \gamma \in \mathcal{P}_{\text{per},x} \mid \rho_\gamma - \mu_{\text{per}} \in \mathcal{C}_\Gamma \right\},$$

where $\mathcal{P}_{\text{per},x}$ is the kinetic energy space defined in (3.10) and \mathcal{C}_Γ is the Coulomb space defined in (3.14).

Lemma 3.5. *The set \mathcal{F}_Γ is not empty. Moreover, for any $\gamma \in \mathcal{F}_\Gamma$,*

$$\int_\Gamma \rho_\gamma = \int_\Gamma \mu_{\text{per}}. \quad (3.16)$$

The proof of Lemma 3.5 relies on an explicit construct of an element in \mathcal{F}_Γ , and can be read in Section 3.4.3.

The periodic rHF ground state energy (per unit cell) of a quasi 1D system can then be written as the following minimization problem:

$$I_{\text{per}} = \inf \left\{ \mathcal{E}_{\text{per},x}(\gamma); \gamma \in \mathcal{F}_\Gamma \right\}, \quad (3.17)$$

The minimization problem similar to (3.17) under the Thomas-Fermi type models has been studied in [BLB00], where the authors proved the uniqueness of the minimizers, and justified the model by a thermodynamic limit argument. For a 3D periodic crystal, the minimization problem (3.17) has been examined in [CLBL01], where the authors showed the existence of minimizers and the uniqueness of the density of the minimizers. The characterization of the minimizers is given in [CDL08a, Theorem 1]: the minimizer is unique and is a spectral projector satisfying a self-consistent equation. The following theorem provides similar results for a quasi 1D system: we show that the minimizer of (3.17) exists, and that the density of the minimizers is unique. Let us emphasize that the unit cell of a quasi 1D system is an unbounded domain Γ , hence we need to deal with the possible escaping of electrons in the \mathbf{r} -direction, a situation which needs not be considered for bounded unit cells as in [CLBL01, CDL08a].

Theorem 3.6 (Existence of rHF ground state). *The minimization problem (3.17) admits a minimizer γ_{per} with density $\rho_{\gamma_{\text{per}}}$ belonging to $L^p_{\text{per},x}(\Gamma)$ for $1 \leq p \leq 3$. Besides, all the minimizers share the same density.*

The proof of Theorem 3.6 relies on a classical variational argument, and can be read in Section 3.4.4.

In order to treat the junction of quasi 1D systems in Section 3.3, it is useful to define and study the mean–field potential $V_{\text{per,sym}}$ generated by the ground state electronic density $\rho_{\gamma_{\text{per}}}$ and the nuclear density μ_{per} . It is also critical to obtain some decay estimates of $V_{\text{per,sym}}$ in the \mathbf{r} -direction. However, for $V_{\text{per,sym}}$ satisfying Poisson’s equation $-\Delta V_{\text{per,sym}} = 4\pi(\rho_{\gamma_{\text{per}}} - \mu_{\text{per}})$, the L^p integrability of $\rho_{\gamma_{\text{per}}}$ obtained in Theorem 3.6 does not imply the decay of the mean-field potential $V_{\text{per,sym}}$ in the \mathbf{r} -direction, given that the Green’s function defined in (3.7) has log-growth in the \mathbf{r} -direction. Moreover, the uniform bound given by the energy functional (3.15) does not provide any L^p bounds or decay property of $V_{\text{per,sym}}$. In this perspective, we introduce the following assumption on $\rho_{\gamma_{\text{per}}}$. Remark that this assumption, which we call “summability condition” is common when treating 2D Poisson’s equation [LL01, Theorem 6.21].

Assumption 2. *The unique ground state density $\rho_{\gamma_{\text{per}}}$ of the problem (3.17) satisfies*

$$\int_{\Gamma} |\mathbf{r}| \rho_{\gamma_{\text{per}}}(x, \mathbf{r}) dx d\mathbf{r} < +\infty. \quad (3.18)$$

With this mild summability condition (3.18) on $\rho_{\gamma_{\text{per}}}$, we prove in Theorem 3.7 that the highest attainable energy (Fermi level) of electrons for a quasi 1D system in its ground state is always negative. This coincides with the physical reality: the additional summability condition on the density is sufficient to guarantee that the mean-field potential tends to 0 in the \mathbf{r} -direction. If the Fermi level is non-negative, electrons can escape to infinity in the \mathbf{r} -direction, decreasing the energy of the system, hence the system is not at ground state. Furthermore, we are able to characterize the unique minimizer as a spectral projector of the mean-field Hamiltonian. We comment on Assumption 2 in Remark 3.9.

Theorem 3.7 (Properties of the rHF ground state with summability condition on the density). *Assume that Assumption 2 holds for the unique ground state density $\rho_{\gamma_{\text{per}}}$ of the minimization problem (3.17).*

1. **(The integrability of mean-field potential.)** *The mean-field potential*

$$V_{\text{per,sym}} := (\rho_{\gamma_{\text{per}}} - \mu_{\text{per,sym}}) \star_{\Gamma} G$$

belongs to $L^p_{\text{per},x}(\Gamma)$ for $2 < p \leq +\infty$. Moreover, $V_{\text{per,sym}}$ is continuous and tends to zero in the \mathbf{r} -direction.

2. **(Spectral properties of the mean-field Hamiltonian.)** *The mean-field Hamiltonian*

$$H_{\text{per}} = \mathcal{B}^{-1} \left(\int_{\Gamma^*} H_{\text{per},\xi} \frac{d\xi}{2\pi} \right) \mathcal{B} = -\frac{1}{2}\Delta + V_{\text{per,sym}}, \quad H_{\text{per},\xi} := -\frac{1}{2}\Delta_{\xi} + V_{\text{per,sym}}, \quad (3.19)$$

is a self-adjoint operator acting on $L^2(\mathbb{R}^3)$ with domain $H^2(\mathbb{R}^3)$ and form domain $H^1(\mathbb{R}^3)$. There exists $N_H \in \mathbb{N}^$ which can be finite or infinite, and a sequence $\{\lambda_n(\xi)\}_{\xi \in \Gamma^*, 1 \leq n \leq N_H}$ such that*

$$\sigma_{\text{ess}}(H_{\text{per},\xi}) = [0, +\infty), \quad \sigma_{\text{disc}}(H_{\text{per},\xi}) = \bigcup_{1 \leq n \leq N_H} \lambda_n(\xi) \subset [-\|V_{\text{per,sym}}\|_{L^\infty}, 0).$$

Moreover, the following spectral decomposition holds:

$$\sigma(H_{\text{per}}) = \sigma_{\text{ess}}(H_{\text{per}}) = \bigcup_{\xi \in \Gamma^*} \sigma(H_{\text{per},\xi}), \quad \bigcup_{\xi \in \Gamma^*} \sigma_{\text{disc}}(H_{\text{per},\xi}) \subseteq \sigma_{\text{ac}}(H_{\text{per}}). \quad (3.20)$$

In particular, $[0, +\infty) \subset \sigma_{\text{ess}}(H_{\text{per}})$.

3. **(The Fermi level is always negative.)** The energy level counting function

$$F(\kappa) : \kappa \mapsto \frac{1}{|\Gamma^*|} \int_{\Gamma^*} \text{Tr}_{L^2_{\text{per},x}(\Gamma)} (\mathbb{1}_{(-\infty, \kappa]}(H_{\text{per},\xi})) d\xi = \frac{1}{|\Gamma^*|} \sum_{n=1}^{N_H} \int_{\Gamma^*} \mathbb{1}(\lambda_n(\xi) \leq \kappa) d\xi$$

is continuous and non-decreasing on $(-\infty, 0]$. The following inequality always holds:

$$N_H = F(0) \geq \int_{\Gamma} \mu_{\text{per},\text{sym}},$$

which means that there are always enough negative energy levels for the electrons. Moreover, there exists $\epsilon_F < 0$ called Fermi level (chemical potential) such that $F(\epsilon_F) = \int_{\Gamma} \mu_{\text{per},\text{sym}} = Z$, which represents the highest attainable energy level by electrons, and can be interpreted as the Lagrange multiplier associated with the charge neutrality condition (3.16).

4. **(The unique minimizer is a spectral projector.)** The minimizer of the problem (3.17) is unique and satisfies the following self-consistent equation:

$$\gamma_{\text{per}} = \mathbb{1}_{(-\infty, \epsilon_F]}(H_{\text{per}}) = \mathcal{B}^{-1} \left(\int_{\Gamma^*} \gamma_{\text{per},\xi} \frac{d\xi}{2\pi} \right) \mathcal{B}, \quad \gamma_{\text{per},\xi} := \mathbb{1}_{(-\infty, \epsilon_F]}(H_{\text{per},\xi}). \quad (3.21)$$

Furthermore, there exist positive constants C_{ϵ_F} and α_{ϵ_F} which depend on the Fermi level ϵ_F , such that

$$0 \leq \rho_{\gamma_{\text{per}}}(x, \mathbf{r}) \leq C_{\epsilon_F} e^{-\alpha_{\epsilon_F} |\mathbf{r}|}. \quad (3.22)$$

The proof of Theorem 3.7 can be read in Section 3.4.6.

Remark 3.8. As the unit cell of the 1D system in the 3D space is an unbounded domain Γ , the decomposed mean-field Hamiltonian $H_{\text{per},\xi}$ does not have a compact resolvent, which is a significant difference compared to the situation considered in [CLBL01, CDL08a].

Remark 3.9. Let us comment on Assumption 2. Remark that the exponential decay of the density (3.22) implies the summability condition (3.18). However, we were not able to directly prove (3.18). This failure is mainly due to the lack of a priori summability bounds for the density matrices in \mathcal{F}_{Γ} . One might argue that we can add the condition (3.18) to the definition of \mathcal{F}_{Γ} . However, the set \mathcal{F}_{Γ} with the condition (3.18) is not closed for the usual weak-* topology when considering a minimizing sequence of (3.15). Another attempt is to use a Schauder fixed-point algorithm as in [Lio87, CSS⁺09] to prove that (3.21) admits a solution. The most crucial step is to guarantee that there are enough negative bound states to meet the charge neutrality constraint (3.16). The number of bound states is controlled by the decay rate of potentials. With exponentially decaying densities we can show that [BLB00, Lemma 2.5] there exists $C \in \mathbb{R}^+$ such that $|V_{\text{per},\text{sym}}(\cdot, \mathbf{r})| \leq C |\mathbf{r}|^{-1}$. Nevertheless this condition is not sufficient to guarantee that the number of bound states is sufficient, as the critical decay rate for numbers of bound states to be finite or infinite is $-|\mathbf{r}|^{-2}$ [RS78, Theorem XIII.6]. In other words, we do not have a uniform bound over the Fermi level ϵ_F at each fixed-point iteration. On the other hand, the summability condition (3.18) is a sufficient but probably not a necessary condition for the negativity of the Fermi level and the characterization of the minimizers. The main difficulty is to control the decay of the mean-field potential $V_{\text{per},\text{sym}}$ in the \mathbf{r} -direction by just controlling the nuclear density $\mu_{\text{per},\text{sym}}$, given that the Green's function defined in (3.7) has log-growth in the \mathbf{r} -direction. Furthermore, different decay scenarios of $V_{\text{per},\text{sym}}$ in the \mathbf{r} -direction lead to different characterizations of the spectrum of the Hamiltonian H_{per} : if $V_{\text{per},\text{sym}}$ is bounded from below, and positive with log-growth when $|\mathbf{r}| \rightarrow \infty$, one can show that the spectrum of $H_{\text{per},\xi}$ is purely discrete and the spectrum of H_{per} has a band structure. The Fermi level of the system could be positive in this case. We are not able to prove the above statements without Assumption 2.

In order to describe the junction of quasi 1D systems, more specifically to guarantee that the Coulomb energy generated by the perturbative state is finite, the integrability of the mean-field potential provided

in Theorem 3.7 is not sufficient in view of Lemma 3.13 below. In order to make use of this result, let us introduce a class of nuclear densities such that the x -averaged density is rotationally invariant in the \mathbf{r} -direction:

$$\mu_{\text{per,sym}}(x, \mathbf{r}) = \sum_{n \in \mathbb{Z}} Z m_s(x - n, \mathbf{r}),$$

where $m_s(x, \mathbf{r})$ is a non-negative $C_c^\infty(\Gamma)$ function such that $\int_{\mathbb{R}^3} m_s = 1$. Moreover, there exists $m_{\text{sym}} \in C_c^\infty(\mathbb{R})$ such that

$$\forall \mathbf{r} \in \mathbb{R}^2, \quad \int_{-1/2}^{1/2} m_s(x, \mathbf{r}) dx \equiv m_{\text{sym}}(|\mathbf{r}|). \quad (3.23)$$

Lemma 3.10. *Suppose that Assumption 2 holds. Under the symmetry condition (3.23) on the nuclear density μ_{per} , all the results of Theorem 3.7 hold for the minimization problem (3.17). Besides, the mean-field potential $V_{\text{per,sym}}$ belongs to $L_{\text{per},x}^p(\Gamma)$ for $1 < p \leq +\infty$.*

The proof of this lemma can be read in Section 3.4.7. The nuclei of many actual materials can be modeled with a smear nuclear density satisfying the condition (3.23): for instance nanotubes and polymers with rotational symmetry in the \mathbf{r} -direction.

3.3 Mean-field stability for the junction of quasi 1D systems

In this section, we construct a rHF model for the junction of two different quasi 1D periodic systems. The junction system is described by periodic nuclei satisfying the symmetry condition (3.23) with different periodicities and possibly different charges per unit cell, occupying separately the left and right half spaces (i.e., $(-\infty, 0] \times \mathbb{R}^2$ and $(0, +\infty) \times \mathbb{R}^2$), see Fig. 1.7. We do not assume any commensurability of the different periodicities. The junction system is therefore *a priori* no longer periodic, making it impossible to define the periodic rHF energy. Inspired by perturbative approaches when treating infinitely extended systems [HLS05a, HLS05b, HLS07, HLS09a, CDL08a], the idea is to find an appropriate reference state which is close enough to the actual one. Section 3.3.1 gives a mathematical description of the junction system. Section 3.3.2 is devoted to a rigorous construction of a reference Hamiltonian H_χ and a reference one-particle density matrix defined as a spectral projector of H_χ . In Section 3.3.3 we construct a perturbative state, which encodes the non-linear effects due to the electron-electron interaction in the rHF approximation, and associate the ground state energy of this perturbative state to some minimization problem in Section 3.3.4.

3.3.1 Mathematical description of the junction system

Consider two quasi 1D periodic systems with periods $a_L > 0$ and $a_R > 0$. The unit cells are respectively denoted by $\Gamma_L := [-\frac{a_L}{2}, \frac{a_L}{2}) \times \mathbb{R}^2$ and $\Gamma_R := [-\frac{a_R}{2}, \frac{a_R}{2}) \times \mathbb{R}^2$ with their duals $\Gamma_L^* := [-\frac{\pi}{a_L}, \frac{\pi}{a_L})$ and $\Gamma_R^* := [-\frac{\pi}{a_R}, \frac{\pi}{a_R})$. We consider nuclear densities fulfilling the symmetry condition (3.23) and suppose that Assumption 2 holds for the ground state densities of both quasi 1D periodic systems. More precisely, let $m_L(x, \mathbf{r})$ and $m_R(x, \mathbf{r})$ be non-negative C_c^∞ functions with supports respectively in Γ_L and Γ_R such that $\int_{\mathbb{R}^3} m_L = 1$ and $\int_{\mathbb{R}^3} m_R = 1$. Assume that there exist $m_{\text{sym},L}, m_{\text{sym},R} \in C_c^\infty(\mathbb{R})$ such that

$$\forall \mathbf{r} \in \mathbb{R}^2, \quad \int_{-a_L/2}^{a_L/2} m_L(x, \mathbf{r}) dx \equiv m_{\text{sym},L}(|\mathbf{r}|), \quad \int_{-a_R/2}^{a_R/2} m_R(x, \mathbf{r}) dx \equiv m_{\text{sym},R}(|\mathbf{r}|).$$

Denoting by $Z_L, Z_R \in \mathbb{N} \setminus \{0\}$ the total charges of the nuclei per unit cells, the smeared periodic nuclear densities are respectively defined as

$$\mu_{\text{per},L}(x, \mathbf{r}) := \sum_{n \in \mathbb{Z}} Z_L m_L(x - a_L n, \mathbf{r}), \quad \mu_{\text{per},R}(x, \mathbf{r}) := \sum_{n \in \mathbb{Z}} Z_R m_R(x - a_R n, \mathbf{r}). \quad (3.24)$$

The periodic Green's functions with period Γ_L and Γ_R are separately defined as

$$G_{a_L}(x, \mathbf{r}) = a_L^{-1} G\left(\frac{x}{a_L}, \mathbf{r}\right), \quad G_{a_R}(x, \mathbf{r}) = a_R^{-1} G\left(\frac{x}{a_R}, \mathbf{r}\right),$$

where $G(\cdot)$ is the periodic Green's function defined in (3.7). One can easily verify that

$$-\Delta G_{a_L}(x, \mathbf{r}) = 4\pi \sum_{n \in \mathbb{Z}} \delta_{(x, \mathbf{r})=(a_L n, \mathbf{0})} \in \mathcal{S}'(\mathbb{R}^3), \quad -\Delta G_{a_R}(x, \mathbf{r}) = 4\pi \sum_{n \in \mathbb{Z}} \delta_{(x, \mathbf{r})=(a_R n, \mathbf{0})} \in \mathcal{S}'(\mathbb{R}^3).$$

According to the results of Theorem 3.7, the following self-consistent equations uniquely define the ground states density matrices associated with the periodic nuclear densities $\mu_{\text{per},L}$ and $\mu_{\text{per},R}$:

$$\begin{aligned} \gamma_{\text{per},L} &:= \mathbb{1}_{(-\infty, \epsilon_L]}(H_{\text{per},L}), & H_{\text{per},L} &:= -\frac{\Delta}{2} + V_{\text{per},L}, & V_{\text{per},L} &:= (\rho_{\text{per},L} - \mu_{\text{per},L}) \star_{\Gamma_L} G_{a_L}, \\ \gamma_{\text{per},R} &:= \mathbb{1}_{(-\infty, \epsilon_R]}(H_{\text{per},R}), & H_{\text{per},R} &:= -\frac{\Delta}{2} + V_{\text{per},R}, & V_{\text{per},R} &:= (\rho_{\text{per},R} - \mu_{\text{per},R}) \star_{\Gamma_R} G_{a_R}, \end{aligned}$$

where the negative constants ϵ_L and ϵ_R are the Fermi levels of the quasi 1D systems. The junction of the quasi 1D systems are described by considering the following nuclear density configuration (see Fig.1.7):

$$\mu_J(x, \mathbf{r}) := \mathbb{1}_{x \leq 0} \cdot \mu_{\text{per},L}(x, \mathbf{r}) + \mathbb{1}_{x > 0} \cdot \mu_{\text{per},R}(x, \mathbf{r}) + v(x, \mathbf{r}), \quad (3.25)$$

where $v(x, \mathbf{r}) \in L^{6/5}(\mathbb{R}^3)$ describes how the junction switches between the underlying nuclear densities. The assumption $v \in L^{6/5}(\mathbb{R}^3)$ ensures that $D(v, v) < +\infty$. Recall that

$$D(f, g) = \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{f(x)g(y)}{|x-y|} dx dy = \frac{1}{4\pi} \int_{\mathbb{R}^3} \frac{\widehat{f}(k)\widehat{g}(k)}{k^2} dk$$

describes the Coulomb interactions in the whole space. Once one sets the nuclear configuration (3.25), electrons are allowed to move in the 3D space. The *infinite* rHF energy functional for the junction system associated with a test density matrix γ_J formally reads

$$\mathcal{E}(\gamma_J) = \text{Tr} \left(-\frac{1}{2} \Delta \gamma_J \right) + \frac{1}{2} D(\rho_{\gamma_J} - \mu_J, \rho_{\gamma_J} - \mu_J). \quad (3.26)$$

Let us also introduce the Coulomb space \mathcal{C} and its dual \mathcal{C}' (Beppo-Levi space [CDL08a]):

$$\mathcal{C} := \{\rho \in \mathcal{S}'(\mathbb{R}^3) \mid \widehat{\rho} \in L^1_{\text{loc}}(\mathbb{R}^3), D(\rho, \rho) < \infty\}, \quad \mathcal{C}' := \{V \in L^6(\mathbb{R}^3) \mid \nabla V \in (L^2(\mathbb{R}^3))^3\}. \quad (3.27)$$

Remark that the ground state energy of the junction system, if it exists, is infinite and there is no period-

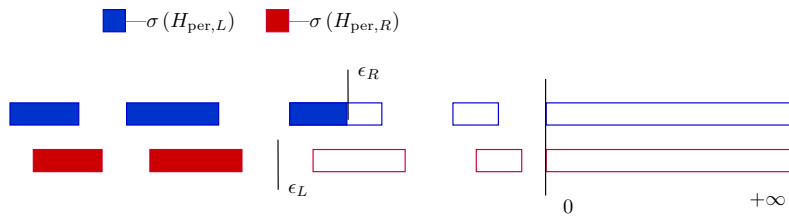
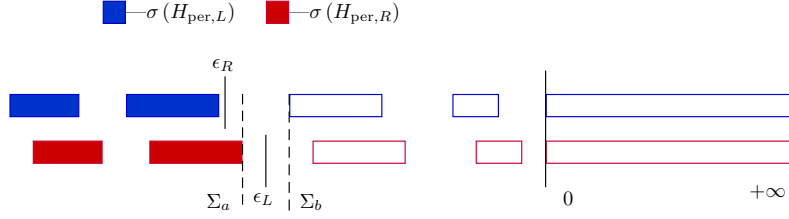


Figure 3.1: Spectrum of $H_{\text{per},L}, H_{\text{per},R}$ in the non-equilibrium regime.

icity in this system, hence usual techniques which essentially consist in considering the energy per unit volume [CLBL01, CDL08a] are not applicable. We next define a reference system such that the difference between the junction system and the reference can be considered as a perturbation. This perturbative approach has been used in [HLS07, HLS05a, HLS09a, CDL08a] in various contexts. The next section is devoted to the rigorous mathematical construction of the reference state and its rHF energy functional.

Figure 3.2: Spectrum of $H_{\text{per},L}$, $H_{\text{per},R}$ in the equilibrium regime.

3.3.2 Reference state for the junction system

In this section, we construct a reference Hamiltonian obtained by a linear combination of the periodic mean-field potentials $V_{\text{per},L}$ and $V_{\text{per},R}$. We prove the validity of this approach by showing that the density generated by this reference state is close to the linear combination of the periodic densities $\rho_{\text{per},L}$ and $\rho_{\text{per},R}$.

Hamiltonian of the reference state. We introduce a class of smoothed cut-off functions. For $\mathbf{x} \in \mathbb{R}^3$, consider:

$$\mathcal{X} := \left\{ \chi \in C^2(\mathbb{R}^3) \mid 0 \leq \chi \leq 1; \chi(\mathbf{x}) = 1 \text{ if } \mathbf{x} \in \left(-\infty, -\frac{a_L}{2}\right] \times \mathbb{R}^2; \chi(\mathbf{x}) = 0 \text{ if } \mathbf{x} \in \left[\frac{a_R}{2}, +\infty\right) \times \mathbb{R}^2 \right\}. \quad (3.28)$$

Fix $\chi \in \mathcal{X}$, let us introduce a reference potential

$$V_\chi := \chi^2 V_{\text{per},L} + (1 - \chi^2) V_{\text{per},R}.$$

We will show in Section 3.3.4 that the choice of $\chi \in \mathcal{X}$ is irrelevant. By Theorem 3.7 and Lemma 3.10 we know that V_χ belongs to $L^p_{\text{loc}}(\mathbb{R}, L^p(\mathbb{R}^2))$ for $1 < p \leq \infty$, is continuous in all directions and tends to zero in the r -direction. By the Kato–Rellich theorem (see for example [Hel13, Theorem 9.10]), there exists a unique self-adjoint operator

$$H_\chi := -\frac{1}{2}\Delta + V_\chi \quad (3.29)$$

on $L^2(\mathbb{R}^3)$ with domain $H^2(\mathbb{R}^3)$ and form domain $H^1(\mathbb{R}^3)$. We next show that the essential spectrum of the reference Hamiltonian H_χ is the union of the essential spectra of $H_{\text{per},L}$ and $H_{\text{per},R}$, which implies that the reference system does not change essentially the unions of possible energy levels of quasi periodic systems, and that there are no surface states which propagate along the junction surface in the r -direction. Note that this is *a priori* not obvious as the cut-off function χ is r -translation invariant (hence not compact), therefore scattering states may occur at the junction surface and escape to infinity in the r -direction. Standard techniques in scattering theory to prove this statement, such as Dirichlet decoupling [DS76, HKSV15], are not applicable in our situation since the junction surface is not compact.

Proposition 3.11 (Spectral properties of the reference state H_χ). *For any $\chi \in \mathcal{X}$, the essential spectrum of H_χ defined in (3.29) satisfies*

$$\sigma_{\text{ess}}(H_\chi) = \sigma_{\text{ess}}(H_{\text{per},L}) \cup \sigma_{\text{ess}}(H_{\text{per},R}).$$

In particular, $[0, +\infty) \subset \sigma_{\text{ess}}(H_\chi)$ and $\sigma_{\text{ess}}(H_\chi)$ does not depend on the shape of the cut-off function $\chi \in \mathcal{X}$ defined in (3.28).

The proof relies on an explicit construction of Weyl sequences associated with H_χ (see Section 3.4.8). Remark that Proposition 3.11 also implies that the reference system essentially preserves the scattering channels of the underlying quasi 1D systems, since the scattering involves the purely absolutely continuous spectrum of a Hamiltonian (see for example [EF07, BJLP16a, BJLP16b]). However, this does not exclude the existence of embedded eigenvalues in the essential spectrum, which may cause additional scattering channels [RR03, RR04]. We prove in Corollary 3.16 that the results in Proposition 3.11 still hold for the nonlinear junction.

Reference state as a spectral projector. Before constructing the reference state, let us discuss different regimes for junction system. From Theorem 3.7 we know that the chemical potentials (Fermi levels) ϵ_L and ϵ_R are negative. Introduce the energy interval

$$I_{\epsilon_F} := [\min(\epsilon_L, \epsilon_R), \max(\epsilon_L, \epsilon_R)].$$

In view of Proposition 3.11, assume that the essential spectrum of H_χ below 0 is purely absolutely continuous, the non-equilibrium regime (Fig. 3.1) corresponds to

$$\sigma_{\text{ac}}(H_\chi) \cap I_{\epsilon_F} \neq \emptyset.$$

In this regime, steady state currents occur and the Landauer-Büttiker conductance can be calculated [BJLP15, BJLP16a, BJLP16b]. When $\mu_{\text{per},L}$ and $\mu_{\text{per},R}$ are identical, the junction system becomes periodic with different chemical potentials ϵ_L and ϵ_R on the left and right half lines. In this case the Thouless conductance [BJLP15] can be defined and it is given by

$$C_T \frac{|\sigma_{\text{ac}}(H_\chi) \cap I_{\epsilon_F}|}{|I_{\epsilon_F}|} > 0,$$

for some positive constant C_T . However it is not the aim of this article to discuss steady state currents for non-equilibrium systems. We instead consider the equilibrium regime (see Fig. 3.2) with the following assumption.

Assumption 3. *The chemical potential ϵ_L and ϵ_R are in a common spectral gap (Σ_a, Σ_b) (equilibrium regime, see Fig. 3.2), where Σ_a is the maximum of the filled bands of $H_{\text{per},L}$ and $H_{\text{per},R}$, and Σ_b is the minimum of the unfilled bands of $H_{\text{per},L}$ and $H_{\text{per},R}$.*

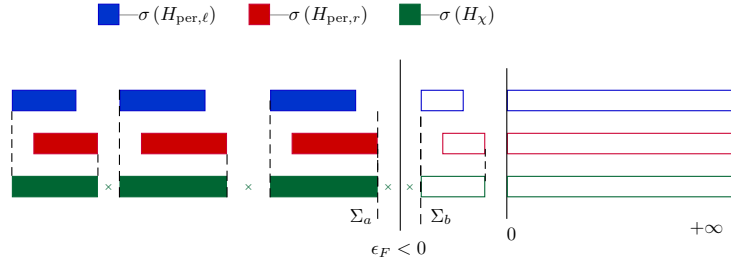


Figure 3.3: Spectrum of $H_{\text{per},L}$, $H_{\text{per},R}$ and H_χ below 0.

Assumption 3 guarantees that the Fermi level of the junction system lies in a spectral gap of H_χ in view of Proposition 3.11, which is a common hypothesis [CDL08a, HLS05a, HLS09a] for 3D periodic insulating and semi-conducting systems. We make this assumption for simplicity. Remark that with approaches proposed in [FLLS11, FLLS13, CCS18] it is possible to extend the results to metallic systems provided that the junction system is in its ground state and no steady state current occurs.

Let us without loss of generality choose the Fermi level $\epsilon_F = \max(\epsilon_L, \epsilon_R) = \sup I_{\epsilon_F}$ and define the reference state γ_χ as the spectral projector associated with the states of H_χ below ϵ_F :

$$\gamma_\chi := \mathbb{1}_{(-\infty, \epsilon_F)}(H_\chi). \quad (3.30)$$

Remark that H_χ can have discrete spectrum in the gap (Σ_a, Σ_b) , with eigenvalues possibly accumulating at Σ_a and Σ_b , and ϵ_F can also be an eigenvalue of H_χ . The definition of (3.30) however excludes the possible bound states with energy ϵ_F .

The following proposition shows that the density ρ_χ of γ_χ is well defined in $L^1_{\text{loc}}(\mathbb{R}^3)$, and is close to the linear combination of the periodic densities $\rho_{\text{per},L}$ and $\rho_{\text{per},R}$, the difference decaying exponentially fast in the x -direction as $|x| \rightarrow \infty$.

Proposition 3.12 (Exponential decay of density). *Under Assumption 3, the spectral projector γ_χ is locally trace class, so that its density ρ_χ is well defined in $L^1_{\text{loc}}(\mathbb{R}^3)$. Moreover,*

$$\chi^2 \rho_{\text{per},L} + (1 - \chi^2) \rho_{\text{per},R} - \rho_\chi \in L^p(\mathbb{R}^3) \text{ for } 1 < p \leq 2.$$

Furthermore, denote by w_a the characteristic function of the unit cube centered at $a \in \mathbb{R}^3$. There exist positive constants C and t such that for all

$$\alpha = (\alpha_x, 0, 0) \in \mathbb{R}^3, \text{ with either } \text{supp}(w_\alpha) \subset (-\infty, a_L/2] \times \mathbb{R}^2 \text{ or } \text{supp}(w_\alpha) \subset [a_R/2, +\infty) \times \mathbb{R}^2,$$

it holds,

$$\int_{\mathbb{R}^3} |w_\alpha (\chi^2 \rho_{\text{per},L} + (1 - \chi^2) \rho_{\text{per},R} - \rho_\chi) w_\alpha| \leq C e^{-t|\alpha|}.$$

The proof can be read in Section 3.4.10.

Fictitious nuclear density of the reference state. The density ρ_χ associated with γ_χ is fixed once the Fermi level ϵ_F is chosen. We can therefore define a fictitious nuclear density μ_χ by imposing that the total electronic density $\rho_\chi - \mu_\chi$ generates the potential V_χ . The fictitious nuclear density μ_χ is given by

$$-\Delta V_\chi = 4\pi (\rho_\chi - \mu_\chi), \quad \mu_\chi := \rho_\chi - (\chi^2 (\rho_{\text{per},L} - \mu_{\text{per},L}) + (1 - \chi^2) (\rho_{\text{per},R} - \mu_{\text{per},R}) + \eta_\chi), \quad (3.31)$$

where η_χ has compact support in the x -direction:

$$\eta_\chi := -\frac{1}{4\pi} (\partial_x^2 (\chi^2) (V_{\text{per},L} - V_{\text{per},R}) + 2\partial_x (\chi^2) \partial_x (V_{\text{per},L} - V_{\text{per},R})). \quad (3.32)$$

Let us emphasize that the Poisson's equation (3.31) is defined on the whole space \mathbb{R}^3 .

The nuclear density of the junction is a fictitious nuclear density plus a perturbation. Once we have defined fictitious nuclear density, we can treat the difference between the real nuclear density of the junction system μ_J and the fictitious nuclear density μ_χ as a perturbative nuclear density. By doing so we can define a finite renormalized energy with respect to the perturbative nuclear density. Note that this idea is similar to the definition of the defect state in [CDL08a] for defects in crystals, and the polarization of the vacuum in the Bogoliubov–Dirac–Fock model [HLS07, HLS05a, HLS09a]. Introduce

$$\nu_\chi := \mu_J - \mu_\chi = (\mathbb{1}_{x \leq 0} - \chi^2) (\mu_{\text{per},L} - \mu_{\text{per},R}) + (\chi^2 \rho_{\text{per},L} + (1 - \chi^2) \rho_{\text{per},R} - \rho_\chi) + \eta_\chi + v. \quad (3.33)$$

In order to guarantee that the perturbative state has a finite Coulomb energy, we need $D(\nu_\chi, \nu_\chi) < +\infty$. A sufficient condition is that ν_χ belongs to $L^{6/5}(\mathbb{R}^3)$. This motivates the following L^p -estimate on η_χ .

Lemma 3.13. *The function η_χ defined in (3.32) belongs to $L^p(\mathbb{R}^3)$ for $1 < p < 6$.*

The proof can be read in Section 3.4.11. In view of Lemma 3.13 and Proposition 3.12, together with the fact that $(\mathbb{1}_{x \leq 0} - \chi^2) (\mu_{\text{per},L} - \mu_{\text{per},R})$ has compact support and v belongs to $L^{6/5}(\mathbb{R}^3)$, it is easy to see that ν_χ belongs to $L^{6/5}(\mathbb{R}^3)$, and hence to the Coulomb space \mathcal{C} defined in (3.27). This means that the perturbative state generated by the nuclear density ν_χ has finite Coulomb energy.

Remark 3.14. *Remark that the integrability of $V_{\text{per},\text{sym}}$ provided by Lemma 3.10 is crucial to deduce Lemma 3.13.*

3.3.3 Definition of the perturbative state

In this section we define a perturbative state associated with the perturbative density ν_χ following the ideas developed in [CDL08a]. We formally derive the rHF energy difference between the junction state γ_J and the reference state γ_χ by writing $\gamma_J = \gamma_\chi + Q_\chi$ with Q_χ a trial density state. In view of (3.26), we formally have

$$\begin{aligned}
\mathcal{E}(\gamma_J) - \mathcal{E}(\gamma_\chi) &\stackrel{\text{formally}}{=} \text{Tr} \left(-\frac{1}{2} \Delta (\gamma_\chi + Q_\chi) \right) + \frac{1}{2} D(\rho_J - \mu_J, \rho_J - \mu_J) \\
&\quad - \text{Tr} \left(-\frac{1}{2} \Delta \gamma_\chi \right) - \frac{1}{2} D(\rho_\chi - \mu_\chi, \rho_\chi - \mu_\chi) \\
&= \text{Tr} \left(-\frac{1}{2} \Delta Q_\chi \right) + D(\rho_\chi - \mu_\chi, \rho_{Q_\chi}) - D(\rho_{Q_\chi}, \nu_\chi) + \frac{1}{2} D(\rho_{Q_\chi}, \rho_{Q_\chi}) \\
&\quad - D(\rho_\chi - \mu_\chi, \nu_\chi) + \frac{1}{2} D(\nu_\chi, \nu_\chi) \\
&= \text{Tr} (H_\chi Q_\chi) - D(\rho_{Q_\chi}, \nu_\chi) + \frac{1}{2} D(\rho_{Q_\chi}, \rho_{Q_\chi}) - D(\rho_\chi - \mu_\chi, \nu_\chi) + \frac{1}{2} D(\nu_\chi, \nu_\chi).
\end{aligned} \tag{3.34}$$

We next give a mathematical definition of the terms in the last equality of (3.34). We expect Q_χ to be a perturbation of the reference state γ_χ . More precisely, we expect Q_χ to be Hilbert-Schmidt. Moreover, we also expect the kinetic energy of Q_χ to be finite. Let Π be an orthogonal projector on the Hilbert space \mathfrak{H} such that both Π and $\Pi^\perp := 1 - \Pi$ have infinite ranks. A self-adjoint compact operator A on \mathfrak{H} is said to be Π -trace class if $A \in \mathfrak{S}_2(\mathfrak{H})$ and both $\Pi A \Pi$ and $\Pi^\perp A \Pi^\perp$ are in $\mathfrak{S}_1(\mathfrak{H})$. For an operator A we define its Π -trace as

$$\text{Tr}_\Pi(A) := \text{Tr}(\Pi A \Pi) + \text{Tr}(\Pi^\perp A \Pi^\perp),$$

and denote by $\mathfrak{S}_1^\Pi(\mathfrak{H})$ the associated set of Π -trace class operators. Since the reference state γ_χ defined in (3.30) is an orthogonal projector on $L^2(\mathbb{R}^3)$, we can define associated γ_χ -trace class operators. For any trial density matrix Q_χ , let us denote by $Q_\chi^{++} := \gamma_\chi^\perp Q_\chi \gamma_\chi^\perp$ and $Q_\chi^{--} := \gamma_\chi Q_\chi \gamma_\chi$, and introduce a Banach space of operators with finite γ_χ -trace and finite kinetic energy as follows:

$$\begin{aligned}
\mathcal{Q}_\chi := \{ Q_\chi \in \mathfrak{S}_1^{\gamma_\chi}(L^2(\mathbb{R}^3)) \mid Q_\chi^* = Q_\chi, \|\nabla|Q_\chi\| \in \mathfrak{S}_2(L^2(\mathbb{R}^3)), \\
\|\nabla|Q_\chi^{++}\| \in \mathfrak{S}_1(L^2(\mathbb{R}^3)), \|\nabla|Q_\chi^{--}\| \in \mathfrak{S}_1(L^2(\mathbb{R}^3)) \},
\end{aligned}$$

equipped with its natural norm

$$\|Q_\chi\|_{\mathcal{Q}_\chi} := \|Q_\chi\|_{\mathfrak{S}_2} + \|Q_\chi^{++}\|_{\mathfrak{S}_1} + \|Q_\chi^{--}\|_{\mathfrak{S}_1} + \|\nabla|Q_\chi\|_{\mathfrak{S}_2} + \|\nabla|Q_\chi^{++}\|_{\mathfrak{S}_1} + \|\nabla|Q_\chi^{--}\|_{\mathfrak{S}_1}.$$

By construction $\text{Tr}_{\gamma_\chi}(Q_\chi) = \text{Tr}(Q_\chi^{++}) + \text{Tr}(Q_\chi^{--})$. For Q to be an admissible perturbation of the reference state γ_χ , Pauli's principle requires that $0 \leq \gamma_\chi + Q_\chi \leq 1$. Let us introduce the following convex set of admissible perturbative states:

$$\mathcal{K}_\chi := \{ Q_\chi \in \mathcal{Q}_\chi \mid -\gamma_\chi \leq Q_\chi \leq 1 - \gamma_\chi \}.$$

Remark that \mathcal{K}_χ is not empty since it contains at least 0. Note also that \mathcal{K}_χ is the convex hull of states in \mathcal{Q}_χ of the special form $\gamma - \gamma_\chi$, where γ is an orthogonal projector [CDL08a]. Furthermore, for any $Q_\chi \in \mathcal{K}_\chi$ a simple algebraic calculation shows that

$$Q_\chi^{++} \geq 0, \quad Q_\chi^{--} \leq 0, \quad 0 \leq Q_\chi^2 \leq Q_\chi^{++} - Q_\chi^{--}.$$

As mentioned in the previous section, the Fermi level ϵ_F can be an eigenvalue of H_χ . Consider $N \in \mathbb{N}^*$ such that $\epsilon_F \in (\Sigma_{N,\chi}, \Sigma_{N+1,\chi}]$, where $\Sigma_{N,\chi} < \Sigma_{N+1,\chi}$ are two eigenvalues of H_χ in the gap (Σ_a, Σ_b) , and let $\Sigma_{N,\chi} = \Sigma_a$ and $\Sigma_{N+1,\chi} = \Sigma_b$ whenever there is no such element. For any $\kappa \in (\Sigma_{N,\chi}, \epsilon_F)$, let us introduce the following rHF kinetic energy of a state $Q_\chi \in \mathcal{Q}_\chi$:

$$\text{Tr}_{\gamma_\chi}(H_\chi Q_\chi) := \text{Tr} \left(|H_\chi - \kappa|^{1/2} (Q_\chi^{++} - Q_\chi^{--}) |H_\chi - \kappa|^{1/2} \right) + \kappa \text{Tr}_{\gamma_\chi}(Q_\chi).$$

By [CDL08a, Corollary 1], the above expression is independent of $\kappa \in (\Sigma_{N,\chi}, \epsilon_F)$. In view of the last line of (3.34) we introduce the following minimization problem

$$E_{\kappa,\chi} = \inf_{Q_\chi \in \mathcal{K}_\chi} \{ \mathcal{E}_\chi(Q_\chi) - \kappa \text{Tr}_{\gamma_\chi}(Q_\chi) \}, \quad (3.35)$$

where

$$\mathcal{E}_\chi(Q_\chi) := \text{Tr}_{\gamma_\chi}(H_\chi Q_\chi) - D(\rho_{Q_\chi}, \nu_\chi) + \frac{1}{2} D(\rho_{Q_\chi}, \rho_{Q_\chi}). \quad (3.36)$$

3.3.4 Properties of the junction system

The following result shows that the minimization problem (3.35) is well posed and admits minimizers.

Proposition 3.15. (Existence of the perturbative ground state) *Assume that Assumption 3 holds. Then there exist minimizers for the problem (3.35). There may be several minimizers, but they all share the same density. Moreover, any minimizer \overline{Q}_χ of (3.35) satisfies the following self-consistent equation:*

$$\begin{cases} \overline{Q}_\chi = \mathbb{1}_{(-\infty, \epsilon_F)}(H_{\overline{Q}_\chi}) - \gamma_\chi + \delta_\chi, \\ H_{\overline{Q}_\chi} = H_\chi + (\rho_{\overline{Q}_\chi} - \nu_\chi) \star |\cdot|^{-1}, \end{cases} \quad (3.37)$$

where δ_χ is a finite-rank self-adjoint operator satisfying $0 \leq \delta_\chi \leq 1$ and $\text{Ran}(\delta_\chi) \subseteq \text{Ker}(H_{\overline{Q}_\chi} - \epsilon_F)$.

The proof is a direct adaptation of several results obtained in [CDL08a], see a short summary in Section 3.4.12 for completeness. Remark that $(\rho_{\overline{Q}_\chi} - \nu_\chi) \star |\cdot|^{-1} \in L^6(\mathbb{R}^3)$ by [CS12, Lemma 16], therefore $(1 - \Delta)^{-1}(\rho_{\overline{Q}_\chi} - \nu_\chi) \star |\cdot|^{-1}$ belongs to \mathfrak{S}_6 by the Kato–Seiler–Simon inequality (3.39), hence $(\rho_{\overline{Q}_\chi} - \nu_\chi) \star |\cdot|^{-1}$ is $-\Delta$ -compact hence H_χ -compact by the boundedness of V_χ , leaving the essential spectrum unchanged. Therefore in view of Proposition 3.11, the following corollary holds.

Corollary 3.16. *For any $\chi \in \mathcal{X}$, and $H_{\overline{Q}_\chi}$ solution of (3.37), it holds*

$$\sigma_{\text{ess}}(H_{\overline{Q}_\chi}) = \sigma_{\text{ess}}(H_{\text{per},L}) \cup \sigma_{\text{ess}}(H_{\text{per},R}), \quad \sigma_{\text{ess}}(H_{\overline{Q}_\chi}) \cap (-\infty, 0] \subseteq \sigma_{\text{ac}}(H_{\overline{Q}_\chi}).$$

In particular, $[0, +\infty) \subset \sigma_{\text{ess}}(H_{\overline{Q}_\chi})$ and $\sigma_{\text{ess}}(H_{\overline{Q}_\chi})$ does not depend on the shape of the cut-off function $\chi \in \mathcal{X}$ defined in (3.28).

The result of Proposition 3.15 can be interpreted as follows: given a cut-off function χ belonging to the class \mathcal{X} defined in (3.28), we can construct a reference state γ_χ and a perturbative ground state \overline{Q}_χ , the sum of which forms the ground state of the junction system. However it is artificial to introduce cut-off functions χ since there are infinitely many possible choices. In view of (3.25), the ground state of the junction system should not depend on the choice of cut-off functions. The following theorem shows that the electronic density of the junction system is indeed independent of the choice of the cut-off function χ .

Theorem 3.17 (Independence of the reference state and uniqueness of ground state density). *The ground state density of the junction system with nuclear density defined in (3.25) under the rHF description is independent of the choice of the cut-off function $\chi \in \mathcal{X}$, i.e., the total electronic density $\rho_J = \rho_\chi + \rho_{Q_\chi}$ is independent of χ , where ρ_χ is the density associated with the spectral projector γ_χ defined in (3.30), and ρ_{Q_χ} is the unique density associated with the solution Q_χ of the minimization problem (3.37).*

The proof can be read in Section 3.4.13. Theorem 3.17 and Proposition 3.15 together imply that

Corollary 3.18. *The ground state of the junction system (3.25) is of the form*

$$\begin{aligned} \mathbb{1}_{(-\infty, \epsilon_F)}(H_\chi + (\rho_{\overline{Q}_\chi} - \nu_\chi) \star |\cdot|^{-1}) + \delta_\chi, \quad 0 \leq \delta_\chi \leq 1, \\ \text{Ran}(\delta_\chi) \subseteq \text{Ker}(H_\chi + (\rho_{\overline{Q}_\chi} - \nu_\chi) \star |\cdot|^{-1} - \epsilon_F), \end{aligned}$$

and its density is independent of the choice of χ .

3.3.5 Perspective: extension to junctions of 2D materials in \mathbb{R}^2

Assume that the periods of 2D materials (with 2D Coulomb interactions, note that we consider a \mathbb{R}^2 plane in \mathbb{R}^3) in \mathbb{R}^2 are commensurate in the y -direction with period $L_y > 0$ but not necessarily commensurate in the x -direction, see Fig 3.4 for an illustration. Remark that semi-infinite 2D materials are special cases of this, as they can be modeled as a junction with vacuum occupying the other half space. Following ideas

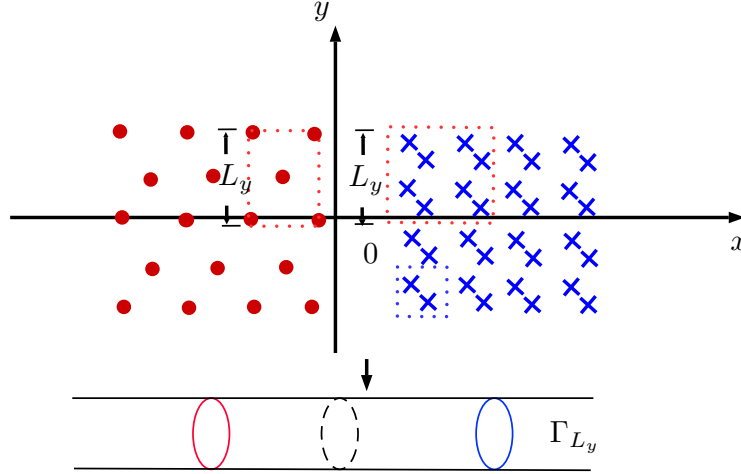


Figure 3.4: Junction of 2D materials which are commensurate in the y -direction. The unit cell of the total junction system is a cylinder Γ_{L_y} .

similar to the one developed in Section 3.2.1 and writing $\Gamma_{L_y} := \mathbb{R} \times [-L_y/2, L_y/2)$ and $\Gamma_{L_y}^* = \left[-\frac{\pi}{L_y}, \frac{\pi}{L_y}\right)$, the following decomposition holds:

$$L^2(\mathbb{R}^2) = \int_{\Gamma_{L_y}^*}^{\oplus} L_{\text{per},y}^2(\Gamma_{L_y}) dq.$$

The partial Bloch transform \mathcal{B}_y can be defined from the dense subspace $C_c^\infty(\mathbb{R}^2)$ of $L^2(\mathbb{R}^2)$ to $L^2\left(\Gamma_{L_y}^*; L_{\text{per},y}^2(\Gamma_{L_y})\right)$ as

$$\forall (x, y) \in \Gamma_{L_y}, \forall q \in \Gamma_{L_y}^*, \quad (\mathcal{B}_y \phi)_q(x, y) := \sum_{k \in L_y \mathbb{Z}} e^{-i(y+k)q} \phi(x, y+k).$$

Its inverse is given by

$$\forall k \in L_y \mathbb{Z}, \text{ for a.a. } (x, y) \in \Gamma_{L_y}, \quad (\mathcal{B}_y^{-1} f)_\bullet(x, y+k) := \frac{1}{|\Gamma_{L_y}^*|} \int_{\Gamma_{L_y}^*} e^{i(k+x)q} f_q(x, y) dq.$$

Under \mathcal{B}_y , the (negative) Laplace operator on $L^2(\mathbb{R}^2)$ is decomposed as

$$-\frac{1}{2}\Delta = \mathcal{B}_y^{-1} \left(\frac{1}{|\Gamma_{L_y}^*|} \int_{\Gamma_{L_y}^*}^{\oplus} -\frac{1}{2}\Delta_q dq \right) \mathcal{B}_y, \quad -\Delta_q = -\partial_x^2 + (i\partial_y - q)^2,$$

with $-\Delta_q$ acting on $L_{\text{per},y}^2(\Gamma_{L_y})$. Given $q \in \Gamma_{L_y}^*$, the junction problem follows exactly the same construction as in Section 3.3 by replacing the space from \mathbb{R}^3 to the cylinder Γ_{L_y} . The latter construction is much simpler as the cylinder is compact in its radius direction, this implies that the cut-off functions used to construct the reference Hamiltonian are periodic in the y -direction. Therefore the cut-off functions are compact in the radius direction, and the reference Hamiltonian has compact resolvent. This simplifies the proofs of Proposition 3.11. With a little bit of abuse, let us still use the same notation as in Section 3.3. We

can construct a reference Hamiltonian H_χ and spectral projector γ_χ which is $L_y\mathbb{Z}$ -translation invariant in the y -direction with χ being $L_y\mathbb{Z}$ -periodic in the y -direction. Moreover, H_χ is decomposed by \mathcal{B}_y

$$H_\chi = \mathcal{B}_y^{-1} \left(\frac{1}{|\Gamma_{L_y}^*|} \int_{\Gamma_{L_y}^*}^\oplus H_{\chi,q} dq \right) \mathcal{B}_y, \quad H_{\chi,q} = -\partial_x^2 + (i\partial_y - q)^2 + V_\chi,$$

$$\gamma_\chi = \mathcal{B}_y^{-1} \left(\frac{1}{|\Gamma_{L_y}^*|} \int_{\Gamma_{L_y}^*}^\oplus \gamma_{\chi,q} dq \right) \mathcal{B}_y, \quad \gamma_{\chi,q} = \mathbb{1}_{(-\infty, \epsilon_F)}(H_{\chi,q}).$$

By a direction adaptation of Proposition 3.11 we obtain that

$$\forall q \in \Gamma_{L_y}^*, \quad \sigma_{\text{ess}}(H_{\chi,q}) = \sigma_{\text{ess}}(H_{\text{per},L,q}) \bigcup \sigma_{\text{ess}}(H_{\text{per},R,q}),$$

where $H_{\text{per},L,q}$ (resp. $H_{\text{per},R,q}$) are the \mathcal{B}_y -decomposed operators of $H_{\text{per},L}$ (resp. $H_{\text{per},R}$). Remark that by [RS78, Theorem XIII.85]

$$\sigma_{\text{ess}}(H_{\text{per},L}) \bigcup \sigma_{\text{ess}}(H_{\text{per},R}) \subseteq \sigma_{\text{ess}}(H_\chi). \quad (3.38)$$

Remark that an equality of the above expression seems physically dubious due to the presence of edge states propagating alongside the junction surface. The perturbative state Q should also possess the same periodicity in the y -direction as H_χ . Using the same techniques in [CCS18] when defining extended defects in the Fermi sea, we can define a new class of perturbations $Q = \mathcal{B}_y^{-1} \left(\int_{\Gamma_{L_y}^*} Q_q \frac{dq}{2\pi} \right) \mathcal{B}_y$ in a suitable class and follow the same procedure as in the quasi 1D case to prove the existence of mean-field ground state.

3.4 Proofs of the results

In order to simplify the notation, in Section 3.4.1 to 3.4.11 when treating the quasi 1D periodic system we denote by \mathfrak{S}_p the Schatten class $\mathfrak{S}_p(L_{\text{per},x}^2(\Gamma))$ for $1 \leq p \leq +\infty$. Unless otherwise specified, starting from Section 3.4.8 we use \mathfrak{S}_p instead of $\mathfrak{S}_p(L^2(\mathbb{R}^3))$ for the proofs of the junction system.

First of all, let us recall the following Kato–Seiler–Simon (KSS) inequality:

Lemma 3.19. ([SS75, Lemma 2.1]) *Let $2 \leq p \leq \infty$. For g, f belonging to $L^p(\mathbb{R}^3)$, the following inequality holds:*

$$\|f(-i\nabla)g(x)\|_{\mathfrak{S}_p(L^2(\mathbb{R}^3))} \leq (2\pi)^{-3/p} \|g\|_{L^p(\mathbb{R}^3)} \|f\|_{L^p(\mathbb{R}^3)}. \quad (3.39)$$

3.4.1 Proof of Lemma 3.1

The proof is an easy adaptation of the proof of the classical Kato–Seiler–Simon inequality (3.39) by replacing the Fourier transform with the mixed Fourier transform \mathcal{F} . Let us prove separately (3.6) for $p = 2$ and $p = +\infty$. The conclusion then follows by an interpolation argument. We use the following kernel representation during the proofs. For $\mathbf{x} = (x, \mathbf{r})$ and $\mathbf{y} = (y, \mathbf{r}')$ belonging to Γ , symbolic calculus shows that the Schwartz kernel $K_{f,\xi}((x, \mathbf{r}), (y, \mathbf{r}'))$ of the operator $f(-i\nabla_\xi)$ acting on $L_{\text{per},x}^2(\Gamma)$ formally reads

$$\begin{aligned} K_{f,\xi}((x, \mathbf{r}), (y, \mathbf{r}')) &= \frac{1}{2\pi} (\mathcal{F}^{-1} \circ \tau_{-\xi}^x f)((x - y), (\mathbf{r} - \mathbf{r}')) \\ &= \frac{1}{4\pi^2} \sum_{n \in \mathbb{Z}} \int_{\mathbb{R}^2} e^{i(2\pi n(x-y) + \mathbf{k} \cdot (\mathbf{r} - \mathbf{r}'))} f(2\pi n + \xi, \mathbf{k}) d\mathbf{k}. \end{aligned} \quad (3.40)$$

Let $p = 2$. In view of the isometry identity (3.4), the convolution equality (3.5) and the kernel representation (3.40), the following estimate holds

$$\begin{aligned} \|f(-i\nabla_\xi)g\|_{\mathfrak{S}_2}^2 &= \frac{1}{4\pi^2} \int_{\Gamma \times \Gamma} |(\mathcal{F}^{-1} \circ \tau_{-\xi}^x f)(\mathbf{x} - \mathbf{y})g(\mathbf{y})|^2 d\mathbf{x} d\mathbf{y} \\ &\leq \frac{1}{4\pi^2} \int_{\Gamma} |g(\mathbf{y})|^2 \left(\int_{\Gamma} |(\mathcal{F}^{-1} \circ \tau_{-\xi}^x f)(\mathbf{x} - \mathbf{y})|^2 d\mathbf{x} \right) d\mathbf{y} \\ &= \frac{1}{4\pi^2} \int_{\Gamma} |g(\mathbf{y})|^2 \sum_{n \in \mathbb{Z}} \left(\int_{\mathbb{R}^2} |f(2\pi n + \xi, \mathbf{k})|^2 d\mathbf{k} \right) d\mathbf{y} \\ &= \frac{1}{4\pi^2} \|g\|_{L_{\text{per},x}^2(\Gamma)}^2 \sum_{n \in \mathbb{Z}} \|f(2\pi n + \xi, \cdot)\|_{L^2(\mathbb{R}^2)}^2, \end{aligned}$$

which proves (3.6) for $p = 2$. For $p = +\infty$, it suffices to prove that for any $\phi \in L_{\text{per},x}^2(\Gamma)$,

$$\|f(-i\nabla_\xi)g\phi\|_{L_{\text{per},x}^2(\Gamma)} \leq \|g\|_{L_{\text{per},x}^\infty(\Gamma)} \sup_{n \in \mathbb{Z}} \|f((2\pi n + \xi, \cdot))\|_{L^\infty(\mathbb{R}^2)} \|\phi\|_{L_{\text{per},x}^2(\Gamma)}.$$

By arguments similar to those used when $p = 2$, we obtain by the isometry (3.4) that

$$\begin{aligned} \|f(-i\nabla_\xi)g\phi\|_{L_{\text{per},x}^2(\Gamma)}^2 &= \sum_{n \in \mathbb{Z}} \int_{\mathbb{R}^2} |\mathcal{F}(g\phi)(n, \mathbf{k})|^2 \left| f((2\pi n + \xi)^2 + \mathbf{k}^2) \right|^2 d\mathbf{k} \\ &\leq \sup_{n \in \mathbb{Z}} \|f((2\pi n + \xi, \cdot))\|_{L^\infty(\mathbb{R}^2)}^2 \|g\phi\|_{L_{\text{per},x}^2(\Gamma)}^2 \\ &\leq \|g\|_{L_{\text{per},x}^\infty(\Gamma)}^2 \sup_{n \in \mathbb{Z}} \|f((2\pi n + \xi, \cdot))\|_{L^\infty(\mathbb{R}^2)}^2 \|\phi\|_{L_{\text{per},x}^2(\Gamma)}^2, \end{aligned}$$

which is (3.6) for $p = +\infty$. Therefore, following the same interpolation arguments as in [SS75, Lemma 2.1] we obtain (3.6) for $2 \leq p \leq +\infty$.

3.4.2 Proof of Lemma 3.3

For $n \in \mathbb{Z}$, let us consider the 2D equation:

$$-\Delta_{\mathbf{r}} G_n + 4\pi^2 n^2 G_n = 2\pi \delta_{\mathbf{r}=0} \quad \text{in } \mathcal{S}'(\mathbb{R}^2).$$

It is well known (see for example [LL01, Lah14]) that the solution of the above equation is

$$G_n(|\mathbf{r}|) = \begin{cases} -\log(|\mathbf{r}|), & n \equiv 0, \\ K_0(2\pi|n||\mathbf{r}|), & |n| \geq 1, \end{cases}$$

where $K_0(\alpha) := \int_0^{+\infty} e^{-\alpha \cosh(t)} dt$ is the modified Bessel function of the second kind. Therefore the Green's function $G(x, \mathbf{r})$ defined in (3.7) can be rewritten as

$$G(x, \mathbf{r}) = 2 \sum_{n \in \mathbb{Z}} e^{2i\pi n x} G_n(\mathbf{r}) \in \mathcal{S}'_{\text{per},x}(\Gamma). \quad (3.41)$$

Applying the Laplacian operator to both sides,

$$-\Delta G(x, \mathbf{r}) = 4\pi \sum_{n \in \mathbb{Z}} e^{2i\pi n x} \delta_{\mathbf{r}=0} \in \mathcal{S}'_{\text{per},x}(\Gamma).$$

On the other hand, by the Poisson summation formula $\sum_{n \in \mathbb{Z}} \delta_{x=n} = \sum_{n \in \mathbb{Z}} e^{2i\pi n x} \in \mathcal{S}'(\mathbb{R})$, we conclude that the Green's function $G(x, \mathbf{r})$ defined in (3.7) satisfies

$$-\Delta G(x, \mathbf{r}) = 4\pi \sum_{n \in \mathbb{Z}} \delta_{(x,\mathbf{r})=(n,0)}.$$

Taking the Fourier transform \mathcal{F} on both sides of (3.41) we obtain that

$$\mathcal{F}G(n, \mathbf{k}) = \frac{2}{4\pi^2 n^2 + |\mathbf{k}|^2} \in \mathcal{S}'(\mathbb{R}^3).$$

Let us now give some estimates on \tilde{G} defined in (3.7). Recall that there exist two positive constants C_0 and C_1 such that [J.71]

$$0 \leq K_0(\alpha) \leq \begin{cases} C_0 |\log(\alpha)|, & \text{when } \alpha \leq 2\pi, \\ C_1 e^{-\alpha} (\pi/2\alpha)^{1/2}, & \text{when } \alpha > 2\pi. \end{cases}$$

For $|\mathbf{r}| > 1$, it holds that

$$|\tilde{G}(x, \mathbf{r})| \leq 2C_1 \sum_{n=1}^{+\infty} \frac{e^{-2\pi n|\mathbf{r}|}}{\sqrt{n|\mathbf{r}|}} \leq \frac{2C_1}{\sqrt{|\mathbf{r}|}} \frac{e^{-2\pi|\mathbf{r}|}}{1 - e^{-2\pi|\mathbf{r}|}} \leq \frac{2C_1}{1 - e^{-2\pi}} \frac{e^{-2\pi|\mathbf{r}|}}{\sqrt{|\mathbf{r}|}}. \quad (3.42)$$

For $|\mathbf{r}| \leq 1$ fixed, there exists $N \geq 1$ such that $N \leq \frac{1}{|\mathbf{r}|} < N + 1$. In particular, for $n > N + 1$ we have $2\pi n|\mathbf{r}| > 2\pi$. There exists therefore a positive constant C such that

$$\begin{aligned} |\tilde{G}(x, \mathbf{r})| &\leq 4C_0 \left| \sum_{n=1}^N \log(2\pi n|\mathbf{r}|) \right| + 2C_1 \sum_{n=N+1}^{\infty} \frac{e^{-2\pi n|\mathbf{r}|}}{\sqrt{n|\mathbf{r}|}} \leq 4C_0 \left| \int_1^{\frac{1}{|\mathbf{r}|}} \log(2\pi t|\mathbf{r}|) dt \right| + 2C_1 \int_{2\pi}^{\infty} e^{-t} dt \\ &= \frac{4C_0}{|\mathbf{r}|} |\log(2\pi) - 1 - |\mathbf{r}| + |\mathbf{r}| \log(2\pi|\mathbf{r}|)| + 2C_1 e^{-2\pi} \leq \frac{C}{|\mathbf{r}|}. \end{aligned} \quad (3.43)$$

Together with (3.42) we deduce that $\tilde{G}(x, \mathbf{r}) \in L^p_{\text{per}, x}(\Gamma)$ for $1 \leq p < 2$. Note that for all $\mathbf{r} \in \mathbb{R}^2 \setminus \{0\}$, it holds $\int_{-1/2}^{1/2} \bar{G}(x, \mathbf{r}) dx \equiv 0$. Consider, for $\mathbf{r} \neq 0$,

$$\bar{G}(x, \mathbf{r}) = \sum_{n \in \mathbb{Z}} \left(\frac{1}{\sqrt{(x-n)^2 + |\mathbf{r}|^2}} - \int_{-1/2}^{1/2} \frac{1}{\sqrt{(x-y-n)^2 + |\mathbf{r}|^2}} dy \right).$$

From [BLB00, Equation (1.8)],

$$-\Delta (\bar{G}(x, \mathbf{r}) - 2 \log(|\mathbf{r}|)) = 4\pi \sum_{k \in \mathbb{Z}} \delta_{(x, \mathbf{r})=(k, 0)} \in \mathcal{S}'(\mathbb{R}^3),$$

with $\bar{G}(x, \mathbf{r}) = \mathcal{O}(\frac{1}{|\mathbf{r}|})$ when $|\mathbf{r}| \rightarrow \infty$ by [BLB00, Lemma 2.2]. Denoting by $u(x, \mathbf{r}) = \tilde{G}(x, \mathbf{r}) - \bar{G}(x, \mathbf{r})$ we therefore obtain that $-\Delta u(x, \mathbf{r}) \equiv 0$. As $u(x, \mathbf{r})$ belongs to $L^1_{\text{loc}}(\mathbb{R}^3)$, by Weyl's lemma for the Laplace equation we obtain that $u(x, \mathbf{r})$ is $C^\infty(\mathbb{R}^3)$. On the other hand, by the decay properties of \tilde{G} and \bar{G} , we deduce that $|u(\cdot, \mathbf{r})| \rightarrow 0$ when $|\mathbf{r}| \rightarrow \infty$ uniformly in x , hence by the maximum modulus principle for harmonic functions we can conclude that $u \equiv 0$, hence $\tilde{G}(x, \mathbf{r}) = \bar{G}(x, \mathbf{r})$.

3.4.3 Proof of Lemma 3.5

We prove this lemma by an explicit construction of a density matrix belonging to \mathcal{F}_Γ . Consider a smooth cut-off function ϱ_{per} which is constant (hence periodic) in the x -direction and has compact support in the \mathbf{r} -direction, such that $0 \leq \varrho_{\text{per}} \leq 1$ and $\int_\Gamma \varrho_{\text{per}}^2 = 1$. Let $\omega \geq 0$ be a parameter to be made precise later. Define

$$\gamma_\omega = \mathcal{B}^{-1} \left(\int_{\Gamma^*} \gamma_{\omega, \xi} \frac{d\xi}{2\pi} \right) \mathcal{B}, \quad \gamma_{\omega, \xi} = A_{\omega, \xi} A_{\omega, \xi}^*, \quad A_{\omega, \xi} := \mathbf{1}_{[0, \omega]}(-\Delta_\xi) \varrho_{\text{per}}. \quad (3.44)$$

It is easy to see that $0 \leq \gamma_\omega \leq 1$, and that $\tau_k^x \gamma_\omega = \gamma_\omega \tau_k^x$ for all $k \in \mathbb{Z}$ by construction. Let us prove that the kinetic energy per unit cell of γ_ω is finite. Denote by $F_\xi(n, \mathbf{k}) = \sqrt{(2\pi n + \xi)^2 + \mathbf{k}^2}$. By the

Kato–Seiler–Simon type inequality (3.6),

$$\begin{aligned} \int_{\Gamma^*} \text{Tr}_{L^2_{\text{per},x}} (\sqrt{1 - \Delta_\xi} \gamma_{\omega,\xi} \sqrt{1 - \Delta_\xi}) d\xi &= \int_{\Gamma^*} \|\sqrt{1 - \Delta_\xi} A_{\omega,\xi}\|_{\mathfrak{S}_2}^2 d\xi \\ &\leq \frac{1}{4\pi^2} \int_{\Gamma^*} \|\varrho_{\text{per}}\|_{L^2_{\text{per},x}(\Gamma)}^2 \left(\sum_{n \in \mathbb{Z}} \left\| \sqrt{1 + F_\xi^2(n, \cdot)} \mathbb{1}_{[0,\omega]} (F_\xi^2(n, \cdot)) \right\|_{L^2(\mathbb{R}^2)}^2 \right) d\xi < +\infty. \end{aligned}$$

The last estimate follows by the condition $(2\pi n + \xi)^2 + \mathbf{k}^2 \leq \omega$ implies that the sum on n is finite and the integration on \mathbf{k} occurs in a compact domain. Hence γ_ω belongs to $\mathcal{P}_{\text{per},x}$. Let us now show that there exists $\omega_* \geq 0$ such that $\rho_{\gamma_{\omega_*}} - \mu_{\text{per},\text{sym}} \in \mathcal{C}_\Gamma$. It is easy to see that the density ρ_{γ_ω} is smooth and compactly supported in Γ by definition. Moreover, in view of the kernel representation (3.40), the kernel $K_{A_{\omega,\xi}}$ of the operator $A_{\omega,\xi}$ is

$$K_{A_{\omega,\xi}}((x, \mathbf{r}), (y, \mathbf{r}')) = \frac{1}{4\pi^2} \sum_{n \in \mathbb{Z}} \int_{\mathbb{R}^2} e^{i(2\pi n(x-y) + \mathbf{k} \cdot (\mathbf{r} - \mathbf{r}'))} \mathbb{1}_{[0,\omega]} (F_\xi^2(n, \mathbf{k})) \varrho_{\text{per}}(y, \mathbf{r}') d\mathbf{k}.$$

Remark that the non-negative function $\omega \mapsto \int_{\Gamma^*} \left(\sum_{n \in \mathbb{Z}} \int_{\mathbb{R}^2} \mathbb{1}_{[0,\omega]} (F_\xi^2(n, \mathbf{k})) d\mathbf{k} \right) d\xi$ is monotonic non-decreasing in ω , equals 0 when $\omega = 0$ and tends to $+\infty$ when $\omega \rightarrow +\infty$. Hence there exists $\omega_* > 0$ such that

$$\begin{aligned} \int_{\Gamma} \rho_{\gamma_{\omega_*}} &= \frac{1}{2\pi} \int_{\Gamma^*} \|A_{\omega_*,\xi}\|_{\mathfrak{S}_2}^2 d\xi = \frac{1}{2\pi} \int_{\Gamma^*} \|K_{A_{\omega,\xi}}\|_{L^2_{\text{per},x}(\Gamma \times \Gamma)}^2 d\xi \\ &= \frac{1}{(2\pi)^3} \int_{\Gamma^*} \int_{\Gamma} \int_{\mathbb{R}^2} \sum_{n \in \mathbb{Z}} \mathbb{1}_{[0,\omega_*]} (F_\xi^2(n, \mathbf{k})) \varrho_{\text{per}}^2(y, \mathbf{r}) dy d\mathbf{r} d\mathbf{k} d\xi \\ &= \frac{1}{(2\pi)^3} \int_{\Gamma^*} \left(\sum_{n \in \mathbb{Z}} \int_{\mathbb{R}^2} \mathbb{1}_{[0,\omega_*]} (F_\xi^2(n, \mathbf{k})) d\mathbf{k} \right) d\xi = \int_{\Gamma} \mu_{\text{per},\text{sym}} > 0. \end{aligned} \quad (3.45)$$

This condition is equivalent to $\mathcal{F}(\rho_{\gamma_{\omega_*}} - \mu_{\text{per}})(0, \mathbf{0}) = 0$. As $\mathbf{k} \mapsto \mathcal{F}(\rho_{\gamma_{\omega_*}} - \mu_{\text{per}})(0, \mathbf{k})$ is $C^1(\mathbb{R}^2)$ and bounded, the function $\mathbf{k} \mapsto |\mathbf{k}|^{-1} \mathcal{F}(\rho_{\gamma_{\omega_*}} - \mu_{\text{per},\text{sym}})(0, \mathbf{k})$ is in $L^2_{\text{loc}}(\mathbb{R}^2)$. In view of this, there exists a positive constant C such that

$$\begin{aligned} \sum_{n \in \mathbb{Z}} \int_{\mathbb{R}^2} \frac{|\mathcal{F}(\rho_{\gamma_{\omega_*}} - \mu_{\text{per},\text{sym}})(n, \mathbf{k})|^2}{|\mathbf{k}|^2 + 4\pi^2 n^2} d\mathbf{k} &\leq \int_{|\mathbf{k}| \leq 2\pi} \frac{|\mathcal{F}(\rho_{\gamma_{\omega_*}} - \mu_{\text{per},\text{sym}})(0, \mathbf{k})|^2}{|\mathbf{k}|^2} d\mathbf{k} \\ &+ \frac{1}{4\pi^2} \left(\int_{|\mathbf{k}| > 2\pi} |\mathcal{F}(\rho_{\gamma_{\omega_*}} - \mu_{\text{per},\text{sym}})(0, \mathbf{k})|^2 d\mathbf{k} + \sum_{n \in \mathbb{Z} \setminus \{0\}} \int_{\mathbb{R}^2} |\mathcal{F}(\rho_{\gamma_{\omega_*}} - \mu_{\text{per},\text{sym}})(n, \mathbf{k})|^2 d\mathbf{k} \right) \\ &\leq C + \frac{1}{4\pi^2} \int_{\Gamma} |\rho_{\gamma_{\omega_*}} - \mu_{\text{per},\text{sym}}|^2 < +\infty. \end{aligned} \quad (3.46)$$

In view of the definition of the Coulomb energy (3.13), we can therefore conclude that

$$D_\Gamma(\rho_{\gamma_{\omega_*}} - \mu_{\text{per},\text{sym}}, \rho_{\gamma_{\omega_*}} - \mu_{\text{per},\text{sym}}) < +\infty.$$

This concludes the proof that the state $\gamma_{\omega_*} \in \mathcal{F}_\Gamma$. Hence \mathcal{F}_Γ is not empty. As any density ρ_γ associated with $\gamma \in \mathcal{P}_{\text{per},x}$ is integrable, we can conclude that (3.16) holds in view of Remark 3.4.

3.4.4 Proof of Theorems 3.6

Let us start by giving a convenient equivalent formulation of the minimization problems (3.17). The operator $-\frac{1}{2}\Delta_\xi$ is not invertible, but the operator $-\frac{1}{2}\Delta_\xi - \kappa$ is positive definite and $|-\frac{1}{2}\Delta_\xi - \kappa|^{-1}$ is bounded for any $\kappa < 0$. Therefore in view of the charge neutrality constraint (3.16), we rewrite the periodic rHF

energy functional (3.15) as follows:

$$\begin{aligned} \forall \gamma \in \mathcal{F}_\Gamma, \quad \mathcal{E}_{\text{per},x}(\gamma) &= \frac{1}{2\pi} \int_{\Gamma^*} \text{Tr}_{L^2_{\text{per},x}(\Gamma)} \left(-\frac{1}{2} \Delta_\xi \gamma_\xi \right) d\xi + \frac{1}{2} D_\Gamma (\rho_\gamma - \mu_{\text{per}}, \rho_\gamma - \mu_{\text{per}}) \\ &= \overline{\mathcal{E}_{\text{per},x,\kappa}}(\gamma) + \frac{\kappa}{2\pi} \int_{\Gamma^*} \text{Tr}_{L^2_{\text{per},x}(\Gamma)} (\gamma_\xi) d\xi = \overline{\mathcal{E}_{\text{per},x,\kappa}}(\gamma) + \kappa \int_\Gamma \mu_{\text{per}}, \end{aligned}$$

with

$$\overline{\mathcal{E}_{\text{per},x,\kappa}}(\gamma) := \frac{1}{2\pi} \int_{\Gamma^*} \text{Tr}_{L^2_{\text{per},x}(\Gamma)} \left(\left| -\frac{1}{2} \Delta_\xi - \kappa \right|^{1/2} \gamma_\xi \left| -\frac{1}{2} \Delta_\xi - \kappa \right|^{1/2} \right) d\xi + \frac{1}{2} D_\Gamma (\rho_\gamma - \mu_{\text{per}}, \rho_\gamma - \mu_{\text{per}}).$$

The parameter κ can be interpreted as the Lagrangian multiplier associated with the charger neutrality constraint. Therefore by fixing $\kappa < 0$, the minimization problem (3.17) is equivalent to the problem

$$\inf \{ \overline{\mathcal{E}_{\text{per},x,\kappa}}(\gamma); \gamma \in \mathcal{F}_\Gamma \}. \quad (3.47)$$

We prove the existence of minimizers and the uniqueness of the density of minimizers for the problem (3.47) (hence of (3.17)) by considering a minimizing sequence, and show that there is no loss of compactness. This approach is rather classical for rHF type models [CLBL01, CDL08a, CLL13, CCS18]. But in our case we need to be careful as electrons might escape to infinity in the r -direction. We show that this is impossible thanks to the Coulomb interactions (Lemma 3.21).

Weak convergence of the minimizing sequence. First of all it is easy to see that the functional $\overline{\mathcal{E}_{\text{per},x,\kappa}}(\cdot)$ is well defined on the non-empty set \mathcal{F}_Γ . Consider a minimizing sequence of $\overline{\mathcal{E}_{\text{per},x,\kappa}}(\cdot)$

$$\left\{ \gamma_n := \mathcal{B}^{-1} \left(\int_{\Gamma^*} \gamma_{n,\xi} \frac{d\xi}{2\pi} \right) \mathcal{B} \right\}_{n \geq 1}$$

on \mathcal{F}_Γ . There exists $C > 0$ such that for all $n \geq 1$:

$$\begin{aligned} 0 &\leq \int_{\Gamma^*} \text{Tr}_{L^2_{\text{per},x}(\Gamma)} \left(\left| -\frac{1}{2} \Delta_\xi - \kappa \right|^{1/2} \gamma_{n,\xi} \left| -\frac{1}{2} \Delta_\xi - \kappa \right|^{1/2} \right) d\xi \leq C, \\ 0 &\leq D_\Gamma (\rho_{\gamma_n} - \mu_{\text{per,sym}}, \rho_{\gamma_n} - \mu_{\text{per,sym}}) \leq C. \end{aligned} \quad (3.48)$$

The kinetic energy bound (3.48) together with the inequality (3.12) implies that the sequence $\{\sqrt{\rho_{\gamma_n}}\}_{n \geq 1}$ is uniformly bounded in $H^1_{\text{per},x}(\Gamma)$ hence in $L^6_{\text{per},x}(\Gamma)$ by Sobolev embeddings. Therefore for all $n \in \mathbb{N}^*$, the density ρ_{γ_n} belongs to $L^p_{\text{per},x}(\Gamma)$ for $1 \leq p \leq 3$. On the other hand, for almost all $\xi \in \Gamma^*$, the operator $\gamma_{n,\xi}$ is a trace-class operator on $L^2_{\text{per},x}(\Gamma)$. As $0 \leq \gamma_{n,\xi}^2 \leq \gamma_{n,\xi} \leq 1$, we obtain that

$$0 \leq \int_{\Gamma^*} \|\gamma_{n,\xi}\|_{\mathfrak{S}_2}^2 d\xi = \int_{\Gamma^*} \text{Tr}_{L^2_{\text{per},x}(\Gamma)} (\gamma_{n,\xi}^2) d\xi \leq \int_{\Gamma^*} \text{Tr}_{L^2_{\text{per},x}(\Gamma)} (\gamma_{n,\xi}) d\xi = 2\pi Z.$$

This implies that the operator-valued function $\xi \mapsto \gamma_{n,\xi}$ is uniformly bounded in $L^2(\Gamma^*; \mathfrak{S}_2)$. Furthermore, the uniform boundedness $0 \leq \gamma_{n,\xi} \leq 1$ also implies that the operator-valued function $\xi \mapsto \gamma_{n,\xi}$ belongs to $L^\infty(\Gamma^*; \mathcal{S}(L^2_{\text{per},x}(\Gamma)))$. Combining these remarks with the uniform energy bound (3.48), we deduce that there exist (up to extraction):

$$\gamma = \mathcal{B}^{-1} \left(\int_{\Gamma^*} \gamma_\xi \frac{d\xi}{2\pi} \right) \mathcal{B}, \quad \overline{\rho}_\gamma \in L^p_{\text{per},x}(\Gamma), \quad \widetilde{\rho}_\gamma - \mu_{\text{per,sym}} \in \mathcal{C}_\Gamma, \quad (3.49)$$

such that $\gamma_n \xrightarrow{*} \gamma$ in the following sense: for any operator-valued function $\xi \mapsto U_\xi \in L^2(\Gamma^*; \mathfrak{S}_2) + L^1(\Gamma^*; \mathfrak{S}_1)$,

$$\int_{\Gamma^*} \text{Tr}_{L^2_{\text{per},x}(\Gamma)} (U_\xi \gamma_n) d\xi \xrightarrow{n \rightarrow \infty} \int_{\Gamma^*} \text{Tr}_{L^2_{\text{per},x}(\Gamma)} (U_\xi \gamma) d\xi. \quad (3.50)$$

The density

$$\rho_{\gamma_n} \rightharpoonup \overline{\rho_\gamma} \text{ weakly in } L^p_{\text{per},x}(\Gamma) \text{ for } 1 < p \leq 3.$$

The total density

$$\rho_{\gamma_n} - \mu_{\text{per,sym}} \rightharpoonup \widetilde{\rho_\gamma} - \mu_{\text{per,sym}} \text{ weakly in } \mathcal{C}_\Gamma.$$

The convergence (3.50) is due to the fact that the predual of $L^\infty(\Gamma^*; \mathcal{S}(L^2_{\text{per},x}(\Gamma)))$ is $L^1(\Gamma^*; \mathfrak{S}_1)$, and that $L^2(\Gamma^*; \mathfrak{S}_2)$ is a Hilbert space.

Remark 3.20. *The convergence of $\gamma_n \xrightarrow{*} \gamma$ in the sense of (3.50) can also be reformulated as the convergence in the sense of the following weak-* topology:*

$$\mathcal{B} \gamma_n \mathcal{B}^{-1} \xrightarrow{n \rightarrow \infty} \mathcal{B} \gamma \mathcal{B}^{-1} \text{ for the weak-* topology of } L^\infty(\Gamma^*; \mathcal{S}(L^2_{\text{per},x}(\Gamma))) \cap L^2(\Gamma^*; \mathfrak{S}_2). \quad (3.51)$$

Denote by $\mathcal{D}_{\text{per},x}(\Gamma)$ the functions which are C^∞ on \mathbb{R} , 1-periodic in the x -direction, and have compact support in the \mathbf{r} -direction. Denote by $\mathcal{D}'_{\text{per},x}(\Gamma)$ the dual space of $\mathcal{D}_{\text{per},x}(\Gamma)$. The following lemma guarantees that the densities obtained by different weak limit processes coincide. In particular there is no loss of compactness in the \mathbf{r} -direction when $|\mathbf{r}| \rightarrow \infty$.

Lemma 3.21 (Consistency of densities). *Denote by ρ_γ the density associated with the density matrix γ obtained in the weak limit (3.49). Then $\rho_\gamma = \overline{\rho_\gamma} = \widetilde{\rho_\gamma}$ in $\mathcal{D}'_{\text{per},x}(\Gamma)$. In particular, $\rho_\gamma = \overline{\rho_\gamma}$ as elements in $L^p_{\text{per},x}(\Gamma)$ for $1 < p \leq 3$ and $\rho_\gamma - \mu_{\text{per,sym}} = \widetilde{\rho_\gamma} - \mu_{\text{per,sym}}$ as elements in \mathcal{C}_Γ .*

We postpone the proof to Section 3.4.5.

The state γ is a minimizer. Let us first show that the kinetic energy of γ obtained by the weak limit (3.50) is finite. To achieve this, consider an orthonormal basis $\{e_i\}_{i \in \mathbb{N}} \subset H^1_{\text{per},x}(\Gamma)$ of $L^2_{\text{per},x}(\Gamma)$, and define the following family of operators for $N \in \mathbb{N}^*$:

$$M_\xi^N := \left| -\frac{1}{2}\Delta_\xi - \kappa \right|^{1/2} \left(\sum_{i=1}^N |e_i\rangle\langle e_i| \right) \left| -\frac{1}{2}\Delta_\xi - \kappa \right|^{1/2}.$$

An easy computation shows that for all $\xi \in \Gamma^*$, the operator M_ξ^N belongs to \mathfrak{S}_2 . Moreover, the function $\xi \mapsto M_\xi^N$ can be seen as an operator-valued function belonging to $L^2(\Gamma^*; \mathfrak{S}_2)$ as $\Gamma^* = [-\pi, \pi]$ is a finite interval. In view of the convergence (3.50) and by choosing $U_\xi = M_\xi^N$ we obtain that (recalling that $\text{Tr}(AB) = \text{Tr}(BA)$ when A, B are Hilbert-Schmidt operators, and $\left| -\frac{1}{2}\Delta_\xi - \kappa \right|^{1/2} \gamma_\xi$ is Hilbert-Schmidt for almost all $\xi \in \Gamma^*$)

$$\begin{aligned} 0 &\leq \int_{\Gamma^*} \text{Tr}_{L^2_{\text{per},x}(\Gamma)} \left(\left| -\frac{1}{2}\Delta_\xi - \kappa \right|^{1/2} \gamma_\xi \left| -\frac{1}{2}\Delta_\xi - \kappa \right|^{1/2} \left(\sum_{i=1}^N |e_i\rangle\langle e_i| \right) \right) d\xi \\ &= \int_{\Gamma^*} \text{Tr}_{L^2_{\text{per},x}(\Gamma)} (M_\xi^N \gamma_\xi) d\xi = \lim_{n \rightarrow \infty} \int_{\Gamma^*} \text{Tr}_{L^2_{\text{per},x}(\Gamma)} (M_\xi^N \gamma_{n,\xi}) d\xi \\ &= \lim_{n \rightarrow \infty} \int_{\Gamma^*} \text{Tr}_{L^2_{\text{per},x}(\Gamma)} \left(\left| -\frac{1}{2}\Delta_\xi - \kappa \right|^{1/2} \gamma_{n,\xi} \left| -\frac{1}{2}\Delta_\xi - \kappa \right|^{1/2} \left(\sum_{i=1}^N |e_i\rangle\langle e_i| \right) \right) d\xi \\ &= \lim_{n \rightarrow \infty} \int_{\Gamma^*} \sum_{i=1}^N \left\langle e_i \left| \left| -\frac{1}{2}\Delta_\xi - \kappa \right|^{1/2} \gamma_{n,\xi} \left| -\frac{1}{2}\Delta_\xi - \kappa \right|^{1/2} \right| e_i \right\rangle d\xi \\ &\leq \liminf_{n \rightarrow \infty} \int_{\Gamma^*} \text{Tr}_{L^2_{\text{per},x}(\Gamma)} \left(\left| -\frac{1}{2}\Delta_\xi - \kappa \right|^{1/2} \gamma_{n,\xi} \left| -\frac{1}{2}\Delta_\xi - \kappa \right|^{1/2} \right) d\xi \leq C', \end{aligned}$$

where the last step we have used the uniform energy bound (3.48). Therefore, by passing to the limit $N \rightarrow +\infty$, by Fatou's lemma we have

$$\begin{aligned} 0 &\leq \int_{\Gamma^*} \text{Tr}_{L^2_{\text{per},x}(\Gamma)} \left(\left| -\frac{1}{2}\Delta_\xi - \kappa \right|^{1/2} \gamma_\xi \left| -\frac{1}{2}\Delta_\xi - \kappa \right|^{1/2} \right) d\xi \\ &\leq \liminf_{n \rightarrow \infty} \int_{\Gamma^*} \text{Tr}_{L^2_{\text{per},x}(\Gamma)} \left(\left| -\frac{1}{2}\Delta_\xi - \kappa \right|^{1/2} \gamma_{n,\xi} \left| -\frac{1}{2}\Delta_\xi - \kappa \right|^{1/2} \right) d\xi \leq C'. \end{aligned} \quad (3.52)$$

Remark that the bound (3.52) also implies that $\sqrt{\rho_\gamma}$ belongs to $H^1_{\text{per},x}(\Gamma)$ by the Hoffmann–Ostenhof inequality (3.12). Hence $\rho_\gamma \in L^p_{\text{per},x}(\Gamma)$ for $1 \leq p \leq 3$. Since $\rho_\gamma - \mu_{\text{per},\text{sym}}$ is an element in \mathcal{C}_Γ by Lemma 3.21, this implies that the charge is neutral by Remark 3.4. That is,

$$\int_{\Gamma} \rho_\gamma = \int_{\Gamma} \mu_{\text{per},\text{sym}}.$$

As $D_\Gamma(\cdot, \cdot)$ defines an inner product on \mathcal{C}_Γ , by the weak convergence (3.49) of $\rho_{\gamma_n} - \mu_{\text{per},\text{sym}}$ to $\widetilde{\rho}_\gamma - \mu_{\text{per},\text{sym}}$ in \mathcal{C}_Γ and the consistency of densities given by Lemma 3.21, we obtain that

$$D_\Gamma(\rho_\gamma - \mu_{\text{per},\text{sym}}, \rho_\gamma - \mu_{\text{per},\text{sym}}) \leq \liminf_{n \rightarrow \infty} D_\Gamma(\rho_{\gamma_n} - \mu_{\text{per},\text{sym}}, \rho_{\gamma_n} - \mu_{\text{per},\text{sym}}). \quad (3.53)$$

In view of (3.52) and (3.53), we conclude that

$$\mathcal{E}_{\text{per},x}(\gamma) \leq \liminf_{n \rightarrow \infty} \mathcal{E}_{\text{per},x}(\gamma_n),$$

which shows that the state γ obtained in (3.49) is a minimizer of the problem (3.17). Let us prove that all minimizers share the same density: consider two minimizers $\bar{\gamma}_1$ and $\bar{\gamma}_2$. By the convexity of \mathcal{F}_Γ it holds that $\frac{1}{2}(\bar{\gamma}_1 + \bar{\gamma}_2) \in \mathcal{F}_\Gamma$. Moreover

$$\mathcal{E}_{\text{per},x} \left(\frac{\bar{\gamma}_1 + \bar{\gamma}_2}{2} \right) = \frac{1}{2} \mathcal{E}_{\text{per},x}(\bar{\gamma}_1) + \frac{1}{2} \mathcal{E}_{\text{per},x}(\bar{\gamma}_2) - \frac{1}{4} D_\Gamma(\rho_{\bar{\gamma}_1} - \rho_{\bar{\gamma}_2}, \rho_{\bar{\gamma}_1} - \rho_{\bar{\gamma}_2}),$$

which shows that $D_\Gamma(\rho_{\bar{\gamma}_1} - \rho_{\bar{\gamma}_2}, \rho_{\bar{\gamma}_1} - \rho_{\bar{\gamma}_2}) \equiv 0$, hence all the minimizers of the problem (3.17) share the same density.

3.4.5 Proof of Lemma 3.21

Equality of $\widetilde{\rho}_\gamma$ and $\bar{\rho}_\gamma$. The proof follows ideas similar to the ones used for the proof of [CCS18, Lemma 3.5] by considering a test function in $\mathcal{D}_{\text{per},x}(\Gamma)$ and replacing the Fourier transform by the mixed Fourier transform defined in (3.3). Consider a test function $w \in \mathcal{D}_{\text{per},x}(\Gamma)$. The weak convergence of $\rho_{\gamma_n} \rightharpoonup \bar{\rho}_\gamma$ in $L^p_{\text{per},x}(\Gamma)$ with $1 < p \leq 3$ implies that

$$\langle \rho_{\gamma_n} - \mu_{\text{per},\text{sym}}, w \rangle_{\mathcal{D}'_{\text{per},x}, \mathcal{D}_{\text{per},x}} \xrightarrow{n \rightarrow \infty} \langle \bar{\rho}_\gamma - \mu_{\text{per},\text{sym}}, w \rangle_{\mathcal{D}'_{\text{per},x}, \mathcal{D}_{\text{per},x}}.$$

On the other hand,

$$\begin{aligned} \langle \rho_{\gamma_n} - \mu_{\text{per},\text{sym}}, w \rangle_{\mathcal{D}'_{\text{per},x}, \mathcal{D}_{\text{per},x}} &= \int_{\Gamma} (\rho_{\gamma_n} - \mu_{\text{per},\text{sym}}) w \\ &= \sum_{n \in \mathbb{Z}} \int_{\mathbb{R}^2} \mathcal{F}(\rho_{\gamma_n} - \mu_{\text{per},\text{sym}})(n, \mathbf{k}) \mathcal{F}w(n, \mathbf{k}) d\mathbf{k} \\ &= 4\pi \sum_{n \in \mathbb{Z}} \int_{\mathbb{R}^2} \frac{\mathcal{F}(\rho_{\gamma_n} - \mu_{\text{per},\text{sym}})(n, \mathbf{k}) \mathcal{F}f(n, \mathbf{k})}{4\pi^2 n^2 + |\mathbf{k}|^2} d\mathbf{k}. \end{aligned} \quad (3.54)$$

where $f = -\frac{1}{4\pi}\Delta w$. Note that f belongs to the Coulomb space \mathcal{C}_Γ defined in (3.14) since for all $n \in \mathbb{Z}$, $\mathcal{F}f(n, \cdot) \in L^1_{\text{loc}}(\mathbb{R}^2)$, and

$$\begin{aligned} D_\Gamma(f, f) &= 4\pi \sum_{n \in \mathbb{Z}} \int_{\mathbb{R}^2} \frac{|\mathcal{F}f(n, \mathbf{k})|^2}{|\mathbf{k}|^2 + 4\pi^2 n^2} d\mathbf{k} = \frac{1}{4\pi} \sum_{n \in \mathbb{Z}} \int_{\mathbb{R}^2} (|\mathbf{k}|^2 + 4\pi^2 n^2) |\mathcal{F}w(n, \mathbf{k})|^2 d\mathbf{k} \\ &= \frac{1}{4\pi} \sum_{n \in \mathbb{Z}} \int_{\mathbb{R}^2} |\mathcal{F}(\nabla w)(n, \mathbf{k})|^2 d\mathbf{k} = \frac{1}{4\pi} \int_\Gamma |\nabla w|^2 < +\infty. \end{aligned}$$

Therefore in view of (3.54), the convergence $D_\Gamma(\rho_{\gamma_n} - \mu_{\text{per, sym}}, f) \xrightarrow{n \rightarrow \infty} D_\Gamma(\widetilde{\rho}_\gamma - \mu_{\text{per, sym}}, f)$ implies that

$$\langle \rho_{\gamma_n} - \mu_{\text{per, sym}}, w \rangle \xrightarrow{n \rightarrow \infty} \langle \widetilde{\rho}_\gamma - \mu_{\text{per, sym}}, w \rangle.$$

The uniqueness of limit in the sense of distribution allows us to conclude.

Equality of ρ_γ and $\overline{\rho}_\gamma$. Let us prove that $\rho_\gamma = \overline{\rho}_\gamma$ in $\mathcal{D}'_{\text{per}, x}(\Gamma)$. The fact that $\rho_{\gamma_n} \rightharpoonup \overline{\rho}_\gamma$ weakly in $L^p_{\text{per}, x}(\Gamma)$ implies that

$$\langle \rho_{\gamma_n}, w \rangle \xrightarrow{n \rightarrow \infty} \langle \overline{\rho}_\gamma, w \rangle.$$

Therefore it suffices to prove that the operator-valued function $\xi \mapsto w\gamma_{n, \xi} \in L^1(\Gamma^*; \mathfrak{S}_1)$ converges in the following sense:

$$\frac{1}{2\pi} \int_{\Gamma^*} \text{Tr}_{L^2_{\text{per}, x}(\Gamma)}(w\gamma_{n, \xi}) d\xi = \langle \rho_{\gamma_n}, w \rangle \xrightarrow{n \rightarrow \infty} \langle \rho_\gamma, w \rangle = \frac{1}{2\pi} \int_{\Gamma^*} \text{Tr}_{L^2_{\text{per}, x}(\Gamma)}(w\gamma_\xi) d\xi. \quad (3.55)$$

The weak convergence (3.50) does not guarantee the above convergence since the function w does not belong to any Schatten class. We prove (3.55) by using the kinetic energy bound (3.48), which implies that the operator-valued function

$$\xi \mapsto \left| -\frac{1}{2}\Delta_\xi - \kappa \right|^{1/2} \gamma_{n, \xi} = \left(\left| -\frac{1}{2}\Delta_\xi - \kappa \right|^{1/2} \gamma_{n, \xi} \left| -\frac{1}{2}\Delta_\xi - \kappa \right|^{1/2} \right) \left| -\frac{1}{2}\Delta_\xi - \kappa \right|^{-1/2}$$

is uniformly bounded in $L^1(\Gamma^*; \mathfrak{S}_1)$ as $\left| -\frac{1}{2}\Delta_\xi - \kappa \right|^{-1/2}$ is uniformly bounded with respect to $\xi \in \Gamma^*$. Moreover, the energy bounded (3.48) also implies that $\xi \mapsto \left| -\frac{1}{2}\Delta_\xi - \kappa \right|^{1/2} \sqrt{\gamma_{n, \xi}}$ is uniformly bounded in $L^2(\Gamma^*; \mathfrak{S}_2)$. Hence the operator-valued function $\xi \mapsto \left| -\frac{1}{2}\Delta_\xi - \kappa \right|^{1/2} \gamma_{n, \xi} = \left| -\frac{1}{2}\Delta_\xi - \kappa \right|^{1/2} \sqrt{\gamma_{n, \xi}} \sqrt{\gamma_{n, \xi}}$ is uniformly bounded in $L^2(\Gamma^*; \mathfrak{S}_2)$ as $0 \leq \gamma_{n, \xi} \leq 1$. Therefore

$$\xi \mapsto \left| -\frac{1}{2}\Delta_\xi - \kappa \right|^{1/2} \gamma_{n, \xi} \text{ is uniformly bounded in } L^1(\Gamma^*; \mathfrak{S}_1) \cap L^2(\Gamma^*; \mathfrak{S}_2),$$

hence in $L^q(\Gamma^*; \mathfrak{S}_q)$ for $1 \leq q \leq 2$ by interpolation. Therefore, up to extraction, the following weak convergence holds: for any operator-valued function $\xi \mapsto W_\xi \in L^{q'}(\Gamma^*; \mathfrak{S}_{q'})$ where $q' = \frac{q}{q-1}$ for $1 < q \leq 2$,

$$\int_{\Gamma^*} \text{Tr}_{L^2_{\text{per}, x}(\Gamma)} \left(W_\xi \left| -\frac{1}{2}\Delta_\xi - \kappa \right|^{1/2} \gamma_{n, \xi} \right) d\xi \xrightarrow{n \rightarrow \infty} \int_{\Gamma^*} \text{Tr}_{L^2_{\text{per}, x}(\Gamma)} \left(W_\xi \left| -\frac{1}{2}\Delta_\xi - \kappa \right|^{1/2} \gamma_\xi \right) d\xi. \quad (3.56)$$

On the other hand by the inequality (3.6) we obtain that for any $\xi \in \Gamma^*$,

$$\left\| w \left| -\frac{1}{2}\Delta_\xi - \kappa \right|^{-1/2} \right\|_{\mathfrak{S}_{q'}} \leq \frac{1}{(2\pi)^{2/q'}} \|w\|_{L^{q'}_{\text{per}, x}(\Gamma)} \left(\sum_{n \in \mathbb{Z}} \int_{\mathbb{R}^2} \frac{2^{q'/2}}{((2\pi n + \xi)^2 + |\mathbf{r}|^2 + 2|\kappa|)^{q'/2}} d\mathbf{r} \right)^{1/q'}.$$

Upon choosing for example $q' = 4$, the right hand side of the above quantity is finite. Therefore upon taking $W_\xi = w \left| -\frac{1}{2}\Delta_\xi - \kappa \right|^{-1/2}$ in (3.56) we obtain that

$$\begin{aligned} \frac{1}{2\pi} \int_{\Gamma^*} \text{Tr}_{L^2_{\text{per},x}(\Gamma)} (w\gamma_{n,\xi}) d\xi &= \frac{1}{2\pi} \int_{\Gamma^*} \text{Tr}_{L^2_{\text{per},x}(\Gamma)} \left(w \left| -\frac{1}{2}\Delta_\xi - \kappa \right|^{-1/2} \left| -\frac{1}{2}\Delta_\xi - \kappa \right|^{1/2} \gamma_{n,\xi} \right) d\xi \\ &\xrightarrow{n \rightarrow \infty} \frac{1}{2\pi} \int_{\Gamma^*} \text{Tr}_{L^2_{\text{per},x}(\Gamma)} \left(w \left| -\frac{1}{2}\Delta_\xi - \kappa \right|^{-1/2} \left| -\frac{1}{2}\Delta_\xi - \kappa \right|^{1/2} \gamma_\xi \right) d\xi = \frac{1}{2\pi} \int_{\Gamma^*} \text{Tr}_{L^2_{\text{per},x}(\Gamma)} (w\gamma_\xi) d\xi. \end{aligned}$$

Hence (3.55) holds. Therefore $\rho_\gamma = \overline{\rho_\gamma}$ in $\mathcal{D}'_{\text{per},x}(\Gamma)$, which concludes the proof of the lemma.

3.4.6 Proof of Theorem 3.7

We first define a mean-field Hamiltonian associated with the problem (3.17), and then show that the Fermi level is always negative. Moreover, the minimizer of (3.17) is uniquely given by the spectral projector of the mean-field Hamiltonian. In the end we show that the density of the minimizer decays exponentially fast in the \mathbf{r} -direction.

Properties of the mean-field potential and Hamiltonian. We begin with the definition of a mean-field potential and a mean-field Hamiltonian, and next study the spectrum of the mean-field Hamiltonian. Consider a minimizer γ_{per} of (3.17) with the unique density $\rho_{\gamma_{\text{per}}} \in L^p_{\text{per},x}(\Gamma)$ where $1 \leq p \leq 3$. Define the mean-field potential

$$V_{\text{per,sym}} := q_{\text{per}} \star_{\Gamma} G, \quad q_{\text{per}} := \rho_{\gamma_{\text{per}}} - \mu_{\text{per,sym}}.$$

which is the solution of Poisson's equation $-\Delta V_{\text{per,sym}} = 4\pi q_{\text{per}}$. Let us prove that $V_{\text{per,sym}}$ belongs to $L^p_{\text{per},x}(\Gamma)$ for $2 < p \leq +\infty$. As μ_{per} is smooth and has compact support in the \mathbf{r} -direction and $\rho_{\gamma_{\text{per}}}$ belongs to $L^p_{\text{per},x}(\Gamma)$ for $1 \leq p \leq 3$, hence $\mathcal{F}q_{\text{per}}(0, \cdot)$ belongs to $L^2(\mathbb{R}^2) \cap L^\infty(\mathbb{R}^2) \cap C^0(\mathbb{R}^2)$ by classical Fourier theory (see for example [RS75]). Moreover, as $\int_{\Gamma} |\mathbf{r}| \rho_{\gamma_{\text{per}}}(x, \mathbf{r}) < +\infty$ by (3.18),

$$\begin{aligned} \left\| \partial_{\mathbf{k}} \mathcal{F}q_{\text{per}}(0, \mathbf{k}) \right\|_{L^\infty(\mathbb{R}^2)} &= \left| \int_{\Gamma} e^{-i\mathbf{r} \cdot \mathbf{k}} \mathbf{r} \cdot q_{\text{per}}(x, \mathbf{r}) dx d\mathbf{r} \right| \\ &\leq \left| \int_{\Gamma} |\mathbf{r}| |\rho_{\gamma_{\text{per}}} + \mu_{\text{per,sym}}|(x, \mathbf{r}) dx d\mathbf{r} \right| < +\infty. \end{aligned} \quad (3.57)$$

This implies that $\mathcal{F}q_{\text{per}}(0, \mathbf{k})$ is $C^1(\mathbb{R}^2)$ and bounded. Remark also that $\mathcal{F}q_{\text{per}}(0, \mathbf{0}) = 0$ by the charge neutrality and that $\mathcal{F}q_{\text{per}}(0, \cdot)$ belongs to $L^2(\mathbb{R}^2) \cap L^\infty(\mathbb{R}^2) \cap C^0(\mathbb{R}^2)$, hence for $1 \leq \alpha < 2$,

$$\begin{aligned} \int_{\mathbb{R}^2} |\mathcal{F}V_{\text{per,sym}}(0, \mathbf{k})|^\alpha d\mathbf{k} &= \int_{\mathbb{R}^2} \frac{|\mathcal{F}q_{\text{per}}(0, \mathbf{k})|^\alpha}{|\mathbf{k}|^{2\alpha}} d\mathbf{k} \\ &\leq \int_{|\mathbf{k}| < 1} \frac{|\mathcal{F}q_{\text{per}}(0, \mathbf{k})|^\alpha}{|\mathbf{k}|^{2\alpha}} d\mathbf{k} + \left(\int_{|\mathbf{k}| \geq 1} |\mathcal{F}q_{\text{per}}(0, \mathbf{k})|^{2\alpha} d\mathbf{k} \right)^{1/2} \left(\int_{|\mathbf{k}| \geq 1} \frac{1}{|\mathbf{k}|^{4\alpha}} d\mathbf{k} \right)^{1/2} < +\infty. \end{aligned} \quad (3.58)$$

Remark that the mixed Fourier transform \mathcal{F} is an isometry from $L^2_{\text{per},x}(\Gamma)$ to $\ell^2(\mathbb{Z}, L^2(\mathbb{R}^2))$ by (3.4). On the other hand,

$$\forall \phi \in \ell^1(\mathbb{Z}, L^1(\mathbb{R}^2)), \quad \|\mathcal{F}^{-1}\phi\|_{L^\infty(\Gamma)} = \sup_{x \in \Gamma} \left| \frac{1}{2\pi} \sum_{n \in \mathbb{Z}} \int_{\mathbb{R}^2} \phi_n(\mathbf{k}) e^{i(2\pi n x + \mathbf{k} \cdot \mathbf{r})} d\mathbf{k} \right| \leq \frac{1}{2\pi} \|\phi\|_{\ell^1(\mathbb{Z}, L^1(\mathbb{R}^2))},$$

By the Riesz–Thorin interpolation theorem (see for example [RS75] and [LL01, Theorem 5.7]), we can deduce a Hausdorff–Young inequality for \mathcal{F}^{-1} : for $1 \leq \alpha \leq 2$ there exists a constant C_α depending on α such that

$$\forall \phi \in \ell^\alpha(\mathbb{Z}, L^\alpha(\mathbb{R}^2)), \quad \|\mathcal{F}^{-1}\phi\|_{L^{\alpha'}_{\text{per},x}(\Gamma)} \leq C_\alpha \|\phi\|_{\ell^\alpha(\mathbb{Z}, L^\alpha(\mathbb{R}^2))}. \quad (3.59)$$

where $\alpha' := \alpha/(\alpha - 1)$. Hence in view of (3.58) and (3.59), for $1 \leq \alpha < 2$ and $2 < \alpha' = \alpha/(\alpha - 1) \leq +\infty$ there exist positive constants $C_{\alpha,1}$, $C_{\alpha,2}$ and $C'_{\alpha,2}$ such that

$$\begin{aligned} \|V_{\text{per,sym}}\|_{L^{\alpha'}_{\text{per},x}(\Gamma)}^\alpha &\leq C_\alpha^\alpha \|\mathcal{F}V_{\text{per,sym}}\|_{\ell^\alpha(\mathbb{Z}, L^\alpha(\mathbb{R}^2))}^\alpha = \frac{C_\alpha^\alpha}{2\pi} \sum_{n \in \mathbb{Z}} \int_{\mathbb{R}^2} |\mathcal{F}V_{\text{per,sym}}(n, \mathbf{k})|^\alpha d\mathbf{k} \\ &= \frac{C_\alpha^\alpha}{2\pi} \int_{\mathbb{R}^2} |\mathcal{F}V_{\text{per,sym}}(0, \mathbf{k})|^\alpha d\mathbf{k} + \frac{C_\alpha^\alpha}{2\pi} \sum_{n \neq 0} \int_{\mathbb{R}^2} \frac{|\mathcal{F}q_{\text{per}}(n, \mathbf{k})|^\alpha}{(4\pi n^2 + |\mathbf{k}|^2)^\alpha} d\mathbf{k} \\ &\leq C_{\alpha,1} + \frac{C_\alpha^\alpha}{2\pi} \left(\sum_{n \neq 0} \int_{\mathbb{R}^2} |\mathcal{F}q_{\text{per}}(n, \mathbf{k})|^{2\alpha} d\mathbf{k} \right)^{1/2} \left(\sum_{n \neq 0} \int_{\mathbb{R}^2} \frac{1}{(4\pi n^2 + |\mathbf{k}|^2)^{2\alpha}} d\mathbf{k} \right)^{1/2} \\ &\leq C_{\alpha,1} + C_{\alpha,2} \|\mathcal{F}q_{\text{per}}\|_{\ell^{2\alpha}(\mathbb{Z}, L^{2\alpha}(\mathbb{R}^2))}^\alpha \leq C_{\alpha,1} + C'_{\alpha,2} \|q_{\text{per}}\|_{L^q_{\text{per},x}(\Gamma)}^\alpha < +\infty, \end{aligned} \quad (3.60)$$

where the last step we have used estimates similar to (3.59) for \mathcal{F} and the fact that q_{per} belongs to $L^q_{\text{per},x}(\Gamma)$ for $4/3 < q := 2\alpha/(2\alpha - 1) \leq 2$. Therefore $V_{\text{per,sym}}$ belongs to $L^p_{\text{per},x}(\Gamma)$ for $2 < p \leq +\infty$. By the elliptic regularity we know that $V_{\text{per,sym}}$ belongs to the Sobolev space $W^{2,p}_{\text{per},x}(\Gamma)$ for $2 < p \leq 3$, where $W^{2,p}_{\text{per},x}(\Gamma)$ is the space of functions, together with their gradients and Hessians, belong to $L^p_{\text{per},x}(\Gamma)$. Approximating $V_{\text{per,sym}}$ by functions in $\mathcal{D}_{\text{per},x}(\Gamma)$, we also deduce that $V_{\text{per,sym}}$ tends to 0 when $|r|$ tends to infinity. The mean-field potential $V_{\text{per,sym}}$ defines a $-\Delta$ -bounded operator on $L^2(\mathbb{R}^3)$ with relative bound zero, hence by the Kato–Rellich theorem (see for example [Hel13, Theorem 9.10]) we know that $H_{\text{per}} = -\frac{1}{2}\Delta + V_{\text{per,sym}}$ uniquely defines a self-adjoint operator on $L^2(\mathbb{R}^3)$ with domain $H^2(\mathbb{R}^3)$ and form domain $H^1(\mathbb{R}^3)$. As H_{per} is \mathbb{Z} -translation invariant in the x -direction,

$$H_{\text{per}} = \mathcal{B}^{-1} \left(\int_{\Gamma^*} H_{\text{per},\xi} \frac{d\xi}{2\pi} \right) \mathcal{B}, \quad H_{\text{per},\xi} := -\frac{1}{2}\Delta_\xi + V_{\text{per,sym}}.$$

Note that the decomposed Hamiltonian $H_{\text{per},\xi}$ does not have a compact resolvent as Γ is not a bounded domain. It is easy to see that $\sigma(-\Delta_\xi) = \sigma_{\text{ess}}(-\Delta_\xi) = [0, +\infty)$. On the other hand, by the inequality (3.6) we have

$$\begin{aligned} &\left\| V_{\text{per,sym}} (1 - \Delta_\xi)^{-1} \right\|_{\mathfrak{S}_2} \\ &\leq \frac{1}{2\pi} \|V_{\text{per,sym}}\|_{L^2_{\text{per},x}(\Gamma)} \left(\sum_{n \in \mathbb{Z}} \int_{\mathbb{R}^2} \frac{1}{((2\pi n + \xi)^2 + |\mathbf{k}|^2 + 1)^2} d\mathbf{k} \right)^{1/2} < +\infty. \end{aligned}$$

In particular $V_{\text{per,sym}}$ is a compact perturbation of $-\Delta_\xi$, and therefore introduces at most countably many eigenvalues below 0 which are bounded from below by $-\|V_{\text{per,sym}}\|_{L^\infty}$. Denote by $\{\lambda_n(\xi)\}_{1 \leq n \leq N_H}$ these (negative) eigenvalues for $N_H \in \mathbb{N}^*$ (N_H can be finite or infinite). Then for all $\xi \in \Gamma^*$,

$$\sigma_{\text{ess}}(H_{\text{per},\xi}) = \sigma_{\text{ess}}(-\Delta_\xi) = [0, +\infty), \quad \sigma_{\text{disc}}(H_{\text{per},\xi}) = \bigcup_{1 \leq n \leq N_H} \lambda_n(\xi).$$

In view of the decomposition (3.19), a result of [RS78, Theorem XIII.85] gives the following spectral decomposition:

$$\sigma_{\text{ess}}(H_{\text{per}}) \supseteq \bigcup_{\xi \in \Gamma^*} \sigma_{\text{ess}}(H_{\text{per},\xi}) = [0, +\infty), \quad \sigma_{\text{disc}}(H_{\text{per}}) \subseteq \bigcup_{\xi \in \Gamma^*} \sigma_{\text{disc}}(H_{\text{per},\xi}) = \bigcup_{\xi \in \Gamma^*} \bigcup_{1 \leq n \leq N_H} \lambda_n(\xi).$$

We also obtain from [RS78, Item (e) of Theorem XIII.85] that

$$\lambda \in \sigma_{\text{disc}}(H_{\text{per}}) \Leftrightarrow \{\xi \in \Gamma^* \mid \lambda \in \sigma_{\text{disc}}(H_{\text{per},\xi})\} \text{ has non-trivial Lebesgue measure.}$$

By the regular perturbation theory of the point spectra [Kat95] (see also [RS78, Section XII.2]) and the approach of Thomas [Tho73, Lemma 1], we know that the eigenvalues $\lambda_n(\xi)$ below 0 are analytical functions of ξ and cannot be constant, so that $\{\xi \in \Gamma^* \mid \lambda \in \sigma_{\text{disc}}(H_{\text{per},\xi})\}$ has trivial Lebesgue measure, and the essential spectrum of H_{per} below 0 is purely absolutely continuous. As a conclusion,

$$\sigma(H_{\text{per}}) = \sigma_{\text{ess}}(H_{\text{per}}) = \bigcup_{\xi \in \Gamma^*} \sigma(H_{\text{per},\xi}).$$

The Fermi level is always negative. Let us prove that the inequality $N_H = F(0) \geq \int_{\Gamma} \mu_{\text{per,sym}}$ always holds. The physical meaning of this statement is that the Fermi level of the quasi 1D system at ground state is always negative when the mean-field potential tends to 0 in the \mathbf{r} -direction. We prove this by contradiction: assume that $F(0) < \int_{\Gamma} \mu_{\text{per,sym}}$, then we can always construct (infinitely many) states belonging to \mathcal{F}_{Γ} with positive energies arbitrarily close to 0 and they decrease the ground state energy of the problem (3.17).

Let us first define a spectral projector representing all the states of H_{per} below 0: for any $\xi \in \Gamma^*$ and $H_{\text{per},\xi}$ defined in (3.19), define

$$\gamma_{\text{per}}^- := \mathbb{1}_{(-\infty, 0]}(H_{\text{per}}), \quad \gamma_{\text{per},\xi}^0 := \mathbb{1}_{(-\infty, 0]}(H_{\text{per},\xi}).$$

Therefore,

$$N_H = F(0) = \frac{1}{|\Gamma^*|} \int_{\Gamma^*} \text{Tr}_{L^2_{\text{per},x}(\Gamma)} (\gamma_{\text{per},\xi}^0) d\xi = \int_{\Gamma} \rho_{\gamma_{\text{per}}^-}. \quad (3.61)$$

The inequality that $F(0) < \int_{\Gamma} \mu_{\text{per,sym}}$ implies that

$$Z_{\text{diff}} := \int_{\Gamma} \mu_{\text{per,sym}} - N_H = \int_{\Gamma} \mu_{\text{per,sym}} - \int_{\Gamma} \rho_{\gamma_{\text{per}}^-} \in \mathbb{N}^*. \quad (3.62)$$

The condition (3.62) implies in particular that $N_H < +\infty$, *i.e.*, that there are at most finitely many states below 0. Let us construct states of H_{per} with positive energies. These states belonging to $L^2(\mathbb{R}^3)$ approximate the plane waves of H_{per} traveling in the \mathbf{r} -direction. For $R > 0$, recall that \mathfrak{B}_R is the ball in \mathbb{R}^3 centered at 0. Consider a smooth function $t(x, \mathbf{r})$ supported in \mathfrak{B}_1 , equal to one in $\mathfrak{B}_{1/2}$ and such that $\|t\|_{L^2(\mathbb{R}^3)} = 1$. For $n \in \mathbb{N}^*$, let us define

$$\psi_n(x, \mathbf{r}) := n^{-3/2} t \left(\frac{(x, \mathbf{r}) - (n^2, (n^2, n^2))}{n} \right).$$

It is easy to see that ψ_n belongs to $L^2(\mathbb{R}^3)$, converges weakly to 0 when n tends to infinity and $\|\psi_n\|_{L^2(\mathbb{R}^3)} = 1$. Moreover, as $V_{\text{per,sym}}$ tends to 0 in the \mathbf{r} -direction, hence for any $\varepsilon > 0$ there exists an integer N_{ε} such that $|V_{\text{per,sym}}(\cdot, (n^2, n^2))| \leq \varepsilon$ when $n \geq N_{\varepsilon}$. Denote by $\{\psi_{n,\xi}\}_{n \in \mathbb{N}^*, \xi \in \Gamma^*}$ the Bloch decomposition \mathcal{B} in the x -direction (see Section 3.2.1 for the definition) of $\{\psi_n\}_{n \in \mathbb{N}^*}$ which belong to $L^2_{\text{per},x}(\Gamma)$. For $n \geq N_{\varepsilon}$, it holds

$$\begin{aligned} \left\| H_{\text{per}} \psi_n \right\|_{L^2(\mathbb{R}^3)}^2 &= \frac{1}{2\pi} \int_{\Gamma^*} \left\| H_{\text{per},\xi} \psi_{n,\xi} \right\|_{L^2_{\text{per},x}(\Gamma)}^2 d\xi \\ &= \left\| -n^{-7/2} \Delta t \left(\frac{\cdot - (n^2, (n^2, n^2))}{n} \right) + V_{\text{per,sym}} \psi_n \right\|_{L^2(\mathbb{R}^3)}^2 \leq 2 \left(\frac{1}{n^4} + \varepsilon^2 \right). \end{aligned} \quad (3.63)$$

Remark that $\gamma_{\text{per},\xi}^0 H_{\text{per},\xi} = \sum_{n=1}^{N_H} \lambda_n(\xi) P_{\{\lambda_n(\xi)\}}(H_{\text{per},\xi})$ is a compact operator, where $P_{\{\cdot\}}(H_{\text{per},\xi})$ the spectral projector of $H_{\text{per},\xi}$. There exists an orthonormal basis $\{e_{n,\xi}\}_{n \geq 1}$ of $L^2_{\text{per},x}(\Gamma)$ with elements in $H^1_{\text{per},x}(\Gamma)$ such that $\gamma_{\text{per},\xi}^0 H_{\text{per},\xi} e_{n,\xi} = \lambda_n(\xi) e_{n,\xi}$ for $1 \leq n \leq N_H$, and $\gamma_{\text{per},\xi}^0 H_{\text{per},\xi} e_{n,\xi} \equiv 0$ for $n > N_H$. Let us construct test density matrices composed by all the states of H_{per} with negative energies and some states with positive energies. More precisely, for $N_0 \in \mathbb{N}^*$ to be made precise later, consider a test density matrix

$$\gamma_{N_0} = \mathcal{B}^{-1} \left(\int_{\Gamma^*} \gamma_{N_0,\xi} \frac{d\xi}{2\pi} \right) \mathcal{B},$$

where

$$\begin{aligned} \gamma_{N_0,\xi} &:= \gamma_{\text{per},\xi}^0 + \sum_{n=N_0+1}^{N_0+Z_{\text{diff}}} (1 - \gamma_{\text{per},\xi}^0) |\psi_{n,\xi}\rangle \langle \psi_{n,\xi}| \\ &= \sum_{n=1}^{+\infty} \gamma_{\text{per},\xi}^0 |e_{n,\xi}\rangle \langle e_{n,\xi}| + \sum_{n=N_0+1}^{N_0+Z_{\text{diff}}} (1 - \gamma_{\text{per},\xi}^0) |\psi_{n,\xi}\rangle \langle \psi_{n,\xi}|. \end{aligned}$$

Lemma 3.22. *For any $N_0 \in \mathbb{N}^*$, the state γ_{N_0} belongs to the admissible set \mathcal{F}_Γ .*

Proof. It is easy to see that $0 \leq \gamma_{N_0} \leq 1$. Remark also that $\text{Ran} \left(\gamma_{\text{per},\xi}^0 \right) = \text{Span} \{e_{n,\xi}\}_{1 \leq n \leq N_H}$ for all $\xi \in \Gamma^*$. The density of γ_{N_0} can be written as

$$\rho_{\gamma_{N_0}} = \frac{1}{2\pi} \int_{\Gamma^*} \sum_{n=1}^{N_H} |e_{n,\xi}|^2 d\xi + \frac{1}{2\pi} \sum_{n=N_0+1}^{N_0+Z_{\text{diff}}} \int_{\Gamma^*} |\psi_{n,\xi}|^2 d\xi.$$

The density $\rho_{\gamma_{N_0}}$ belongs to $L^p_{\text{per}}(\Gamma)$ for $1 \leq p \leq 3$ as $\{e_{n,\xi}\}_{n \geq 1}$ and $\{\psi_{n,\xi}\}_{n \geq 1}$ belong to $H^1_{\text{per},x}(\Gamma)$. Besides, in view of (3.61),

$$\begin{aligned} \int_{\Gamma} \rho_{\gamma_{N_0}} &= \frac{1}{2\pi} \int_{\Gamma^*} \text{Tr}_{L^2_{\text{per},x}(\Gamma)} (\gamma_{\text{per},\xi}^0) d\xi + \frac{1}{2\pi} \sum_{n=N_0+1}^{N_0+Z_{\text{diff}}} \int_{\Gamma} \int_{\Gamma^*} |\psi_{n,\xi}|^2 d\xi \\ &= N_H + \sum_{n=N_0+1}^{N_0+Z_{\text{diff}}} \int_{\mathbb{R}^3} |\psi_n|^2 = N_H + Z_{\text{diff}} = \int_{\Gamma} \mu_{\text{per,sym}}. \end{aligned} \quad (3.64)$$

A simple calculation shows that $|\nabla|\gamma_{N_0,\xi}|\nabla|$ is trace-class on $L^2_{\text{per},x}(\Gamma)$. Hence γ_{N_0} belongs to $\mathcal{P}_{\text{per},x}$. Let us show that $\rho_{\gamma_{N_0}} - \mu_{\text{per,sym}}$ belongs to \mathcal{C}_Γ . Following calculations similar to the ones leading to (3.46), we only need to prove that $\mathbf{k} \mapsto |\mathbf{k}|^{-1} \mathcal{F}(\rho_{\gamma_{N_0}} - \mu_{\text{per,sym}})(0, \mathbf{k})$ is square-integrable near $\mathbf{k} = \mathbf{0}$ since $\rho_{\gamma_{N_0}} - \mu_{\text{per,sym}}$ belongs to $L^2_{\text{per},x}(\Gamma)$. Remark that $\mathcal{F}(\rho_{\gamma_{N_0}} - \mu_{\text{per,sym}})(0, \mathbf{0}) = \int_{\Gamma} \rho_{\gamma_{N_0}} - \mu_{\text{per,sym}} = 0$ and

$$\begin{aligned} \left| \partial_{\mathbf{k}} \mathcal{F}(\rho_{\gamma_{N_0}} - \mu_{\text{per,sym}})(0, \mathbf{0}) \right| &= \left| \int_{\Gamma} \mathbf{r} \left(\rho_{\gamma_{N_0}} - \mu_{\text{per,sym}} \right) (x, \mathbf{r}) dx d\mathbf{r} \right| \\ &\leq \frac{1}{2\pi} \sum_{n=1}^{N_H} \int_{\Gamma^*} \int_{\Gamma} |\mathbf{r}| |e_{n,\xi}|^2 (x, \mathbf{r}) dx d\mathbf{r} d\xi + \sum_{n=N_0+1}^{N_0+Z_{\text{diff}}} \int_{\mathbb{R}^3} |\mathbf{r}| |\psi_n|^2 (x, \mathbf{r}) dx d\mathbf{r} \\ &\quad + \int_{\Gamma} |\mathbf{r}| \mu_{\text{per,sym}}(x, \mathbf{r}) dx d\mathbf{r} < +\infty, \end{aligned}$$

where we have used the fact that the eigenfunctions of $H_{\text{per},\xi}$ associated with negative eigenvalues decay exponentially (see [HS95, Theorem 3.4] and [CT73, Theorem 1]) so that $\int_{\Gamma} |\mathbf{r}| |e_{n,\xi}|^2 (x, \mathbf{r}) dx d\mathbf{r} < +\infty$ for $1 \leq n \leq N_H$ and $\xi \in \Gamma^*$, and the fact that $\{\psi_n\}_{N_0+1 \leq n \leq N_0+Z_{\text{diff}}}$ have compact support in the \mathbf{r} -direction by definition. Therefore $\mathcal{F}(\rho_{\gamma_{N_0}} - \mu_{\text{per,sym}})(0, \mathbf{k})$ is C^1 near $\mathbf{k} = \mathbf{0}$. The conclusion then follows by arguments similar to those leading to (3.46) in Section 3.4.3. \square

Lemma 3.22 implies that we can construct many admissible states in \mathcal{F}_Γ by varying N_0 . Let us show that we can always find N_0 such that γ_{N_0} decreases the ground state energy of (3.17) if $N_H < \int_{\Gamma} \mu_{\text{per,sym}}$.

Given a minimizer $\bar{\gamma}$ of (3.17), simple expansion of the energy functional around minimal shows that $\bar{\gamma}$ also minimizes the functional (see [CDL08a])

$$\gamma \mapsto \int_{\Gamma^*} \text{Tr}_{L^2_{\text{per},x}(\Gamma)} (H_{\text{per},\xi} \gamma_\xi) d\xi$$

on \mathcal{F}_Γ . Therefore, given $N_0 \in \mathbb{N}^*$ we have

$$\begin{aligned} 0 &\leq \int_{\Gamma^*} \text{Tr}_{L^2_{\text{per},x}(\Gamma)} (H_{\text{per},\xi} (\gamma_{N_0,\xi} - \bar{\gamma}_\xi)) d\xi = \int_{\Gamma^*} \text{Tr}_{L^2_{\text{per},x}(\Gamma)} (\gamma_{\text{per},\xi}^0 H_{\text{per},\xi} (\gamma_{N_0,\xi} - \bar{\gamma}_\xi)) d\xi \\ &\quad + \int_{\Gamma^*} \text{Tr}_{L^2_{\text{per},x}(\Gamma)} ((1 - \gamma_{\text{per},\xi}^0) H_{\text{per},\xi} (\gamma_{N_0,\xi} - \bar{\gamma}_\xi)) d\xi \\ &= M + \int_{\Gamma^*} \text{Tr}_{L^2_{\text{per},x}(\Gamma)} ((1 - \gamma_{\text{per},\xi}^0) H_{\text{per},\xi} \gamma_{N_0,\xi}) d\xi - \int_{\Gamma^*} \text{Tr}_{L^2_{\text{per},x}(\Gamma)} ((1 - \gamma_{\text{per},\xi}^0) H_{\text{per},\xi} \bar{\gamma}_\xi) d\xi, \end{aligned} \quad (3.65)$$

where, since $0 \leq \overline{\gamma}_\xi \leq 1$ and $\{\lambda_n(\cdot)\}_{1 \leq n \leq N_H} < 0$,

$$\begin{aligned} M &:= \int_{\Gamma^*} \text{Tr}_{L^2_{\text{per},x}(\Gamma)} (\gamma_{\text{per},\xi}^0 H_{\text{per},\xi} (\gamma_{N_0,\xi} - \overline{\gamma}_\xi)) d\xi = \int_{\Gamma^*} \sum_{n=1}^{N_H} \lambda_n(\xi) \langle e_{n,\xi} | 1 - \gamma_{\text{per},\xi}^0 \overline{\gamma}_\xi | e_{n,\xi} \rangle d\xi \\ &= \int_{\Gamma^*} \sum_{n=1}^{N_H} \lambda_n(\xi) \langle e_{n,\xi} | 1 - \overline{\gamma}_\xi | e_{n,\xi} \rangle d\xi \leq 0. \end{aligned} \quad (3.66)$$

In view of (3.63) and by a Cauchy-Schwarz inequality, we deduce that, for $N_0 \geq N_\varepsilon$:

$$\begin{aligned} &\int_{\Gamma^*} \text{Tr}_{L^2_{\text{per},x}(\Gamma)} ((1 - \gamma_{\text{per},\xi}^0) H_{\text{per},\xi} \gamma_{N_0,\xi}) d\xi \\ &= \int_{\Gamma^*} \sum_{n=N_0+1}^{N_0+Z_{\text{diff}}} \sum_{m=1}^{+\infty} \langle e_{m,\xi} | H_{\text{per},\xi} | \psi_{n,\xi} \rangle \langle \psi_{n,\xi} | e_{m,\xi} \rangle d\xi \\ &\leq \int_{\Gamma^*} \sum_{n=N_0+1}^{N_0+Z_{\text{diff}}} \left(\sum_{m=1}^{+\infty} |\langle \psi_{n,\xi} | e_{m,\xi} \rangle|^2 \right)^{1/2} \left(\sum_{m=1}^{+\infty} |\langle e_{m,\xi} | H_{\text{per},\xi} | \psi_{n,\xi} \rangle|^2 \right)^{1/2} d\xi \\ &= \int_{\Gamma^*} \sum_{n=N_0+1}^{N_0+Z_{\text{diff}}} \|\psi_{n,\xi}\|_{L^2_{\text{per},x}(\Gamma)} \|H_{\text{per},\xi} \psi_{n,\xi}\|_{L^2_{\text{per},x}(\Gamma)} d\xi \\ &\leq 2\pi \sum_{n=N_0+1}^{N_0+Z_{\text{diff}}} \left(\frac{1}{2\pi} \int_{\Gamma^*} \|\psi_{n,\xi}\|_{L^2_{\text{per},x}(\Gamma)}^2 d\xi \right)^{1/2} \left(\frac{1}{2\pi} \int_{\Gamma^*} \|H_{\text{per},\xi} \psi_{n,\xi}\|_{L^2_{\text{per},x}(\Gamma)}^2 d\xi \right)^{1/2} \\ &\leq 2\sqrt{2}\pi \sum_{n=N_0+1}^{N_0+Z_{\text{diff}}} \left(\frac{1}{n^4} + \varepsilon^2 \right)^{1/2} \leq 2\sqrt{2}\pi Z_{\text{diff}} \left(\frac{1}{N_0^4} + \varepsilon^2 \right)^{1/2}. \end{aligned} \quad (3.67)$$

Moreover, by definition of $\overline{\gamma}_{\text{per}}$

$$\begin{aligned} &\int_{\Gamma^*} \text{Tr}_{L^2_{\text{per},x}(\Gamma)} ((1 - \gamma_{\text{per},\xi}^0) H_{\text{per},\xi} \overline{\gamma}_\xi) \\ &= \int_{\Gamma^*} \text{Tr}_{L^2_{\text{per},x}(\Gamma)} (|H_{\text{per},\xi}|^{1/2} (1 - \gamma_{\text{per},\xi}^0) \overline{\gamma}_\xi (1 - \gamma_{\text{per},\xi}^0) |H_{\text{per},\xi}|^{1/2}) \\ &= \int_{\Gamma^*} \text{Tr}_{L^2_{\text{per},x}(\Gamma)} \left((|H_{\text{per},\xi}|^{1/2} (1 - \Delta_\xi)^{-1/2}) (1 - \Delta_\xi)^{1/2} |H_{\text{per},\xi}|^{1/2} (1 - \gamma_{\text{per},\xi}^0) \overline{\gamma}_\xi (1 - \gamma_{\text{per},\xi}^0) \right) \\ &= \int_{\Gamma^*} \text{Tr}_{L^2_{\text{per},x}(\Gamma)} \left((1 - \Delta_\xi)^{1/2} |H_{\text{per},\xi}|^{1/2} (1 - \gamma_{\text{per},\xi}^0) \overline{\gamma}_\xi (1 - \gamma_{\text{per},\xi}^0) |H_{\text{per},\xi}|^{1/2} (1 - \Delta_\xi)^{-1/2} \right) \\ &= \int_{\Gamma^*} \text{Tr}_{L^2_{\text{per},x}(\Gamma)} (|H_{\text{per},\xi}|^{1/2} (1 - \gamma_{\text{per},\xi}^0) \overline{\gamma}_\xi (1 - \gamma_{\text{per},\xi}^0) |H_{\text{per},\xi}|^{1/2}) \geq 0. \end{aligned} \quad (3.68)$$

We distinguish in the inequality (3.66) the cases $M \equiv 0$ or $M < 0$. When $M \equiv 0$, the inequality (3.66) implies that $\overline{\gamma}_\xi \gamma_{\text{per},\xi}^0 = \gamma_{\text{per},\xi}^0$ for almost all $\xi \in \Gamma^*$. In view of the inequalities (3.67) and (3.68), the inequality (3.65) implies that,

$$\forall N_0 \geq N_\varepsilon, \quad 0 \leq \int_{\Gamma^*} \text{Tr}_{L^2_{\text{per},x}(\Gamma)} ((1 - \gamma_{\text{per},\xi}^0) H_{\text{per},\xi} \overline{\gamma}_\xi) d\xi \leq 2\sqrt{2}\pi Z_{\text{diff}} \left(\frac{1}{N_0^4} + \varepsilon^2 \right)^{1/2}. \quad (3.69)$$

By letting N_0 tend to infinity, it is easy to deduce that $(1 - \gamma_{\text{per},\xi}^0) \overline{\gamma}_\xi = 0$ for almost all $\xi \in \Gamma^*$. Together with the fact that $\overline{\gamma}_\xi \gamma_{\text{per},\xi}^0 = \gamma_{\text{per},\xi}^0$ we deduce that $\overline{\gamma}_\xi \equiv \gamma_{\text{per},\xi}^0$ for almost all $\xi \in \Gamma^*$. In view of (3.61) and (3.62), by the charge neutrality we obtain that

$$Z_{\text{diff}} = \int_{\Gamma} \mu_{\text{per},\text{sym}} - N_H = \int_{\Gamma} \rho_{\overline{\gamma}} - N_H = \frac{1}{|\Gamma^*|} \int_{\Gamma^*} \text{Tr}_{L^2_{\text{per},x}(\Gamma)} (\gamma_{\text{per},\xi}^0) d\xi - N_H \equiv 0.$$

Hence $\int_{\Gamma} \mu_{\text{per,sym}} = N_H = F(0)$. This also implies that the minimizer of the problem (3.17) equals to γ_{per}^- when $N_H = F(0) = \int_{\Gamma} \mu_{\text{per,sym}}$ and $Z_{\text{diff}} \equiv 0$. When $M < 0$ and $Z_{\text{diff}} \neq 0$, we can always find $\varepsilon > 0$ and $N_0 \geq N_{\varepsilon}$ such that $2\sqrt{2}\pi Z_{\text{diff}} \left(\frac{1}{N_0^4} + \varepsilon^2\right)^{1/2} \leq -M/2$. In view of the the inequalities (3.67) and (3.68), the inequality (3.65) implies that

$$\forall N_0 \geq N_{\varepsilon}, \quad 0 \leq \int_{\Gamma^*} \text{Tr}_{L^2_{\text{per},x}(\Gamma)} \left((1 - \gamma_{\text{per},\xi}^0) H_{\text{per},\xi} \overline{\gamma_{\xi}} \right) d\xi \leq M/2 < 0,$$

which leads to contradiction. We can finally conclude that $F(0) \geq \int_{\Gamma} \mu_{\text{per,sym}}$, so that the Fermi level of the quasi 1D system is always non-positive. In the following paragraph we show that the Fermi level can be chosen to be strictly negative.

Form of the minimizer and decay of the density of minimizers. We have already shown that if $N_H = F(0) \equiv \int_{\Gamma} \mu_{\text{per,sym}}$ then the 1D system has a unique minimizer which is equal to γ_{per}^- . This also implies that for almost all $\xi \in \Gamma^*$, the operator $H_{\text{per},\xi}$ has N_H strictly negative eigenvalues below 0, therefore we can always choose the Fermi level $\epsilon_F \in (\max_{\xi \in \Gamma^*} \lambda_{N_H}(\xi), 0)$. If $F(0) > \int_{\Gamma} \mu_{\text{per,sym}}$, it is clear that there exists $\epsilon_F < 0$ such that $F(\epsilon_F) = \int_{\Gamma} \mu_{\text{per,sym}}$ as $F(\kappa)$ is a non-decreasing function on $(-\infty, 0]$ with range in $[0, F(0)]$. The form of the minimizer and the uniqueness is a direct adaptation of [CDL08a, Theorem 1] by using a spectral projector decomposition similar to (A.2) of [CDL08a, Theorem 1], that is, the unique minimizer can be written as

$$\gamma_{\text{per}} = \mathbb{1}_{(-\infty, \epsilon_F]}(H_{\text{per}}) = \mathcal{B}^{-1} \left(\int_{\Gamma^*} \gamma_{\text{per},\xi} \frac{d\xi}{2\pi} \right) \mathcal{B} = \mathcal{B}^{-1} \left(\int_{\Gamma^*} \sum_{n=1}^{N_H} \mathbb{1}(\lambda_n(\xi) \leq \epsilon_F) |e_{n,\xi}\rangle \langle e_{n,\xi}| \right) \mathcal{B}, \quad (3.70)$$

where $\gamma_{\text{per},\xi} := \mathbb{1}_{(-\infty, \epsilon_F]}(H_{\text{per},\xi})$. The Fermi level $\epsilon_F < 0$ can be considered as the Lagrange multiplier associated with the charge neutrality condition

$$F(\epsilon_F) = \int_{\Gamma} \rho_{\gamma_{\text{per}}} = \int_{\Gamma} \mu_{\text{per,sym}}.$$

Once the unique minimizer is shown to be a spectral projector, we can use the exponential decay property of the eigenfunctions of $H_{\text{per},\xi}$ in the \mathbf{r} -direction via the Combe–Thomas estimate [CT73, Theorem 1]: for almost all $\xi \in \Gamma^*$, there exist positive constant $C(\xi)$ and $\alpha(\xi)$ such that

$$\forall (x, \mathbf{r}) \in \Gamma, \quad \forall 1 \leq n \leq N_H, \quad |e_{n,\xi}(x, \mathbf{r})| \leq C(\xi) e^{-\alpha(\xi)|\mathbf{r}|}.$$

On the other hand, the fact that $\int_{\Gamma} \mu_{\text{per,sym}} = F(\epsilon_F) < +\infty$ implies that there exist only finitely many states of $H_{\text{per},\xi}$ below ϵ_F for all $\xi \in \Gamma^*$. Therefore there exist positive constants C_{ϵ_F} and α_{ϵ_F} such that

$$0 \leq \rho_{\gamma_{\text{per}}}(x, \mathbf{r}) \leq \frac{1}{2\pi} \int_{\Gamma^*} \sum_{n=1}^{N_H} \mathbb{1}(\lambda_n(\xi) \leq \epsilon_F) C^2(\xi) e^{-2\alpha(\xi)|\mathbf{r}|} d\xi \leq C_{\epsilon_F} e^{-\alpha_{\epsilon_F}|\mathbf{r}|}.$$

Remark that the above exponential decay result of the density coincides with Assumption 2 that

$$\int_{\Gamma} |\mathbf{r}| \rho_{\gamma_{\text{per}}}(x, \mathbf{r}) dx d\mathbf{r} < +\infty.$$

3.4.7 Proof of Lemma 3.10

Assume that (3.23) holds, that is $\mu_{\text{per}}(x, \mathbf{r}) \equiv \mu_{\text{per}}(x, |\mathbf{r}|)$ has radial symmetry in the \mathbf{r} -direction. It is clear that the results of Theorem 3.7 hold. We employ the same notations as in Theorem 3.7 in the sequel. By the uniqueness of density, $\rho_{\gamma_{\text{per}}}$ enjoys the same radial symmetry in the \mathbf{r} -direction. Recall that $q_{\text{per}} =$

$\rho_{\gamma_{\text{per}}} - \mu_{\text{per,sym}}$. Together with the facts that $\int_{\Gamma} |\mathbf{r}| \rho_{\gamma_{\text{per}}}(x, \mathbf{r}) dx d\mathbf{r} < +\infty$ and that μ_{per} has compact support in the \mathbf{r} -direction. The radial symmetry in the \mathbf{r} -direction implies that

$$\int_{\Gamma} \mathbf{r} \cdot q_{\text{per}}(x, \mathbf{r}) dx d\mathbf{r} \equiv 0. \quad (3.71)$$

Remark also that the exponential decay of density implies that $\int_{\Gamma} |\mathbf{r}|^2 |q_{\text{per}}(x, \mathbf{r})| dx d\mathbf{r} < +\infty$. Following calculations similar to the those in (3.57), (3.58) and (3.60), it is easy to deduce that $\partial_{\mathbf{k}} \mathcal{F} q_{\text{per}}(0, \mathbf{k}) \equiv 0$ and $\partial_{\mathbf{k}}^2 \mathcal{F} q_{\text{per}}(0, \mathbf{k})$ is continuous and bounded, so that $\mathcal{F} V_{\text{per,sym}}(0, \cdot)$ belongs to $L^2(\mathbb{R}^2)$, and $V_{\text{per,sym}}$ also belongs to $L^2_{\text{per},x}(\Gamma)$. Let us prove that $V_{\text{per,sym}} \in L^p_{\text{per},x}(\Gamma)$ for $1 < p < 2$ (for which we can conclude that $V_{\text{per,sym}}$ belongs to $L^p_{\text{per},x}(\Gamma)$ for $1 < p \leq +\infty$). Let us rewrite $V_{\text{per,sym}}$ as

$$V_{\text{per,sym}}(x, \mathbf{r}) = (q_{\text{per}} \star_{\Gamma} G)(x, \mathbf{r}) = \left(q_{\text{per}} \star_{\Gamma} \tilde{G} \right)(x, \mathbf{r}) + T(\mathbf{r}), \quad (3.72)$$

where

$$T(\mathbf{r}) = -2 \int_{\mathbb{R}^2} \overline{q_{\text{per}}}(\mathbf{r}') \log(|\mathbf{r} - \mathbf{r}'|) d\mathbf{r}', \quad \overline{q_{\text{per}}}(\mathbf{r}) := \int_{-1/2}^{1/2} q_{\text{per}}(x, \mathbf{r}) dx.$$

Recall that $\mu_{\text{per,sym}}$ has compact support in the \mathbf{r} -direction, hence there exist positive constants C_q, α_q such that

$$\forall (x, \mathbf{r}) \in \mathbb{R}^3, \quad |q_{\text{per}}(\cdot, \mathbf{r})| \leq C_q e^{-\alpha_q |\mathbf{r}|}, \quad |\overline{q_{\text{per}}}(\mathbf{r})| \leq C_q e^{-\alpha_q |\mathbf{r}|}.$$

As \tilde{G} belongs to $L^p_{\text{per},x}(\Gamma)$ for $1 \leq p < 2$, by Young's convolution inequality we deduce that $q_{\text{per}} \star_{\Gamma} \tilde{G}$ belongs to $L^t_{\text{per},x}(\Gamma)$ for $1 \leq t \leq +\infty$.

It remains to prove that $T(\mathbf{r})$ belongs to $L^p(\mathbb{R}^2)$ for $1 < p < 2$. Let us use the partition $\mathbb{R}^2 = \{|\mathbf{r}| \leq 2R\} \cup \{|\mathbf{r}| > 2R\}$ for the integration domain of $T(\mathbf{r})$. Note first that $\log(|\mathbf{r}|)$ is $L^t_{\text{loc}}(\mathbb{R}^2)$ for $1 \leq t < +\infty$. Therefore, by a Cauchy-Schwarz inequality, there exists a positive constant $C_{R,1}$ such that for $p' = p/(p-1) \in (2, +\infty)$:

$$\begin{aligned} \left(\int_{|\mathbf{r}| \leq 2R} |T(\mathbf{r})|^p d\mathbf{r} \right)^{1/p} &= 2 \left(\int_{|\mathbf{r}| \leq 2R} \left| \int_{\mathbb{R}^2} \overline{q_{\text{per}}}(\mathbf{r}') \log(|\mathbf{r} - \mathbf{r}'|) d\mathbf{r}' \right|^p d\mathbf{r} \right)^{1/p} \\ &\leq 2 \left(\int_{|\mathbf{r}| \leq 2R} \left| \int_{|\mathbf{r}'| \leq 3R} \overline{q_{\text{per}}}(\mathbf{r}') \log(|\mathbf{r} - \mathbf{r}'|) d\mathbf{r}' \right|^p d\mathbf{r} \right)^{1/p} \\ &\quad + 2C_q \left(\int_{|\mathbf{r}| \leq 2R} \left| \int_{|\mathbf{r}'| > 3R} e^{-\alpha_q |\mathbf{r}'|} |\log(|\mathbf{r} - \mathbf{r}'|)| d\mathbf{r}' \right|^p d\mathbf{r} \right)^{1/p} \\ &\leq 2 \left(\int_{|\mathbf{r}'| \leq 3R} |\overline{q_{\text{per}}}|^p \right)^{1/p} \left(\int_{|\mathbf{r}| \leq 2R} \left(\int_{|\mathbf{r}'| \leq 3R} |\log(|\mathbf{r} - \mathbf{r}'|)|^{p'} d\mathbf{r}' \right)^{p/p'} d\mathbf{r} \right)^{1/p} \\ &\quad + 2C_q \left(\int_{|\mathbf{r}| \leq 2R} \left| \int_{|\mathbf{r}'| > 3R} e^{-\alpha_q |\mathbf{r}'|} |\log(|(R, R) - \mathbf{r}'|)| d\mathbf{r}' \right|^p d\mathbf{r} \right)^{1/p} \\ &\leq C_{R,1}. \end{aligned} \quad (3.73)$$

Let us look at the integration domain $\{|\mathbf{r}| > 2R\}$. Remark that by the charge neutrality condition and the radial symmetry condition (3.71), it holds, for any $\mathbf{r} \neq 0$,

$$\int_{\mathbb{R}^2} \overline{q_{\text{per}}}(\mathbf{r}') \log(|\mathbf{r}|) d\mathbf{r}' \equiv 0, \quad \int_{\mathbb{R}^2} \overline{q_{\text{per}}}(\mathbf{r}') \frac{\mathbf{r}' \cdot \mathbf{r}}{|\mathbf{r}|^2} d\mathbf{r}' \equiv 0.$$

Denote by

$$Q(\mathbf{r}, \mathbf{r}') := \log(|\mathbf{r} - \mathbf{r}'|) - \log(|\mathbf{r}|) - \frac{\mathbf{r}' \cdot \mathbf{r}}{|\mathbf{r}|^2} = \frac{1}{2} \log \left(1 - \frac{2\mathbf{r}\mathbf{r}'}{|\mathbf{r}|^2} + \frac{|\mathbf{r}'|^2}{|\mathbf{r}|^2} \right) - \frac{\mathbf{r}' \cdot \mathbf{r}}{|\mathbf{r}|^2}.$$

Then $T(\mathbf{r}) = -2 \int_{\mathbb{R}^2} \overline{q_{\text{per}}}(\mathbf{r}') Q(\mathbf{r}, \mathbf{r}') d\mathbf{r}'$. Remark that when $|\mathbf{r}| > 2R$ and $\frac{|\mathbf{r}'|}{|\mathbf{r}|} \leq \varepsilon_R$ for $\varepsilon_R > 0$ fixed. A Taylor expansion shows that there exists a positive constant C such that $|Q(\mathbf{r}, \mathbf{r}')| \leq C \frac{|\mathbf{r}'|^2}{|\mathbf{r}|^2}$. This motivates the following partition of \mathbb{R}^2 given $|\mathbf{r}| > 2R$:

$$\mathbb{R}^2 = \mathbb{B}_{\varepsilon_R} \cup \mathbb{B}_{\varepsilon_R}^c, \quad \mathbb{B}_{\varepsilon_R} := \left\{ \mathbf{r}' \in \mathbb{R}^2 \mid \frac{|\mathbf{r}'|}{|\mathbf{r}|} \leq \varepsilon_R \right\}.$$

Hence

$$T(\mathbf{r}) = T_{\text{int}}(\mathbf{r}) + T_{\text{ext}}(\mathbf{r}), \quad T_{\text{int}}(\mathbf{r}) := \int_{\mathbb{B}_{\varepsilon_R}} \overline{q_{\text{per}}}(\mathbf{r}') Q(\mathbf{r}, \mathbf{r}') d\mathbf{r}', \quad T_{\text{ext}}(\mathbf{r}) := \int_{\mathbb{B}_{\varepsilon_R}^c} \overline{q_{\text{per}}}(\mathbf{r}') Q(\mathbf{r}, \mathbf{r}') d\mathbf{r}'.$$

Therefore, for $1 < p < 2$,

$$\begin{aligned} \int_{|\mathbf{r}| > 2R} |T_{\text{int}}(\mathbf{r})|^p d\mathbf{r} &\leq 2C^p \int_{|\mathbf{r}| > 2R} \left| \int_{\mathbb{B}_{\varepsilon_R}} \overline{q_{\text{per}}}(\mathbf{r}') \frac{|\mathbf{r}'|^2}{|\mathbf{r}|^2} d\mathbf{r}' \right|^p d\mathbf{r} \\ &\leq 2C^p \int_{|\mathbf{r}| > 2R} \left| \int_{|\mathbf{r}'| \leq \varepsilon_R |\mathbf{r}|} e^{-\alpha_q |\mathbf{r}'|} |\mathbf{r}'|^2 d\mathbf{r}' \right|^p |\mathbf{r}|^{-2p} d\mathbf{r} < +\infty. \end{aligned} \quad (3.74)$$

Similarly,

$$\begin{aligned} \int_{|\mathbf{r}| > 2R} |T_{\text{ext}}(\mathbf{r})|^p d\mathbf{r} &\leq C_1 \int_{|\mathbf{r}| > 2R} \left| \int_{|\mathbf{r}'| > \varepsilon_R |\mathbf{r}|} e^{-\alpha_q |\mathbf{r}'|} |Q(\mathbf{r}, \mathbf{r}')| d\mathbf{r}' \right|^p d\mathbf{r} \\ &\leq C_1 \int_{|\mathbf{r}| > 2R} \left| \int_{|\mathbf{r}'| > \varepsilon_R |\mathbf{r}|} e^{-\alpha_q \varepsilon_R |\mathbf{r}|/2} e^{-\alpha_q |\mathbf{r}'|/2} |Q(\mathbf{r}, \mathbf{r}')| d\mathbf{r}' \right|^p d\mathbf{r} < +\infty. \end{aligned} \quad (3.75)$$

In view of (3.73), (3.74) and (3.75) we conclude that $T(\mathbf{r})$ belongs to $L^p(\mathbb{R}^2)$ for $1 < p < 2$. This leads to the conclusion that $V_{\text{per, sym}}$ belongs to $L^p_{\text{per}, x}(\Gamma)$ for $1 < p \leq +\infty$.

3.4.8 Proof of Proposition 3.11

Let us emphasize that the function χ being translation-invariant in the \mathbf{r} -direction makes it difficult to control the compactness in the \mathbf{r} -direction across the junction surface. Our geometry is very different from the cylindrical geometry considered in [HKS15] for instance which automatically provides compactness in the \mathbf{r} -direction.

The proof of $\sigma_{\text{ess}}(H_{\text{per}, L}) \cup \sigma_{\text{ess}}(H_{\text{per}, R}) \subseteq \sigma_{\text{ess}}(H_\chi)$ is relatively easier than the converse inclusion. Intuitively, the a_L -periodicity (resp. a_R -periodicity) implies that the Weyl sequences of $H_{\text{per}, L}$ (resp. $H_{\text{per}, R}$) after a translation by na_L (resp. na_R -translation) are still Weyl sequences of $H_{\text{per}, L}$ (resp. $H_{\text{per}, R}$) for any $n \in \mathbb{Z}$. This suggests that one can construct Weyl sequences of H_χ by properly translating Weyl sequences of $H_{\text{per}, L}$ or $H_{\text{per}, R}$, as H_χ is a linear interpolation of $H_{\text{per}, L}$ and $H_{\text{per}, R}$ hence behaves like $H_{\text{per}, L}$ or $H_{\text{per}, R}$ away from the junction surface. The construction of Weyl sequences of either $H_{\text{per}, L}$ or $H_{\text{per}, R}$ from Weyl sequences of H_χ is much more difficult, as the support of Weyl sequences is essentially away from any compact set, making it difficult to control their behaviors. One naive approach should be to cut-off Weyl sequences of H_χ by the function χ in order to construct Weyl sequences of $H_{\text{per}, L}$. However, one quickly remarks that the commutator $[-\Delta, \chi]$ is not $-\Delta$ -compact, hence it is difficult to ensure that the cut-off sequence is a Weyl sequence of $H_{\text{per}, L}$. Another naive approach is to use a cut-off function χ_c which has compact support in the \mathbf{r} -direction. However as mentioned before, it is also difficult to ensure that the Weyl sequences leave any mass in the support of χ_c as Weyl sequences essentially have supports away from any compact. We construct a special Weyl sequence of H_χ from $H_{\text{per}, L}$ (or $H_{\text{per}, R}$) by a suitable cut-off function which introduces $-\Delta$ -compact perturbations to solve this difficulty.

The proof is organized as follows: we first prove that $[0, +\infty) \subset \sigma_{\text{ess}}(H_\chi)$ by an explicit construction of Weyl sequences with positive energies, as $[0, +\infty)$ belongs to the essential spectrum of $H_{\text{per}, L}$ and $H_{\text{per}, R}$.

We next prove for any $\lambda < 0$ such that $\lambda \in \sigma_{\text{ess}}(H_{\text{per},L}) \cup \sigma_{\text{ess}}(H_{\text{per},R})$, λ also belongs to $\sigma_{\text{ess}}(H_\chi)$. Finally we prove that $\sigma_{\text{ess}}(H_\chi)$ is included in $\sigma_{\text{ess}}(H_{\text{per},L}) \cup \sigma_{\text{ess}}(H_{\text{per},R})$ by a rather technical construction of a Weyl sequence.

The essential spectrum $\sigma_{\text{ess}}(H_\chi)$ contains $[0, +\infty)$. Recall that a sequence $\{\psi_n\}_{n \in \mathbb{N}^*}$ is a Weyl sequence of an operator O on $L^2(\mathbb{R}^3)$ associated with $\lambda \in \mathbb{R}$ if the following properties are satisfied:

- for all n , ψ_n is in the domain of the operator O and $\|\psi_n\|_{L^2(\mathbb{R}^3)} = 1$;
- the sequence $\psi_n \rightharpoonup 0$ weakly in $L^2(\mathbb{R}^3)$;
- $\lim_{n \rightarrow +\infty} \|(O - \lambda)\psi_n\|_{L^2(\mathbb{R}^3)} = 0$.

Consider a $C_c^\infty(\mathbb{R})$ function $f(z)$ supported on $[0, 1]$ with $\int_{\mathbb{R}} |f|^2 = 1$, and $g \in C_c(\mathbb{R}^2)$ supported on the unit disk centered at 0 and such that $\int_{\mathbb{R}^2} |g|^2 = 1$. For any $\lambda > 0$, consider a sequence of functions $\{\psi_n\}_{n \in \mathbb{N}^*}$ defined as follows:

$$\psi_n(x, y, z) := n^{-3/2} e^{i\sqrt{\lambda}z} f((z - 2n)/n) g(x/n, y/n).$$

It is easy to see that $\int_{\mathbb{R}^3} |\psi_n|^2 = 1$ for all $n \in \mathbb{N}^*$, and that ψ_n tends weakly to 0 in $L^2(\mathbb{R}^3)$. On the other hand

$$\begin{aligned} (H_\chi - \lambda)\psi_n(x, y, z) &= \left(-n^{-2} f''((z - 2n)/n) - 2i\sqrt{\lambda} n^{-1} f'((z - 2n)/n) \right) n^{-3/2} e^{i\sqrt{\lambda}z} g(x/n, y/n) \\ &\quad - n^{-7/2} e^{i\sqrt{\lambda}z} f((z - 2n)/n) (\Delta g)(x/n, y/n) + V_\chi \psi_n(x, y, z). \end{aligned}$$

Recall also that by the results of Theorem 3.7, there exists for any $\epsilon > 0$ an integer N_ϵ such that

$$|V_\chi(x, y, 2n)| \leq \epsilon \text{ when } n \geq N_\epsilon.$$

Therefore, for $n \geq N_\epsilon$, there exists a positive constant C such that

$$\begin{aligned} \|(H_\chi - \lambda)\psi_n\|_{L^2(\mathbb{R}^3)} &\leq \frac{1}{n^2} \|f''\|_{L^2(\mathbb{R})} \|g\|_{L^2(\mathbb{R}^2)} + \frac{2\sqrt{\lambda}}{n} \|f'\|_{L^2(\mathbb{R})} \|g\|_{L^2(\mathbb{R}^2)} + \frac{1}{n^2} \|f\|_{L^2(\mathbb{R})} \|\Delta g\|_{L^2(\mathbb{R}^2)} \\ &\quad + \left(n^{-3} \int_{\mathbb{R}^2} \left(\int_{2n}^{3n} |V_\chi(x, y, z) f((z - 2n)/n)|^2 dz \right) |g(x/n, y/n)|^2 dx dy \right)^{1/2} \\ &\leq \frac{C}{n} + \left(\int_{\mathbb{R}^2} \int_0^1 |V_\chi(nx, ny, 2n + nz) f(z)|^2 |g(x, y)|^2 dz dx dy \right)^{1/2} \\ &\leq \frac{C}{n} + \epsilon \|f\|_{L^2(\mathbb{R})} \|g\|_{L^2(\mathbb{R}^2)} = \frac{C}{n} + \epsilon. \end{aligned}$$

This shows that $\{\psi_n\}_{n \in \mathbb{N}^*}$ is a Weyl sequence of H_χ associated with $\lambda > 0$. Since that 0 is an accumulation point of $\sigma_{\text{ess}}(H_\chi)$, it holds $[0, +\infty) \subset \sigma_{\text{ess}}(H_\chi)$.

The union of $\sigma_{\text{ess}}(H_{\text{per},L}) \cup \sigma_{\text{ess}}(H_{\text{per},R})$ is included in $\sigma_{\text{ess}}(H_\chi)$. Without loss of generality we prove that a negative λ_L belonging to $\sigma_{\text{ess}}(H_{\text{per},L})$ also belongs to $\sigma_{\text{ess}}(H_\chi)$. Consider a Weyl sequence $\{w_n\}_{n \in \mathbb{N}^*}$ for $H_{\text{per},L}$ associated with λ_L . Let us construct a Weyl sequence for H_χ from $\{w_n\}_{n \in \mathbb{N}^*}$. Fix $n \in \mathbb{N}^*$, there exists a sequence $\{v_{k,n}\}_{k \in \mathbb{N}^*}$ belonging to $C_c^\infty(\mathbb{R}^3)$ such that for all $\epsilon > 0$, there exists a $K_n \in \mathbb{N}^*$ such that for any $k \geq K_n$,

$$\|v_{k,n} - w_n\|_{H^2(\mathbb{R}^3)} \leq \epsilon. \quad (3.76)$$

It is easy to see that $v_{K_n,n}$ tends weakly to 0 in $L^2(\mathbb{R}^3)$ as $n \rightarrow \infty$ since w_n converges weakly to 0. As $v_{K_n,n}$ has compact support, for any fixed $n \in \mathbb{N}^*$ and for $m \in \mathbb{N}^*$ large enough,

$$\text{supp}(\tau_{a_L m}^x v_{K_n,n}) \cap \left(([-a_L/2, +\infty) \times \mathbb{R}^2) \cup \mathfrak{B}_n \right) = \emptyset, \quad (3.77)$$

where \mathfrak{B}_n denotes the ball of radius n centered at 0 in \mathbb{R}^3 . Remark that the above equality also ensures that $\tau_{a_L m}^x v_{K_n, n}$ tends weakly to 0 in $L^2(\mathbb{R}^3)$ when $m \rightarrow +\infty$ for n fixed. In view of (3.76) and (3.77), we introduce $\widetilde{w}_n := \tau_{a_L m_n}^x v_{K_n, n}$ for $n \in \mathbb{N}^*$ so that (3.77) is satisfied. This implies that \widetilde{w}_n tends weakly to 0 in $L^2(\mathbb{R}^3)$ when $n \rightarrow +\infty$. Moreover, in view of (3.76) and by the definition of the Weyl sequence

$$\begin{aligned} \left\| (H_\chi - \lambda_L) \widetilde{w}_n \right\|_{L^2} &= \left\| (H_\chi - \lambda_L) \tau_{a_L m_n}^x v_{K_n, n} \right\|_{L^2} = \left\| (H_{\text{per}, L} - \lambda_L) \tau_{a_L m_n}^x v_{K_n, n} \right\|_{L^2} \\ &\leq \left\| \tau_{a_L m_n}^x (H_{\text{per}, L} - \lambda_L) (v_{K_n, n} - w_n) \right\|_{L^2} + \left\| \tau_{a_L m_n}^x (H_{\text{per}, L} - \lambda_L) w_n \right\|_{L^2} \\ &\leq (1 + \|V_{\text{per}, L}\|_{L^\infty} + |\lambda_L|) \left\| v_{K_n, n} - w_n \right\|_{H^2} + \left\| (H_{\text{per}, L} - \lambda_L) w_n \right\|_{L^2} \xrightarrow{n \rightarrow +\infty} 0. \end{aligned}$$

Therefore the sequence $\widetilde{w}_n / \|\widetilde{w}_n\|_{L^2}$ is a Weyl sequence of H_χ associated with λ_L . This leads to the conclusion that

$$\sigma_{\text{ess}}(H_{\text{per}, L}) \cup \sigma_{\text{ess}}(H_{\text{per}, R}) \subseteq \sigma_{\text{ess}}(H_\chi). \quad (3.78)$$

The essential spectrum $\sigma_{\text{ess}}(H_\chi)$ is included in $\sigma_{\text{ess}}(H_{\text{per}, L}) \cup \sigma_{\text{ess}}(H_{\text{per}, R})$. We prove that for strictly negative $\lambda \in \sigma_{\text{ess}}(H_\chi)$, it holds that $\lambda \in \sigma_{\text{ess}}(H_{\text{per}, L}) \cup \sigma_{\text{ess}}(H_{\text{per}, R})$. The main technique is to use spreading sequences (Zhislin sequences) [GS11, Definition 5.12], which are special Weyl sequences for which the supports of the functions move off to infinity. More precisely, a sequence $\{\psi_n\}_{n \in \mathbb{N}^*}$ is a spreading sequence of an operator O on $L^2(\mathbb{R}^3)$ associated with λ if the following properties are satisfied:

- for all n , ψ_n is in the domain of the operator O and $\|\psi_n\|_{L^2(\mathbb{R}^3)} = 1$;
- for any bounded set $\mathcal{G} \subset \mathbb{R}^3$, $\text{supp}(\psi_n) \cap \mathcal{G} = \emptyset$ for n sufficiently large. As a consequence, $\psi_n \rightharpoonup 0$ weakly in $L^2(\mathbb{R}^3)$;
- $\lim_{n \rightarrow +\infty} \|(O - \lambda) \psi_n\|_{L^2(\mathbb{R}^3)} = 0$.

As $V_{\text{per}, L}$ and $V_{\text{per}, R}$ are continuous and bounded by Theorem 3.7, it holds by [GS11, Theorem 5.14] that

$$\sigma_{\text{ess}}(H_\theta) = \{\lambda \in \mathbb{C} \mid \text{there is a spreading sequence for } H_\theta \text{ and } \lambda\}$$

with H_θ being H_χ , $H_{\text{per}, L}$ or $H_{\text{per}, R}$. The results of Theorem 3.7 also imply that, for any $\varepsilon > 0$, there exists a constant \mathcal{R}_ε such that

$$\max \left(\|V_{\text{per}, L} \mathbf{1}_{|\mathbf{r}| > \mathcal{R}_\varepsilon}\|_{L^\infty(\mathbb{R}^3)}, \|V_{\text{per}, R} \mathbf{1}_{|\mathbf{r}| > \mathcal{R}_\varepsilon}\|_{L^\infty(\mathbb{R}^3)} \right) < \varepsilon. \quad (3.79)$$

Consider a spreading sequence $\{\phi_n\}_{n \in \mathbb{N}^*}$ for H_χ associated with $\lambda < 0$. For all $n \in \mathbb{N}^*$,

$$\text{either } \|\phi_n\|_{L^2((0, +\infty) \times \mathbb{R}^2)} \geq 1/2 \text{ or } \|\phi_n\|_{L^2((-\infty, 0] \times \mathbb{R}^2)} \geq 1/2.$$

Without loss of generality, we assume in the sequel that there exists a sub-sequence $\{\phi_n\}_{n \in \mathbb{N}^*}$ such that, for n sufficiently large, $\|\phi_n\|_{L^2((0, +\infty) \times \mathbb{R}^2)} \geq 1/2$. We next construct a Weyl sequence of $H_{\text{per}, R}$ from $\{\phi_n\}_{n \in \mathbb{N}^*}$ by constructing a special weight function ρ which has a non-trivial mass on $(0, +\infty) \times \mathbb{R}^2$, and whose derivatives decay rapidly:

$$\rho(x) := \frac{\int_{-\infty}^x \eta(y) dy}{\|\eta\|_{L^1(\mathbb{R})}},$$

where

$$\eta = \frac{e^{-2\sqrt{-\lambda}|x|}}{3\lambda} - \frac{2e^{-\sqrt{-\lambda}|x|}}{3\lambda}$$

is the solution of the following one-dimensional Yukawa equation

$$-\eta'' - \lambda\eta = e^{-2\sqrt{-\lambda}|x|}. \quad (3.80)$$

The following lemma summarizes some properties of the weight function ρ .

Lemma 3.23. *It holds that $0 \leq \rho \leq 1$ and $\lim_{n \rightarrow \infty} \|\rho \phi_n\|_{L^2} \neq 0$. Moreover,*

$$\|\rho'' \phi_n + 2\rho' \partial_x \phi_n\|_{L^2} \xrightarrow{n \rightarrow \infty} 0, \quad \rho \chi^2 (V_{\text{per},L} - V_{\text{per},R}) \in L^2(\mathbb{R}^3). \quad (3.81)$$

We postpone the proof of this lemma to Section 3.4.9. Define $w_n := \rho \phi_n / \|\rho \phi_n\|_{L^2}$. Let us show that $\{w_n\}_{n \in \mathbb{N}^*}$ is a spreading sequence of $H_{\text{per},R}$ associated with λ . First of all, the sequence $\{w_n\}_{n \in \mathbb{N}^*}$ is well defined at least for large n as $\lim_{n \rightarrow \infty} \|\rho \phi_n\|_{L^2} \neq 0$. It is also easy to see that $\|w_n\|_{L^2} = 1$ for all $n \in \mathbb{N}^*$. For any bounded set $\mathcal{G} \in \mathbb{R}^3$, it holds $\text{supp}(w_n) \cap \mathcal{G} = \emptyset$ for n sufficiently large as $\{\phi_n\}_{n \in \mathbb{N}^*}$ is a spreading sequence. Note that

$$(H_{\text{per},R} - \lambda) w_n = \frac{1}{\|\rho \phi_n\|_{L^2}} (\rho (H_\chi - \lambda) \phi_n + A_\chi \phi_n), \quad (3.82)$$

where $A_\chi := -\frac{1}{2}\rho'' - \rho' \partial_x + \rho \chi^2 (V_{\text{per},L} - V_{\text{per},R})$. As $\lim_{n \rightarrow \infty} \|(H_\chi - \lambda) \phi_n\|_{L^2} = 0$ by definition of the spreading sequence, it follows that $\lim_{n \rightarrow \infty} \|\rho (H_\chi - \lambda) \phi_n\|_{L^2} \leq \lim_{n \rightarrow \infty} \|(H_\chi - \lambda) \phi_n\|_{L^2} = 0$. It therefore suffices to prove that (possibly up to extraction) $\lim_{n \rightarrow \infty} \|A_\chi \phi_n\|_{L^2} = 0$. By the Kato–Seiler–Simon inequality (3.39) we obtain that

$$\left\| (1 - \Delta)^{-1} \rho \chi^2 (V_{\text{per},L} - V_{\text{per},R}) \right\|_{\mathfrak{S}_2} \leq \frac{1}{2\sqrt{\pi}} \left\| \rho \chi^2 (V_{\text{per},L} - V_{\text{per},R}) \right\|_{L^2(\mathbb{R}^3)}.$$

In particular $\rho \chi^2 (V_{\text{per},L} - V_{\text{per},R})$ is $-\Delta$ -compact, hence $H_{\text{per},R}$ -compact by the boundedness of $V_{\text{per},R}$. As the sequence $H_{\text{per},R} w_n$ is bounded in $L^2(\mathbb{R}^3)$, the $H_{\text{per},R}$ -compactness of $\rho \chi^2 (V_{\text{per},L} - V_{\text{per},R})$ implies that $\rho \chi^2 (V_{\text{per},L} - V_{\text{per},R}) w_n$ converges strongly to some function $v \in L^2(\mathbb{R}^3)$. On the other hand, for any $f \in L^2(\mathbb{R}^3)$,

$$(v, f)_{L^2} = \lim_{n \rightarrow +\infty} (\rho \chi^2 (V_{\text{per},L} - V_{\text{per},R}) w_n, f)_{L^2} = \lim_{n \rightarrow +\infty} (w_n, \rho \chi^2 (V_{\text{per},L} - V_{\text{per},R}) f)_{L^2} = 0,$$

where we have used the fact that $w_n \rightharpoonup 0$ and $\rho \chi^2 (V_{\text{per},L} - V_{\text{per},R}) \in L^\infty(\mathbb{R}^3)$ so

$$\rho \chi^2 (V_{\text{per},L} - V_{\text{per},R}) f \in L^2(\mathbb{R}^3).$$

Therefore by the uniqueness of weak limit, $\rho \chi^2 (V_{\text{per},L} - V_{\text{per},R}) w_n$ converges strongly to $v \equiv 0$. Together with (3.81) we conclude that $\lim_{n \rightarrow \infty} \|A \phi_n\|_{L^2} = 0$. Therefore in view of (3.82), it holds

$$\lim_{n \rightarrow \infty} \|(H_{\text{per},R} - \lambda) w_n\|_{L^2} = 0.$$

Hence $\{w_n\}_{n \in \mathbb{N}}$ is a spreading sequence of $H_{\text{per},R}$ associated with $\lambda < 0$. This implies that for any spreading sequence of H_χ associated with $\lambda < 0$, we can construct a spreading sequence for either $H_{\text{per},L}$ or $H_{\text{per},R}$ associated with $\lambda < 0$, depending on whether (up to extraction) the spreading sequence of H_χ has non-trivial mass on $((-\infty, 0] \times \mathbb{R}^2)$ or $((0, +\infty) \times \mathbb{R}^2)$. This allows us to conclude that

$$\sigma_{\text{ess}}(H_\chi) \subseteq \sigma_{\text{ess}}(H_{\text{per},L}) \cup \sigma_{\text{ess}}(H_{\text{per},R}). \quad (3.83)$$

By gathering (3.78) and (3.83) we conclude that $\sigma_{\text{ess}}(H_\chi) \equiv \sigma_{\text{ess}}(H_{\text{per},L}) \cup \sigma_{\text{ess}}(H_{\text{per},R})$. In particular, $\sigma_{\text{ess}}(H_\chi)$ is independent of the function $\chi \in \mathcal{X}$.

3.4.9 Proof of Lemma 3.23

The solution of the one-dimensional Yukawa equation (3.80) is

$$0 < \eta(x) = \int_{\mathbb{R}} \frac{e^{-\sqrt{-\lambda}|x-y|}}{2\sqrt{-\lambda}} e^{-2\sqrt{-\lambda}|y|} dy \leq \int_{\mathbb{R}} \frac{e^{-\sqrt{-\lambda}(|x|+|y|)}}{2\sqrt{-\lambda}} dy \leq \frac{1}{-\lambda} e^{-\sqrt{-\lambda}|x|}. \quad (3.84)$$

This implies that η belongs to $L^p(\mathbb{R})$ for $1 \leq p \leq +\infty$. As $\eta > 0$ is integrable, the weight function $\rho(x) = \frac{\int_{-\infty}^x \eta(y) dy}{\|\eta\|_{L^1(\mathbb{R})}}$ is well defined. It is easy to see that $0 \leq \rho \leq 1$. Since $\|\phi_n\|_{L^2((0,+\infty) \times \mathbb{R}^2)} \geq 1/2$ for n large enough and $\rho(x) \geq \frac{1}{2}$ for $x \geq 0$, hence $\lim_{n \rightarrow \infty} \|\rho \phi_n\|_{L^2(\mathbb{R}^3)} \neq 0$.

Let us next prove that $\|\rho'' \phi_n + 2\rho' \partial_x \phi_n\|_{L^2} \xrightarrow{n \rightarrow \infty} 0$. In view of (3.84),

$$\begin{aligned} |\eta'(x)| &= \frac{1}{2} \left| \int_{-\infty}^{\infty} e^{-\sqrt{-\lambda}|x-y|-2\sqrt{-\lambda}|y|} (\mathbf{1}_{x \leq y} - \mathbf{1}_{x > y}) dy \right| \\ &\leq \int_{-\infty}^{+\infty} e^{-\sqrt{-\lambda}|x-y|-2\sqrt{-\lambda}|y|} dy = \sqrt{-\lambda} \eta(x) \leq \frac{1}{\sqrt{-\lambda}} e^{-\sqrt{-\lambda}|x|}. \end{aligned}$$

Combining the above inequality with (3.84) we obtain that

$$\begin{aligned} \|\rho'' \phi_n + 2\rho' \partial_x \phi_n\|_{L^2(\mathbb{R}^3)}^2 &= \frac{\|\eta' \phi_n + 2\eta \partial_x \phi_n\|_{L^2(\mathbb{R}^3)}^2}{\|\eta\|_{L^1(\mathbb{R})}^2} \leq \frac{2}{\|\eta\|_{L^1(\mathbb{R})}^2} \int_{\mathbb{R}^3} \left((\eta')^2 |\phi_n|^2 + 4\eta^2 |\partial_x \phi_n|^2 \right) \\ &\leq \frac{2}{|\lambda| \|\eta\|_{L^1(\mathbb{R})}^2} \int_{\mathbb{R}^3} e^{-2\sqrt{-\lambda}|\cdot|} |\phi_n|^2 + \frac{8\|\eta\|_{L^\infty}}{\|\eta\|_{L^1(\mathbb{R})}^2} \int_{\mathbb{R}^3} \eta |\partial_x \phi_n|^2. \end{aligned} \quad (3.85)$$

It suffices to prove that each of the previous integrals tends to 0 when $n \rightarrow \infty$. Remark that the integrands of these terms appear when one does an explicit calculation of $(\eta(-\Delta - \lambda)\phi_n, (-\Delta - \lambda)\phi_n)$. Let us therefore first prove that

$$(\eta(-\Delta - \lambda)\phi_n, (-\Delta - \lambda)\phi_n)_{L^2(\mathbb{R}^3)} \xrightarrow{n \rightarrow \infty} 0.$$

For this purpose, we prove that $\|\eta(-\Delta - \lambda)\phi_n\|_{L^2(\mathbb{R}^3)} \xrightarrow{n \rightarrow \infty} 0$ strongly and $(-\Delta - \lambda)\phi_n \xrightarrow{n \rightarrow \infty} 0$ weakly in $L^2(\mathbb{R}^3)$. In view of (3.84), for any $\varepsilon > 0$ there exists $x_\varepsilon > 0$ such that when $|x| > x_\varepsilon$, $0 \leq \eta(x) \leq \varepsilon$. Together with (3.79) and the fact that $\{\phi_n\}_{n \in \mathbb{N}^*}$ is a spreading sequence, it holds

$$\begin{aligned} \|\eta V_\chi \phi_n\|_{L^2(\mathbb{R}^3)}^2 &= \int_{\mathbb{R} \times \{|r| > R_\varepsilon\}} |\eta V_\chi \phi_n|^2 + \int_{[-x_0, x_0] \times \{|r| \leq R_\varepsilon\}} |\eta V_\chi \phi_n|^2 + \int_{[-x_0, x_0]^c \times \{|r| \leq R_\varepsilon\}} |\eta V_\chi \phi_n|^2 \\ &\leq \varepsilon \|\eta\|_{L^\infty(\mathbb{R})}^2 + \|\eta V_\chi\|_{L^\infty(\mathbb{R})}^2 \left\| \phi_n \mathbf{1}_{[-x_0, x_0] \times \{|r| \leq R_\varepsilon\}} \right\|_{L^2(\mathbb{R})}^2 + \varepsilon \|V_\chi\|_{L^\infty(\mathbb{R}^3)}^2 \xrightarrow{n \rightarrow \infty} 0. \end{aligned}$$

The above convergence allows us to conclude that

$$\|\eta(-\Delta - \lambda)\phi_n\|_{L^2(\mathbb{R}^3)} \leq \|\eta(H_\chi - \lambda)\phi_n\|_{L^2(\mathbb{R}^3)} + \|\eta V_\chi \phi_n\|_{L^2(\mathbb{R}^3)} \xrightarrow{n \rightarrow \infty} 0. \quad (3.86)$$

Moreover, for all $n \in \mathbb{N}^*$, ϕ_n belongs to $H^2(\mathbb{R}^3)$, which is continuously embedded in $L^\infty(\mathbb{R}^3)$. Approximating ϕ_n by $C_c^\infty(\mathbb{R}^3)$ functions we deduce that $\lim_{|x| \rightarrow \infty} |\phi_n(x)| = 0$. Furthermore, remark that for any $\psi \in C_c^\infty(\mathbb{R}^3)$ it holds

$$((-\Delta - \lambda)\phi_n, \psi)_{L^2(\mathbb{R}^3)} = (\phi_n, (-\Delta - \lambda)\psi)_{L^2(\mathbb{R}^3)} \xrightarrow{n \rightarrow \infty} 0,$$

which implies the weak convergence $(-\Delta - \lambda)\phi_n \xrightarrow{n \rightarrow \infty} 0$ by the density of $C_c^\infty(\mathbb{R}^3)$ in $L^2(\mathbb{R}^3)$. Together with the strong convergence (3.86) and an integration by parts, this leads to,

$$\begin{aligned} (\eta(-\Delta - \lambda)\phi_n, (-\Delta - \lambda)\phi_n)_{L^2(\mathbb{R}^3)} &= \int_{\mathbb{R}^3} \eta |\Delta \phi_n|^2 + \eta \lambda \overline{\Delta \phi_n} \phi_n + \lambda \eta \Delta \phi_n \overline{\phi_n} + \eta \lambda^2 |\phi_n|^2 \\ &= \int_{\mathbb{R}^3} \eta |\Delta \phi_n|^2 - \lambda \eta' \partial_x (|\phi_n|^2) - 2\eta \lambda |\nabla \phi_n|^2 + \lambda^2 \eta |\phi_n|^2 \\ &= \int_{\mathbb{R}^3} \eta |\Delta \phi_n|^2 + (\lambda \eta'' + \lambda^2 \eta) |\phi_n|^2 + 2\eta |\lambda| |\nabla \phi_n|^2 \xrightarrow{n \rightarrow \infty} 0. \end{aligned}$$

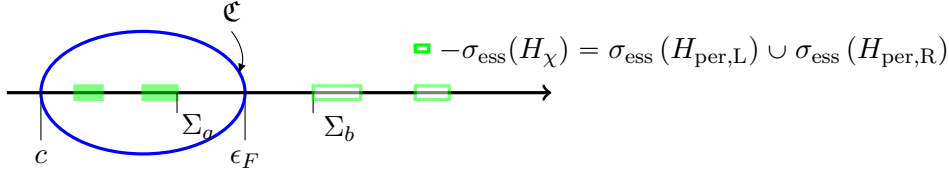


Figure 3.5: The essential spectrum of H_χ , $H_{\text{per},L}$ and $H_{\text{per},R}$, and the contour \mathfrak{C} .

In view of (3.80) we have $(\lambda\eta'' + \lambda^2\eta) = -\lambda e^{-2\sqrt{-\lambda}|\cdot|} > 0$, hence the integrand of the above integral is positive. This implies that

$$\int_{\mathbb{R}^3} e^{-2\sqrt{-\lambda}|\cdot|} |\phi_n|^2 \xrightarrow{n \rightarrow \infty} 0, \quad \int_{\mathbb{R}^3} \eta |\nabla \phi_n|^2 \xrightarrow{n \rightarrow \infty} 0. \quad (3.87)$$

In view of (3.85) and (3.87), we deduce that $\|\rho''\phi_n + 2\rho'\partial_x\phi_n\|_{L^2(\mathbb{R}^3)}^2 \xrightarrow{n \rightarrow \infty} 0$. Let us finally prove that

$$\rho\chi^2(V_{\text{per},L} - V_{\text{per},R}) \in L^2(\mathbb{R}^3).$$

By definition of χ , the function $\rho\chi^2$ has support in $(-\infty, a_R/2]$ and is equal to $\rho(x)$ when $x \in (-\infty, -a_L/2)$. Remark also that (3.84) implies that

$$\forall x < 0, \quad \rho(x) \leq \frac{1}{\|\eta\|_{L^1}} \int_{-\infty}^x \frac{1}{|\lambda|} e^{-\sqrt{-\lambda}|y|} dy \leq \frac{1}{|\lambda|^{3/2} \|\eta\|_{L^1}} e^{\sqrt{-\lambda}x}.$$

Hence, as $V_{\text{per},L} \in L^s_{\text{per},x}(\Gamma_L)$ for $1 < s \leq \infty$ by Theorem 3.7,

$$\begin{aligned} \int_{\mathbb{R}^3} (\rho\chi^2 V_{\text{per},L})^2 &= \int_{(-\infty, -a_L/2) \times \mathbb{R}^2} (\rho V_{\text{per},L})^2 + \int_{[-a_L/2, a_R/2] \times \mathbb{R}^2} (\rho\chi^2 V_{\text{per},L})^2 \\ &\leq \frac{\|V_{\text{per},L}\|_{L^2(\Gamma_{a_L})}^2}{|\lambda|^{3/2} \|\eta\|_{L^1(\mathbb{R})}^2} \sum_{n=0}^{+\infty} e^{-2\sqrt{-\lambda}a_L n} + \int_{[-a_L/2, a_R/2] \times \mathbb{R}^2} V_{\text{per},L}^2 < +\infty. \end{aligned}$$

This implies that $\rho\chi^2 V_{\text{per},L} \in L^2(\mathbb{R}^3)$. Similar arguments show that $\rho\chi^2 V_{\text{per},R} \in L^2(\mathbb{R}^3)$, which concludes the proof of the lemma.

3.4.10 Proof of Proposition 3.12

In view of Proposition 3.11, consider a contour \mathfrak{C} in the complex plane enclosing the spectrum of H_χ below the Fermi level ϵ_F without intersecting it, crossing the real axis at

$$c < \inf \{-\|V_{\text{per},L}\|_{L^\infty}, -\|V_{\text{per},R}\|_{L^\infty}\}.$$

See Fig. 3.5. This is possible even if ϵ_F is an eigenvalue: one can always slightly move the curve \mathfrak{C} below ϵ_F in order to bypass ϵ_F but still enclose all the spectrum of H_χ below ϵ_F . Let us introduce the following estimates, which are useful to characterize the decay property of densities.

Lemma 3.24 (Combes-Thomas estimate [Klo95, CT73, GK03]). *Consider $H := -\frac{1}{2}\Delta + V$ with $V \in L^\infty(\mathbb{R}^3)$. Let p, q be positive integers such that $pq > 3/2$. Then there exists $\varepsilon > 0$ and a positive constant $C(p, q)$ such that for any $\zeta \notin \sigma(H)$, and any $(\alpha, \beta) \in \mathbb{Z}^3 \times \mathbb{Z}^3$,*

$$\left\| w_\alpha (\zeta - H)^{-p} w_\beta \right\|_{\mathfrak{S}_q} \leq C(p, q) \left(1 + \frac{1}{\theta(\zeta, V)} \right)^{4p} e^{-\varepsilon\theta(\zeta, V)|\alpha - \beta|}, \quad (3.88)$$

where $\theta(\zeta, V) = \frac{\text{dist}(\zeta, \sigma(H))}{|\zeta| + \|V\|_{L^\infty} + 1}$.

Since V_χ belongs to $L^\infty(\mathbb{R}^3)$, the following lemma is a direct adaption of [CDL08a, Lemma 1]:

Lemma 3.25. *Under Assumption 3, there exist two positive constants c_1, c_2 such that*

$$\forall \zeta \in \mathfrak{C}, \quad c_1(1 - \Delta) \leq |H_\chi - \zeta| \leq c_2(1 - \Delta)$$

as operators on $L^2(\mathbb{R}^3)$, where recall that \mathfrak{C} is a contour in the complex plane enclosing the spectrum of H_χ below the Fermi level ϵ_F without intersecting it, crossing the real axis at $c < \inf \{-\|V_{\text{per},L}\|_{L^\infty}, -\|V_{\text{per},R}\|_{L^\infty}\}$. In particular

$$\left\| |H_\chi - \zeta|^{1/2}(1 - \Delta)^{-1/2} \right\| \leq \sqrt{c_2}, \quad \left\| |H_\chi - \zeta|^{-1/2}(1 - \Delta)^{1/2} \right\| \leq \frac{1}{\sqrt{c_1}}.$$

Moreover, $(H_\chi - \zeta)(1 - \Delta)^{-1}$ and its inverse are bounded operators.

Let us turn to the proof of Proposition 3.12. First of all let us show that γ_χ is locally trace class. Consider $\varrho \in C_c^\infty(\mathbb{R}^3)$. Remark that γ_χ is a spectral projector. In view of Lemma 3.25, by Cauchy's resolvent formula and the Kato–Seiler–Simon inequality (3.39), there exists a positive constant C_χ such that

$$\|\varrho \gamma_\chi \varrho\|_{\mathfrak{S}_1} = \|\varrho \gamma_\chi \gamma_\chi \varrho\|_{\mathfrak{S}_1} = \|\varrho \gamma_\chi\|_{\mathfrak{S}_2}^2 = \left\| \varrho \oint_{\mathfrak{C}} \frac{1}{2i\pi} \frac{1}{\zeta - H_\chi} d\zeta \right\|_{\mathfrak{S}_2}^2 \leq C_\chi \left\| \varrho \frac{1}{1 - \Delta} \right\|_{\mathfrak{S}_2}^2 \leq \frac{C_\chi}{4\pi} \|\varrho\|_{L^2(\mathbb{R}^3)}^2.$$

This implies that γ_χ is locally trace class so that its density ρ_χ is well defined in $L^1_{\text{loc}}(\mathbb{R}^3)$. Let us prove that $\chi^2 \rho_{\text{per},L} + (1 - \chi^2) \rho_{\text{per},R} - \rho_\chi$ belongs to $L^p(\mathbb{R}^3)$ for $1 < p \leq 2$. It is difficult to directly compare the difference of $\chi^2 \rho_{\text{per},L} + (1 - \chi^2) \rho_{\text{per},R}$ and ρ_χ . We construct to this end a density operator γ_d whose density ρ_d is equal to $\chi^2 \rho_{\text{per},L} + (1 - \chi^2) \rho_{\text{per},R} - \rho_\chi$:

$$\gamma_d := \gamma_{d,1} + \gamma_{d,2}, \quad \gamma_{d,1} := \chi (\gamma_{\text{per},L} - \gamma_\chi) \chi, \quad \gamma_{d,2} := \sqrt{1 - \chi^2} (\gamma_{\text{per},R} - \gamma_\chi) \sqrt{1 - \chi^2}. \quad (3.89)$$

Remark that if $\gamma_d \in \mathfrak{S}_1$, then $\text{Tr}_{L^2(\mathbb{R}^3)}(\gamma_d) = \chi^2 \rho_{\text{per},L} + (1 - \chi^2) \rho_{\text{per},R} - \rho_\chi$.

The density ρ_d is in $L^p(\mathbb{R}^3)$ for $1 < p \leq 2$. The proof that $\rho_d \in L^p(\mathbb{R}^3)$ relies on duality arguments: denoting by $q = \frac{p}{p-1} \in [2, +\infty)$, we prove that for any $W \in L^q(\mathbb{R}^3)$ there exists some $K_q > 0$ such that $|\text{Tr}_{L^2(\mathbb{R}^3)}(\gamma_d W)| \leq K_q \|W\|_{L^q}$. By Cauchy's formula we have

$$\begin{aligned} \gamma_{d,1} &= \frac{1}{2\pi i} \oint_{\mathfrak{C}} \chi \left(\frac{1}{z - H_{\text{per},L}} - \frac{1}{\zeta - H_\chi} \right) \chi d\zeta, \\ \gamma_{d,2} &= \frac{1}{2\pi i} \oint_{\mathfrak{C}} \sqrt{1 - \chi^2} \left(\frac{1}{\zeta - H_{\text{per},R}} - \frac{1}{\zeta - H_\chi} \right) \sqrt{1 - \chi^2} d\zeta. \end{aligned} \quad (3.90)$$

Let us prove that there exists $K_q^1 > 0$ such that

$$|\text{Tr}_{L^2(\mathbb{R}^3)}(\gamma_{d,1} W)| \leq K_q^1 \|W\|_{L^q}.$$

It is easily shown that a similar inequality holds for $\gamma_{d,2}$. Denote by $V_d := (1 - \chi^2)(V_{\text{per},L} - V_{\text{per},R}) \in L^\infty(\mathbb{R}^3)$. Remark that the function $V_d \chi$ has compact support in the x -direction and that $V_d \chi$ belongs to $L^r(\mathbb{R}^3)$ for $1 < r \leq +\infty$ by Theorem 3.7. For any $\zeta \in \mathfrak{C}$, the integrand of $\gamma_{d,1}$ writes

$$D(\zeta) := \chi \left(\frac{1}{\zeta - H_{\text{per},L}} - \frac{1}{\zeta - H_\chi} \right) \chi = \chi \frac{1}{\zeta - H_{\text{per},L}} V_d \frac{1}{\zeta - H_\chi} \chi.$$

Remark that χ being translation-invariant in the r -direction, it is not in any L^p space in \mathbb{R}^3 , which prevents us from using the standard techniques such as calculating the commutator $[-\Delta, \chi]$ to give Schatten class estimates on $\gamma_{d,1}$. By writing $1 = \gamma_{\text{per},L} + \gamma_{\text{per},L}^\perp$ and $1 = \gamma_\chi + \gamma_\chi^\perp$, the following decomposition holds

$$D(\zeta) = \chi \frac{\gamma_{\text{per},L}}{\zeta - H_{\text{per},L}} V_d \frac{1}{\zeta - H_\chi} \chi + \chi \frac{\gamma_{\text{per},L}^\perp}{\zeta - H_{\text{per},L}} V_d \frac{\gamma_\chi}{\zeta - H_\chi} \chi + \chi \frac{\gamma_{\text{per},L}}{\zeta - H_{\text{per},L}} V_d \frac{\gamma_\chi^\perp}{\zeta - H_\chi} \chi. \quad (3.91)$$

By the residue theorem,

$$\int_{\mathfrak{C}} \chi \frac{\gamma_{\text{per},L}^\perp}{\zeta - H_{\text{per},L}} V_d \frac{\gamma_\chi^\perp}{\zeta - H_\chi} \chi d\zeta \equiv 0. \quad (3.92)$$

To estimate other terms in (3.91) we rely on the following Lemmas 3.26 and 3.27.

Lemma 3.26. *Consider a self-adjoint operator $H = -\Delta + V$ defined on $L^2(\mathbb{R}^3)$ with domain $H^2(\mathbb{R}^2)$ and $V \in L^\infty(\mathbb{R}^3)$. For $E \in \mathbb{R} \setminus \sigma(H)$ denote by $\gamma = \mathbb{1}_{(-\infty, E]}(H)$. Then for any $a, b \in \mathbb{R}$, the operator $(1 - \Delta)^a \gamma (1 - \Delta)^b$ is bounded. Moreover, if $\gamma \in \mathfrak{S}_k$ for some $k \geq 1$, then $(1 - \Delta)^a \gamma (1 - \Delta)^b \in \mathfrak{S}_k$.*

Proof. Similarly as in Lemma 3.25 it can be shown that for any $\zeta \in \mathbb{R} \setminus \sigma(H)$ the operator $(\zeta - H)^{-a} (1 - \Delta)^a$ and its inverse are bounded. Fix $\delta > 0$ and define $\lambda_0 := -\|V\|_{L^\infty} - \delta$. Then $\lambda_0 \notin \sigma(H)$. By writing $\gamma = \gamma^2$, there exists a positive constant C such that

$$\left\| (1 - \Delta)^a \gamma (1 - \Delta)^b \right\|_{\mathfrak{S}_k} \leq C \left\| (\lambda_0 - H)^a \gamma (\lambda_0 - H)^b \right\|_{\mathfrak{S}_k} = C \left\| \gamma^2 (\lambda_0 - H)^{a+b} \right\|_{\mathfrak{S}_k} < +\infty,$$

as $\gamma \in \mathfrak{S}_k$ and $\gamma(\lambda_0 - H)^{a+b}$ is a bounded operator. The proof of the boundedness in operator norm follows the same lines. \square

Lemma 3.27. *For any $1 < p \leq 2$, there exist positive constants $d_{p,1}$ and $d_{p,2}$, such that*

$$\forall \zeta \in \mathfrak{C}, \quad \left\| \chi \frac{\gamma_{\text{per},L}}{\zeta - H_{\text{per},L}} V_d \right\|_{\mathfrak{S}_p} \leq d_{p,1} \|V_d \chi\|_{L^p(\mathbb{R}^3)}, \quad \left\| V_d \frac{\gamma_\chi}{\zeta - H_\chi} \chi \right\|_{\mathfrak{S}_p} \leq d_{p,2} \|V_d \chi\|_{L^p(\mathbb{R}^3)}. \quad (3.93)$$

Proof. Let us prove the statement for $\chi \gamma_{\text{per},L} (\zeta - H_{\text{per},L})^{-1} V_d$, the proof of the bound of $V_d \gamma_\chi (\zeta - H_\chi)^{-1} \chi$ follows similar arguments. Fix $R > 0$. Recall that \mathfrak{B}_R is the ball in \mathbb{R}^3 centered at 0 with radius R . Denote by φ_R the characteristic function of \mathfrak{B}_R . For any $R > 0$, by the Kato–Seiler–Simon inequality (3.39) and the boundedness of $(1 - \Delta)(\zeta - H_{\text{per},L})^{-1}$ it is easy to see that $\varphi_R \chi (\zeta - H_{\text{per},L})^{-1}$ and $(\zeta - H_{\text{per},L})^{-1} V_d \varphi_R$ belong to \mathfrak{S}_2 . The operator $\gamma_{\text{per},L} (\zeta - H_{\text{per},L})^m$ is a bounded for any $m \in \mathbb{R}$ in view of Lemma 3.27. Therefore

$$\varphi_R \left(\chi \frac{\gamma_{\text{per},L}}{\zeta - H_{\text{per},L}} V_d \right) \varphi_R = \left(\varphi_R \chi \frac{1}{\zeta - H_{\text{per},L}} \right) \gamma_{\text{per},L} (\zeta - H_{\text{per},L}) \left(\frac{1}{\zeta - H_{\text{per},L}} V_d \varphi_R \right) \in \mathfrak{S}_1.$$

Let us first prove that for any $1 \leq p \leq 2$, there exists a positive constant $d_{p,1}$ only depending on p such that for any $R > 0$,

$$\left\| \varphi_R \chi \frac{\gamma_{\text{per},L}}{\zeta - H_{\text{per},L}} V_d \varphi_R \right\|_{\mathfrak{S}_p} \leq d_{p,1} \|V_d \varphi_R^2 \chi\|_{L^p(\mathbb{R}^3)}. \quad (3.94)$$

We first prove (3.94) for $p = 1$ and $p = 2$, and conclude by an interpolation argument for $1 \leq p \leq 2$. Consider $p = 1$. By the cyclicity of the trace and the Kato–Seiler–Simon inequality (3.39),

$$\begin{aligned} \left\| \varphi_R \chi \frac{\gamma_{\text{per},L}}{\zeta - H_{\text{per},L}} V_d \varphi_R \right\|_{\mathfrak{S}_1} &= \left\| \varphi_R \chi \frac{1}{\zeta - H_{\text{per},L}} \gamma_{\text{per},L} (\zeta - H_{\text{per},L}) \frac{1}{\zeta - H_{\text{per},L}} V_d \varphi_R \right\|_{\mathfrak{S}_1} \\ &= \left\| \gamma_{\text{per},L} (\zeta - H_{\text{per},L}) \frac{1}{\zeta - H_{\text{per},L}} V_d \varphi_R^2 \chi \frac{1}{\zeta - H_{\text{per},L}} \right\|_{\mathfrak{S}_1} \\ &\leq c \left\| \frac{1}{|1 - \Delta|} |V_d \varphi_R^2 \chi| \frac{1}{|1 - \Delta|} \right\|_{\mathfrak{S}_1} \\ &= c \left\| \frac{1}{|1 - \Delta|} |V_d \varphi_R^2 \chi|^{1/2} \right\|_{\mathfrak{S}_2}^2 \leq d_{1,1} \|V_d \varphi_R^2 \chi\|_{L^1}. \end{aligned}$$

Let us next prove (3.94) for $p = 2$. Use again the cyclicity of the trace and the Kato–Seiler–Simon inequality (3.39),

$$\begin{aligned}
\left\| \varphi_{RX} \frac{\gamma_{\text{per},L}}{\zeta - H_{\text{per},L}} V_d \varphi_R \right\|_{\mathfrak{S}_2}^2 &= \left\| V_d \varphi_R \frac{\gamma_{\text{per},L}}{\zeta - H_{\text{per},L}} \varphi_R^2 \chi^2 \frac{\gamma_{\text{per},L}}{\zeta - H_{\text{per},L}} V_d \varphi_R \right\|_{\mathfrak{S}_1} \\
&= \left\| \frac{\gamma_{\text{per},L}}{\zeta - H_{\text{per},L}} \varphi_R^2 \chi^2 \frac{\gamma_{\text{per},L}}{\zeta - H_{\text{per},L}} V_d^2 \varphi_R^2 \right\|_{\mathfrak{S}_1} \\
&\leq c' \left\| \varphi_R^2 \chi^2 \frac{1}{\zeta - H_{\text{per},L}} \gamma_{\text{per},L} (\zeta - H_{\text{per},L}) \frac{1}{\zeta - H_{\text{per},L}} V_d^2 \varphi_R^2 \right\|_{\mathfrak{S}_1} \\
&= c' \left\| \gamma_{\text{per},L} (\zeta - H_{\text{per},L}) \frac{1}{\zeta - H_{\text{per},L}} V_d^2 \varphi_R^4 \chi^2 \frac{1}{\zeta - H_{\text{per},L}} \right\|_{\mathfrak{S}_1} \\
&\leq c'' \left\| \frac{1}{\zeta - H_{\text{per},L}} V_d^2 \varphi_R^4 \chi^2 \frac{1}{\zeta - H_{\text{per},L}} \right\|_{\mathfrak{S}_1} \\
&= c'' \left\| |V_d \varphi_R^2 \chi| \frac{1}{\zeta - H_{\text{per},L}} \right\|_{\mathfrak{S}_2}^2 \leq d_{2,1}^2 \|V_d \varphi_R^2 \chi\|_{L^2}^2.
\end{aligned}$$

By the interpolation arguments we can conclude (3.94) for $1 \leq p \leq 2$. Remark that for $1 < p \leq 2$ the following uniform bound holds:

$$\left\| \varphi_{RX} \frac{\gamma_{\text{per},L}}{\zeta - H_{\text{per},L}} V_d \varphi_R \right\|_{\mathfrak{S}_p} \leq d_{p,1} \|V_d \varphi_R^2 \chi\|_{L^p(\mathbb{R}^3)} \leq d_{p,1} \|V_d \chi\|_{L^p(\mathbb{R}^3)}.$$

By passing the limit $R \rightarrow +\infty$ we can conclude the proof. \square

Consider $W \in L^q(\mathbb{R}^3)$ for $q = \frac{p}{p-1} \in [2, +\infty)$. In view of (3.91), (3.92) and (3.93), by manipulations similar to the ones used in the proof of Lemma 3.27, and the Hölder's inequality for Schatten class operators (see for example [RS75, Proposition 5]), we obtain that

$$\begin{aligned}
\|\gamma_{d,1} W\|_{\mathfrak{S}_1} &= \frac{1}{2\pi} \left\| \oint_{\mathfrak{e}} D(\zeta) d\zeta W \right\|_{\mathfrak{S}_1} \\
&= \left\| \oint_{\mathfrak{e}} \chi \frac{\gamma_{\text{per},L}}{\zeta - H_{\text{per},L}} V_d \frac{1}{\zeta - H_\chi} \chi W + \chi \frac{\gamma_{\text{per},L}^\perp}{\zeta - H_{\text{per},L}} V_d \frac{\gamma_\chi}{\zeta - H_\chi} \chi W d\zeta \right\|_{\mathfrak{S}_1} \\
&\leq \left\| \oint_{\mathfrak{e}} \left(\chi \frac{\gamma_{\text{per},L}}{\zeta - H_{\text{per},L}} V_d \right) \frac{1}{\zeta - H_\chi} (1 - \Delta) \left(\frac{1}{1 - \Delta} \chi W \right) d\zeta \right\|_{\mathfrak{S}_1} \\
&\quad + \left\| \oint_{\mathfrak{e}} \left(W \chi \frac{1}{1 - \Delta} \right) (1 - \Delta) \frac{\gamma_{\text{per},L}^\perp}{\zeta - H_{\text{per},L}} \left(V_d \frac{\gamma_\chi}{\zeta - H_\chi} \chi \right) d\zeta \right\|_{\mathfrak{S}_1} \\
&\leq C \|V_d \chi\|_{L^p(\mathbb{R}^3)} \left\| \frac{1}{1 - \Delta} \chi W \right\|_{\mathfrak{S}_q} \leq K_q^1 \|W\|_{L^q(\mathbb{R}^3)},
\end{aligned} \tag{3.95}$$

where we have used the Kato–Seiler–Simon inequality (3.39) as well as the fact that $\|\chi\|_{L^\infty} = 1$. Similar estimates hold for $\gamma_{d,2}$. We therefore can conclude that $\rho_d = \chi^2 \rho_{\text{per},L} + (1 - \chi^2) \rho_{\text{per},R} - \rho_\chi$ belongs to $L^p(\mathbb{R}^3)$ for $1 < p \leq 2$.

Decay rate in the x -direction. Let us show that the density difference $\chi^2 \rho_{\text{per},L} + (1 - \chi^2) \rho_{\text{per},R} - \rho_\chi$ decays exponentially fast in the x -direction. Note that there exists $N_L \in \mathbb{N}$ such that $N_L - 1 < a_L/2 \leq N_L$.

Denote by $\mathbb{D}_{a_L} := [-a_L/2, +\infty) \times \mathbb{R}^2$, we prove the exponential decay when $\text{supp}(w_\alpha) \subset \mathbb{R}^3 \setminus \mathbb{D}_{a_L}$. Denote by

$$\alpha := (\alpha_x, 0, 0) \in (\mathbb{R}, 0, 0), \quad \beta = (\beta_x, \beta_y, \beta_z) \in \mathbb{Z}^3, \quad \beta_x \geq -N_L.$$

We have

$$\mathbb{1}_{\mathbb{D}_{a_L}} \left(\sum_{\beta_x \geq -N_L}^{+\infty} \sum_{\beta_y, \beta_z \in \mathbb{Z}} w_\beta \right) = \mathbb{1}_{\mathbb{D}_{a_L}}, \quad \mathbb{1}_{\mathbb{D}_{a_L}} V_d = V_d, \quad \alpha_x < -\frac{a_L}{2} < -N_L + 1 \leq \beta_x + 1.$$

The above relations imply, together with (3.93), the Combes–Thomas estimate (3.88) and arguments similar to ones used in (3.95), that there exist a positive constants C_1 and t_1 such that, for $1 < p \leq 2$ and $q = \frac{p}{p-1} \geq 2$,

$$\begin{aligned} \|w_\alpha \gamma_d w_\alpha\|_{\mathfrak{S}_1} &= \|w_\alpha \gamma_{d,1} w_\alpha\|_{\mathfrak{S}_1} \\ &= \left\| \frac{1}{2\pi i} \oint_{\mathfrak{C}} \left(w_\alpha \chi \frac{\gamma_{\text{per},L}}{\zeta - H_{\text{per},L}} V_d \frac{1}{\zeta - H_\chi} \chi w_\alpha + w_\alpha \chi \frac{\gamma_{\text{per},L}^\perp}{\zeta - H_{\text{per},L}} V_d \frac{\gamma_\chi}{\zeta - H_\chi} \chi w_\alpha \right) d\zeta \right\|_{\mathfrak{S}_1} \\ &\leq \left\| \frac{1}{2\pi i} \oint_{\mathfrak{C}} \left(w_\alpha \chi \frac{\gamma_{\text{per},L}}{\zeta - H_{\text{per},L}} V_d \right) \left(\mathbb{1}_{\mathbb{D}_{a_L}} \frac{1}{\zeta - H_\chi} \chi w_\alpha \right) d\zeta \right\|_{\mathfrak{S}_1} \\ &\quad + \left\| \frac{1}{2\pi i} \oint_{\mathfrak{C}} \left(w_\alpha \chi \frac{\gamma_{\text{per},L}^\perp}{\zeta - H_{\text{per},L}} \mathbb{1}_{\mathbb{D}_{a_L}} \right) \left(V_d \frac{\gamma_\chi}{\zeta - H_\chi} \chi w_\alpha \right) d\zeta \right\|_{\mathfrak{S}_1} \\ &\leq K \sum_{\beta_x \geq -N_L}^{+\infty} \sum_{\beta_y, \beta_z \in \mathbb{Z}}^{+\infty} e^{-t_1(\beta_x - \alpha_x)} e^{-t_1|\beta_y|} e^{-t_1|\beta_z|} \leq C_1 e^{-t_1|\alpha_x|}. \end{aligned}$$

The last step relies on the uniform distance of $\zeta \in \mathfrak{C}$ to $\sigma(H_\chi)$ and $\sigma(H_{\text{per},L})$. Similar estimates hold when the support of w_α is in $[a_R/2, +\infty) \times \mathbb{R}^2$. There exist therefore positive constants C and t such that $\|w_\alpha \gamma_d w_\alpha\|_{\mathfrak{S}_1} = \int_{\mathbb{R}^3} |w_\alpha \rho_d w_\alpha| \leq C e^{-t|\alpha|}$, which concludes the proof.

3.4.11 Proof of Lemma 3.13

From the last item of the Theorem 3.7 we know that $V_{\text{per},L} \in L^p_{\text{per},x}(\Gamma_L)$ (resp. $V_{\text{per},R} \in L^p_{\text{per},x}(\Gamma_R)$) for $1 < p \leq +\infty$. Remark also that $\partial_x^2(\chi^2)$, $\partial_x(\chi^2)$ are uniformly bounded and have support in $[-a_L/2, a_R/2] \times \mathbb{R}^2$. It therefore suffices to obtain the L^p -estimates on $\partial_x V_{\text{per},L}$ and $\partial_x V_{\text{per},R}$. We treat $\partial_x V_{\text{per},L}$, the L^p -estimates of $\partial_x V_{\text{per},R}$ following similar arguments. First of all in view of the form of the minimizer (3.70), by the Cauchy–Schwarz inequality

$$\begin{aligned} \partial_x \rho_{\text{per},L} &= \partial_x \left(\frac{1}{2\pi} \int_{\Gamma_L^*} \sum_{n \geq 1} \mathbb{1}(\lambda_n(\xi) \leq \epsilon_L) |e_n(\xi, \cdot)|^2 d\xi \right) \\ &\leq \frac{1}{\pi} \int_{\Gamma_L^*} \left(\sum_{n \geq 1} \mathbb{1}(\lambda_n(\xi) \leq \epsilon_L) |\partial_x |e_n(\xi, \cdot)||^2 \right)^{1/2} \left(\sum_{n \geq 1} \mathbb{1}(\lambda_n(\xi) \leq \epsilon_L) |e_n(\xi, \cdot)|^2 \right)^{1/2} d\xi \\ &\leq \frac{1}{\pi} \sqrt{K_{\xi,L}} \sqrt{\rho_{\text{per},L}}, \end{aligned}$$

where $K_{\xi,L}(\mathbf{x}) := \int_{\Gamma_L^*} \sum_{n \geq 1} \mathbb{1}(\lambda_n(\xi) \leq \epsilon_L) |\partial_x e_n(\xi, \mathbf{x})|^2 d\xi$. We also have used the fact that $|\nabla|f|| \leq |\nabla f|$ for any complex-valued function f . In view of the potential decomposition (3.72), the term $T(\mathbf{r})$ does not contribute to the x -directional derivative, hence

$$|\partial_x V_{\text{per},L}| = \left| (\partial_x (\rho_{\text{per},L} - \mu_{\text{per},L})) \star \widetilde{G_{a_L}} \right| \leq \left(\frac{1}{2\pi} \sqrt{K_{\xi,L}} \sqrt{\rho_{\text{per},L}} + |\partial_x \mu_{\text{per},L}| \right) \star \left| \widetilde{G_{a_L}} \right|.$$

On the other hand, finite kinetic energy condition (3.10) implies that $K_{\xi,L} \in L^1_{\text{per},x}(\Gamma_L)$. Moreover, $\sqrt{\rho_{\text{per},L}}$ belongs to $H^1_{\text{per},x}(\Gamma_L)$ hence to $L^s_{\text{per},x}(\Gamma_L)$ for $2 \leq s \leq 6$. Therefore, by Hölder's inequality, for $p, m \geq 1$:

$$\int_{\Gamma_L} (K_{\xi,L} \rho_{\text{per},L})^{p/2} \leq \left(\int_{\Gamma_L} K_{\xi,L}^{pm/2} \right)^{1/m} \left(\int_{\Gamma_L} \rho_{\text{per},L}^{pm/(2(m-1))} \right)^{(m-1)/m},$$

with the conditions $pm = 2$ and $2 \leq pm/(m-1) \leq 6$. This is the case for $4/3 \leq m \leq 2$ and $1 \leq p \leq 3/2$ so that $(K_{\xi,L} \rho_{\text{per},L})^{1/2}$ belongs to $L^p_{\text{per},x}(\Gamma_L)$ for $1 \leq p \leq 3/2$. As $\partial_x \mu_{\text{per},L}$ is in $L^p_{\text{per},x}(\Gamma_L)$ for any $1 \leq p \leq +\infty$ and $\widetilde{G_{a_L}} \in L^q_{\text{per},x}(\Gamma_L)$ for $1 \leq q < 2$ by Lemma 3.3, we obtain by Young's convolution inequality that $\partial_x V_{\text{per},L} \in L^s_{\text{per},x}(\Gamma_L)$ for $1 \leq s < 6$. This allows us to conclude the lemma.

3.4.12 Proof of Proposition 3.15

The following statements ensure that the problem (3.35) is well-defined: a duality argument shows that densities of operators in \mathcal{Q}_χ are well defined. The energy functional (3.36) is well defined and is bounded from below. The proofs are direct adaptations of [CDL08a, Proposition 1, Lemma 2, Corollary 1 and Corollary 2].

1. For any $Q_\chi \in \mathcal{Q}_\chi$, it holds that $Q_\chi W \in \mathfrak{S}_1^{\gamma_\chi}$ for $W = W_1 + W_2 \in \mathcal{C}' + L^2(\mathbb{R}^3)$. Moreover, there exists a positive constant C_χ such that:

$$|\text{Tr}_{\gamma_\chi}(Q_\chi W)| \leq C_\chi \|Q_\chi\|_{\mathcal{Q}_\chi} (\|W_1\|_{\mathcal{C}'} + \|W_2\|_{L^2(\mathbb{R}^3)}).$$

Moreover, there exists a uniquely defined function $\rho_{Q_\chi} \in \mathcal{C} \cap L^2(\mathbb{R}^3)$ such that

$$\forall W = W_1 + W_2 \in \mathcal{C}' + L^2(\mathbb{R}^3), \quad \text{Tr}_{\gamma_\chi}(Q_\chi W) = \langle \rho_{Q_\chi}, W_1 \rangle_{\mathcal{C}', \mathcal{C}} + \int_{\mathbb{R}^3} \rho_{Q_\chi} W_2.$$

The linear map $Q_\chi \in \mathcal{Q}_\chi \mapsto \rho_{Q_\chi} \in \mathcal{C} \cap L^2(\mathbb{R}^3)$ is continuous:

$$\|\rho_{Q_\chi}\|_{\mathcal{C}} + \|\rho_{Q_\chi}\|_{L^2(\mathbb{R}^2)} \leq C_\chi \|Q_\chi\|_{\mathcal{Q}_\chi}.$$

Moreover, if $Q_\chi \in \mathfrak{S}_1 \subset \mathfrak{S}_1^{\gamma_\chi}$, then $\rho_{Q_\chi}(\mathbf{x}) = Q_\chi(\mathbf{x}, \mathbf{x})$ where $Q_\chi(\mathbf{x}, \mathbf{x})$ the integral kernel of Q_χ .

2. For any $\kappa \in (\Sigma_{N,\chi}, \epsilon_F)$ and any state $Q_\chi \in \mathcal{K}_\chi$, the following inequality holds

$$\begin{aligned} 0 \leq c_1 \text{Tr} \left((1 - \Delta)^{1/2} (Q_\chi^{++} - Q_\chi^{--}) (1 - \Delta)^{1/2} \right) &\leq \text{Tr}_{\gamma_\chi}(H_\chi Q_\chi) - \kappa \text{Tr}_{\gamma_\chi}(Q_\chi) \\ &\leq c_2 \text{Tr} \left((1 - \Delta)^{1/2} (Q_\chi^{++} - Q_\chi^{--}) (1 - \Delta)^{1/2} \right), \end{aligned}$$

where c_1 and c_2 are the same constants as in Lemma 3.25.

3. Assume that Assumption 3 holds. There are positive constants \tilde{d}_1, \tilde{d}_2 , such that

$$\begin{aligned} \mathcal{E}_\chi(Q_\chi) - \kappa \text{Tr}_{\gamma_\chi}(Q_\chi) &\geq \tilde{d}_1 (\|Q_\chi^{++}\|_{\mathfrak{S}_1} + \|Q_\chi^{--}\|_{\mathfrak{S}_1} + \|\|\nabla|Q_\chi^{++}| \nabla\|\|_{\mathfrak{S}_1} + \|\|\nabla|Q_\chi^{--}| \nabla\|\|_{\mathfrak{S}_1}) \\ &\quad + \tilde{d}_2 (\|\|\nabla|Q_\chi\|\|_{\mathfrak{S}_2}^2 + \|Q_\chi\|_{\mathfrak{S}_2}^2) - \frac{1}{2} D(\nu_\chi, \nu_\chi). \end{aligned}$$

Hence $\mathcal{E}_\chi(\cdot) - \kappa \text{Tr}_{\gamma_\chi}(\cdot)$ is bounded from below and coercive on \mathcal{K}_χ .

The existence and the form of the minimizers are direct adaptations of [CDL08a, Theorem 2].

3.4.13 Proof of Theorem 3.17

We prove this theorem by taking two arbitrary cut-off functions χ_1, χ_2 belonging to \mathcal{X} , and prove that $\rho_{\chi_1} + \rho_{Q_{\chi_1}} = \rho_{\chi_2} + \rho_{Q_{\chi_2}}$. For $i = 1, 2$, consider the reference states associated with the Hamiltonian H_{χ_i} . Denote by γ_{χ_i} the spectral projector of H_{χ_i} below ϵ_F and by Q_{χ_i} the solutions of (3.37) associated with χ_i . Consider a test state

$$\tilde{Q} := \gamma_{\chi_1} + Q_{\chi_1} - \gamma_{\chi_2}. \quad (3.96)$$

We show that \tilde{Q} is a minimizer of the problem (3.35) associated with the cut-off function χ_2 , so that $\rho_{\tilde{Q}} \equiv \rho_{Q_{\chi_2}}$ by the uniqueness of the density of the minimizer provided by Proposition 3.15. Note that Assumption 3 and Proposition 3.11 guarantee that there is a common spectral gap for H_{χ_i} and $\sigma_{\text{ess}}(H_{\chi_1}) = \sigma_{\text{ess}}(H_{\chi_2})$. We first show that the test state \tilde{Q} belongs to the convex set

$$\mathcal{K}_{\chi_2} := \{Q \in \mathcal{Q}_{\chi_2} \mid -\gamma_{\chi_2} \leq Q \leq 1 - \gamma_{\chi_2}\},$$

hence is an admissible state for the minimization problem (3.35) associated with χ_2 . We next show that \tilde{Q} is a minimizer.

The test state \tilde{Q} belongs to \mathcal{K}_{χ_2} . We begin by proving that \tilde{Q} is in \mathcal{Q}_{χ_2} . Let us prove that \tilde{Q} is γ_{χ_2} -trace class. The following lemma will be useful.

Lemma 3.28. *The difference of the spectral projectors $\gamma_{\chi_1} - \gamma_{\chi_2}$ belongs to $\mathfrak{S}_1^{\gamma_{\chi_2}}$. Moreover,*

$$|\nabla|(\gamma_{\chi_1} - \gamma_{\chi_2}) \in \mathfrak{S}_2, \quad (\gamma_{\chi_1} - \gamma_{\chi_2})|\nabla| \in \mathfrak{S}_2. \quad (3.97)$$

Proof. By Cauchy's resolvent formula and the Kato–Seiler–Simon inequality (3.39),

$$\begin{aligned} \|\gamma_{\chi_1} - \gamma_{\chi_2}\|_{\mathfrak{S}_2} &= \left\| \frac{1}{2i\pi} \oint_{\mathfrak{C}} (\zeta - H_{\chi_1})^{-1} (\chi_1^2 - \chi_2^2) (V_{\text{per},L} - V_{\text{per},R}) (\zeta - H_{\chi_2})^{-1} d\zeta \right\|_{\mathfrak{S}_2} \\ &\leq C \left\| (1 - \Delta)^{-1} (\chi_1^2 - \chi_2^2) (V_{\text{per},L} - V_{\text{per},R}) \right\|_{\mathfrak{S}_2} \\ &\leq \frac{C}{2\sqrt{\pi}} \left\| (\chi_1^2 - \chi_2^2) (V_{\text{per},L} - V_{\text{per},R}) \right\|_{L^2} < +\infty. \end{aligned} \quad (3.98)$$

The results of Lemma 3.25 imply that $|\nabla|(\zeta - H_{\chi_i})^{-1}$ is uniformly bounded with respect to $\zeta \in \mathfrak{C}$. By calculations similar to (3.98),

$$\left\| |\nabla|(\gamma_{\chi_1} - \gamma_{\chi_2}) \right\|_{\mathfrak{S}_2} \leq c_1 \left\| (\chi_1^2 - \chi_2^2) (V_{\text{per},L} - V_{\text{per},R}) (1 - \Delta)^{-1} \right\|_{\mathfrak{S}_2} < +\infty. \quad (3.99)$$

Hence $(\gamma_{\chi_1} - \gamma_{\chi_2})|\nabla|$ also belongs to \mathfrak{S}_2 since it is the adjoint of $|\nabla|(\gamma_{\chi_1} - \gamma_{\chi_2})$. On the other hand, as γ_{χ_1} is a bounded operator, in view of (3.98) and by writing $\gamma_{\chi_1} - \gamma_{\chi_2} = \gamma_{\chi_2}^\perp - \gamma_{\chi_1}^\perp$ and using the fact that $\gamma_{\chi_i} + \gamma_{\chi_i}^\perp = 1$,

$$\begin{aligned} \gamma_{\chi_2}^\perp (\gamma_{\chi_1} - \gamma_{\chi_2}) \gamma_{\chi_2}^\perp &= \gamma_{\chi_2}^\perp \gamma_{\chi_1} \gamma_{\chi_2}^\perp = (\gamma_{\chi_1} - \gamma_{\chi_2}) \gamma_{\chi_1} (\gamma_{\chi_1} - \gamma_{\chi_2}) \in \mathfrak{S}_1, \\ \gamma_{\chi_2} (\gamma_{\chi_1} - \gamma_{\chi_2}) \gamma_{\chi_2} &= -\gamma_{\chi_2} \gamma_{\chi_1}^\perp \gamma_{\chi_2} = -(\gamma_{\chi_2} - \gamma_{\chi_1}) \gamma_{\chi_1}^\perp (\gamma_{\chi_2} - \gamma_{\chi_1}) \in \mathfrak{S}_1. \end{aligned} \quad (3.100)$$

Together with (3.98) we conclude that $\gamma_{\chi_1} - \gamma_{\chi_2}$ belongs to $\mathfrak{S}_1^{\gamma_{\chi_2}}$. \square

The following lemma is a consequence of [HLS05a, Lemma 1] and the fact that $\gamma_{\chi_1} - \gamma_{\chi_2} \in \mathfrak{S}_2$.

Lemma 3.29. *Any self-adjoint operator A is in $\mathfrak{S}_1^{\gamma_{\chi_1}}$ if and only if A is in $\mathfrak{S}_1^{\gamma_{\chi_2}}$. Moreover $\text{Tr}_{\gamma_{\chi_1}}(A) = \text{Tr}_{\gamma_{\chi_2}}(A)$.*

The fact that $Q_{\chi_1} \in \mathfrak{S}_1^{\gamma_{\chi_1}}$ implies that $|\nabla|Q_{\chi_1} \in \mathfrak{S}_2$, and $Q_{\chi_1} \in \mathfrak{S}_1^{\gamma_{\chi_2}}$ by Lemma 3.29. In view of this and Lemma 3.28 we know that $\tilde{Q} = \gamma_{\chi_1} - \gamma_{\chi_2} + Q_{\chi_1}$ belongs to $\mathfrak{S}_1^{\gamma_{\chi_2}}$. The inequality (3.99) implies that $|\nabla|\tilde{Q} = |\nabla|Q_{\chi_1} + |\nabla|(\gamma_{\chi_1} - \gamma_{\chi_2}) \in \mathfrak{S}_2$. It remains to prove that $|\nabla|\gamma_{\chi_2}^\perp \tilde{Q} \gamma_{\chi_2}^\perp |\nabla| \in \mathfrak{S}_1$ and $|\nabla|\gamma_{\chi_2} \tilde{Q} \gamma_{\chi_2} |\nabla| \in \mathfrak{S}_1$. In view of (3.96) we have

$$\begin{aligned} |\nabla|\gamma_{\chi_2}^\perp \tilde{Q} \gamma_{\chi_2}^\perp |\nabla| &= |\nabla|\gamma_{\chi_2}^\perp Q_{\chi_1} \gamma_{\chi_2}^\perp |\nabla| + |\nabla|\gamma_{\chi_2}^\perp (\gamma_{\chi_1} - \gamma_{\chi_2}) \gamma_{\chi_2}^\perp |\nabla|, \\ |\nabla|\gamma_{\chi_2} \tilde{Q} \gamma_{\chi_2} |\nabla| &= |\nabla|\gamma_{\chi_2} Q_{\chi_1} \gamma_{\chi_2} |\nabla| + |\nabla|\gamma_{\chi_2} (\gamma_{\chi_1} - \gamma_{\chi_2}) \gamma_{\chi_2} |\nabla|. \end{aligned} \quad (3.101)$$

We estimate (3.101) term by term. By Lemma 3.26 we know that $\| |\nabla|\gamma_{\chi_i} \| \leq \| |\nabla|(1-\Delta)^{-1} \| \| (1-\Delta)\gamma_{\chi_i} \| < \infty$. Moreover, by writing $\gamma_{\chi_2}^\perp = 1 - \gamma_{\chi_1} + \gamma_{\chi_1} - \gamma_{\chi_2}$ and $\gamma_{\chi_2} = \gamma_{\chi_1} + \gamma_{\chi_2} - \gamma_{\chi_1}$, in view of (3.99),

$$\begin{aligned} & \left\| |\nabla|\gamma_{\chi_2}^\perp Q_{\chi_1} \gamma_{\chi_2}^\perp |\nabla| \right\|_{\mathfrak{S}_1} \\ &= \left\| |\nabla|\gamma_{\chi_1}^\perp Q_{\chi_1} \gamma_{\chi_1}^\perp |\nabla| + |\nabla|\gamma_{\chi_1}^\perp Q_{\chi_1} (\gamma_{\chi_1} - \gamma_{\chi_2}) |\nabla| + |\nabla|(\gamma_{\chi_1} - \gamma_{\chi_2}) Q_{\chi_1} \gamma_{\chi_2}^\perp |\nabla| \right\|_{\mathfrak{S}_1} \\ &\leq \left\| |\nabla|\gamma_{\chi_1}^\perp Q_{\chi_1} \gamma_{\chi_1}^\perp |\nabla| \right\|_{\mathfrak{S}_1} + \left\| |\nabla|Q_{\chi_1} (\gamma_{\chi_1} - \gamma_{\chi_2}) |\nabla| \right\|_{\mathfrak{S}_1} + \left\| |\nabla|\gamma_{\chi_1} Q_{\chi_1} (\gamma_{\chi_1} - \gamma_{\chi_2}) |\nabla| \right\|_{\mathfrak{S}_1} \\ &\quad + \left\| |\nabla|(\gamma_{\chi_1} - \gamma_{\chi_2}) Q_{\chi_1} \gamma_{\chi_2} |\nabla| \right\|_{\mathfrak{S}_1} + \left\| |\nabla|(\gamma_{\chi_1} - \gamma_{\chi_2}) Q_{\chi_1} |\nabla| \right\|_{\mathfrak{S}_1} \\ &\leq \left\| |\nabla|\gamma_{\chi_1}^\perp Q_{\chi_1} \gamma_{\chi_1}^\perp |\nabla| \right\|_{\mathfrak{S}_1} + \left\| |\nabla|Q_{\chi_1} \right\|_{\mathfrak{S}_2} \left\| (\gamma_{\chi_1} - \gamma_{\chi_2}) |\nabla| \right\|_{\mathfrak{S}_2} + \left\| |\nabla|\gamma_{\chi_1} \right\|_{\mathfrak{S}_2} \left\| Q_{\chi_1} \right\|_{\mathfrak{S}_2} \left\| (\gamma_{\chi_1} - \gamma_{\chi_2}) |\nabla| \right\|_{\mathfrak{S}_2} \\ &\quad + \left\| \gamma_{\chi_2} |\nabla| \right\|_{\mathfrak{S}_2} \left\| Q_{\chi_1} \right\|_{\mathfrak{S}_2} \left\| |\nabla|(\gamma_{\chi_1} - \gamma_{\chi_2}) \right\|_{\mathfrak{S}_2} + \left\| Q_{\chi_1} |\nabla| \right\|_{\mathfrak{S}_2} \left\| |\nabla|(\gamma_{\chi_1} - \gamma_{\chi_2}) \right\|_{\mathfrak{S}_2} < \infty, \end{aligned}$$

and similarly

$$\begin{aligned} & \left\| |\nabla|\gamma_{\chi_2} Q_{\chi_1} \gamma_{\chi_2} |\nabla| \right\|_{\mathfrak{S}_1} \\ &= \left\| |\nabla|\gamma_{\chi_1} Q_{\chi_1} \gamma_{\chi_1} |\nabla| + |\nabla|\gamma_{\chi_1} Q_{\chi_1} (\gamma_{\chi_2} - \gamma_{\chi_1}) |\nabla| + |\nabla|(\gamma_{\chi_2} - \gamma_{\chi_1}) Q_{\chi_1} \gamma_{\chi_2} |\nabla| \right\|_{\mathfrak{S}_1} \\ &\leq \left\| |\nabla|\gamma_{\chi_1} Q_{\chi_1} \gamma_{\chi_1} |\nabla| \right\|_{\mathfrak{S}_1} + \left\| |\nabla|\gamma_{\chi_1} Q_{\chi_1} (\gamma_{\chi_1} - \gamma_{\chi_2}) |\nabla| \right\|_{\mathfrak{S}_1} + \left\| |\nabla|(\gamma_{\chi_1} - \gamma_{\chi_2}) Q_{\chi_1} \gamma_{\chi_2} |\nabla| \right\|_{\mathfrak{S}_1} \\ &\leq \left\| |\nabla|\gamma_{\chi_1} Q_{\chi_1} \gamma_{\chi_1} |\nabla| \right\|_{\mathfrak{S}_1} + \left\| |\nabla|\gamma_{\chi_1} \right\|_{\mathfrak{S}_2} \left\| Q_{\chi_1} \right\|_{\mathfrak{S}_2} \left\| (\gamma_{\chi_1} - \gamma_{\chi_2}) |\nabla| \right\|_{\mathfrak{S}_2} \\ &\quad + \left\| \gamma_{\chi_2} |\nabla| \right\|_{\mathfrak{S}_2} \left\| Q_{\chi_1} \right\|_{\mathfrak{S}_2} \left\| |\nabla|(\gamma_{\chi_1} - \gamma_{\chi_2}) \right\|_{\mathfrak{S}_2} < \infty, \end{aligned}$$

From (3.100) we know that

$$\begin{aligned} \left\| |\nabla|\gamma_{\chi_2}^\perp (\gamma_{\chi_1} - \gamma_{\chi_2}) \gamma_{\chi_2}^\perp |\nabla| \right\|_{\mathfrak{S}_1} &= \left\| |\nabla|(\gamma_{\chi_1} - \gamma_{\chi_2}) \gamma_{\chi_1} (\gamma_{\chi_1} - \gamma_{\chi_2}) |\nabla| \right\|_{\mathfrak{S}_1} \\ &\leq \left\| |\nabla|(\gamma_{\chi_1} - \gamma_{\chi_2}) \right\|_{\mathfrak{S}_2}^2 < \infty, \\ \left\| |\nabla|\gamma_{\chi_2} (\gamma_{\chi_1} - \gamma_{\chi_2}) \gamma_{\chi_2} |\nabla| \right\|_{\mathfrak{S}_1} &= \left\| |\nabla|(\gamma_{\chi_2} - \gamma_{\chi_1}) \gamma_{\chi_1}^\perp (\gamma_{\chi_2} - \gamma_{\chi_1}) |\nabla| \right\|_{\mathfrak{S}_1} \\ &\leq \left\| |\nabla|(\gamma_{\chi_1} - \gamma_{\chi_2}) \right\|_{\mathfrak{S}_2}^2 < \infty. \end{aligned}$$

This shows that $|\nabla|\gamma_{\chi_2}^\perp \tilde{Q} \gamma_{\chi_2}^\perp |\nabla| \in \mathfrak{S}_1$ and $|\nabla|\gamma_{\chi_2} \tilde{Q} \gamma_{\chi_2} |\nabla| \in \mathfrak{S}_1$. In view of (3.101), this allows us to conclude that $\tilde{Q} \in \mathcal{Q}_{\chi_2}$. On the other hand, it is easy to see that $-\gamma_{\chi_2} \leq \tilde{Q} = \gamma_{\chi_1} + Q_{\chi_1} - \gamma_{\chi_2} \leq 1 - \gamma_{\chi_2}$, which shows that \tilde{Q} belongs to the convex set \mathcal{K}_{χ_2} .

The state \tilde{Q} is a minimizer. We now prove that \tilde{Q} is a minimizer of the problem (3.35) associated with the cut-off function χ_2 . As $\tilde{Q} \in \mathcal{K}_{\chi_2}$, the fact that Q_{χ_2} is a minimizer implies that

$$\mathcal{E}_{\chi_2}(\tilde{Q}) - \kappa \text{Tr}_{\gamma_{\chi_2}}(\tilde{Q}) \geq \mathcal{E}_{\chi_2}(Q_{\chi_2}) - \kappa \text{Tr}_{\gamma_{\chi_2}}(Q_{\chi_2}). \quad (3.102)$$

Define $\Theta := \tilde{Q} - Q_{\chi_2} = Q_{\chi_1} - Q_{\chi_2} + \gamma_{\chi_1} - \gamma_{\chi_2}$. The inequality (3.102) can therefore also be written as

$$\mathcal{E}_{\chi_2}(\Theta) - \kappa \text{Tr}_{\gamma_{\chi_2}}(\Theta) + D(\rho_{\Theta}, \rho_{Q_{\chi_2}}) \geq 0. \quad (3.103)$$

It is easy to see that $-1 \leq \Theta \leq 1$ and Θ belongs to \mathcal{Q}_{χ_2} (but not necessarily to the convex set \mathcal{K}_{χ_2}), which also implies that the density ρ_{Θ} of Θ is well defined and belongs to the Coulomb space \mathcal{C} (see Section 3.4.12). Therefore (3.103) is well defined. Introduce another state by exchanging the indices 1 and 2 in the definition of \tilde{Q} :

$$\tilde{\tilde{Q}} := \gamma_{\chi_2} + Q_{\chi_2} - \gamma_{\chi_1}.$$

Proceeding as before, it can be shown that $\tilde{\tilde{Q}} \in \mathcal{K}_{\chi_1}$. By definition $Q_{\chi_1} = \Theta + \tilde{\tilde{Q}}$. Since Q_{χ_1} minimizes the problem (3.35) associated with χ_1 and $\tilde{\tilde{Q}} \in \mathcal{K}_{\chi_1}$,

$$\mathcal{E}_{\chi_1}(\tilde{\tilde{Q}}) - \kappa \text{Tr}_{\gamma_{\chi_1}}(\tilde{\tilde{Q}}) \geq \mathcal{E}_{\chi_1}(\Theta + \tilde{\tilde{Q}}) - \kappa \text{Tr}_{\gamma_{\chi_1}}(\Theta + \tilde{\tilde{Q}}).$$

The above equation can be simplified as

$$\mathcal{E}_{\chi_1}(\Theta) - \kappa \text{Tr}_{\gamma_{\chi_1}}(\Theta) + D(\rho_{\Theta}, \rho_{\tilde{\tilde{Q}}}) \leq 0. \quad (3.104)$$

Let us show that the left hand sides of (3.103) and (3.104) are equal. First of all as Θ belongs to \mathcal{Q}_{χ_2} , we know that $\text{Tr}_{\gamma_{\chi_2}}(\Theta) = \text{Tr}_{\gamma_{\chi_1}}(\Theta)$ by Lemma 3.29. Remark also that $\rho_{\tilde{\tilde{Q}}} = \rho_{\chi_2} - \rho_{\chi_1} + \rho_{Q_{\chi_2}}$. By Lemma 3.29

$$\begin{aligned} & \mathcal{E}_{\chi_2}(\Theta) - \kappa \text{Tr}_{\gamma_{\chi_2}}(\Theta) + D(\rho_{\Theta}, \rho_{Q_{\chi_2}}) - \left(\mathcal{E}_{\chi_1}(\Theta) - \kappa \text{Tr}_{\gamma_{\chi_1}}(\Theta) + D(\rho_{\Theta}, \rho_{\tilde{\tilde{Q}}}) \right) \\ &= \text{Tr}_{\gamma_{\chi_2}}((-\Delta + V_{\chi_2})\Theta) - D(\rho_{\Theta}, \nu_{\chi_2}) + \frac{1}{2}D(\rho_{\Theta}, \rho_{\Theta}) - \text{Tr}_{\gamma_{\chi_1}}((-\Delta + V_{\chi_1})\Theta) + D(\rho_{\Theta}, \nu_{\chi_1}) \\ & \quad - \frac{1}{2}D(\rho_{\Theta}, \rho_{\Theta}) - \kappa(\text{Tr}_{\gamma_{\chi_2}}(\Theta) - \text{Tr}_{\gamma_{\chi_1}}(\Theta)) + D(\rho_{\Theta}, \rho_{Q_{\chi_2}}) - D(\rho_{\Theta}, \rho_{\tilde{\tilde{Q}}}) \\ &= \text{Tr}_{\gamma_{\chi_2}}((-\Delta + V_{\chi_2})\Theta) - \text{Tr}_{\gamma_{\chi_1}}((-\Delta + V_{\chi_1})\Theta) + D(\rho_{\Theta}, \rho_{\chi_1} + \nu_{\chi_1} - \rho_{\chi_2} - \nu_{\chi_2}) \\ &= \text{Tr}_{\gamma_{\chi_2}}((V_{\chi_2} - V_{\chi_1})\Theta) + D(\rho_{\Theta}, \rho_{\chi_1} + \nu_{\chi_1} - \rho_{\chi_2} - \nu_{\chi_2}). \end{aligned} \quad (3.105)$$

We show that (3.105) is equal to zero by first showing that $(V_{\chi_2} - V_{\chi_1})\Theta \in \mathfrak{S}_1 \subset \mathfrak{S}_1^{\gamma_{\chi_2}}$. We start by showing that $(1 - \Delta)Q_{\chi_i} \in \mathfrak{S}_2$. By Cauchy's resolvent formula,

$$Q_{\chi_i} = \frac{1}{2i\pi} \oint_{\mathfrak{c}} \left(\frac{1}{z - H_{\overline{Q_{\chi_i}}}} - \frac{1}{z - H_{\chi_i}} \right) d\zeta = Q_{1,i} + Q_{2,i} + Q_{3,i},$$

where

$$\begin{aligned} Q_{1,i} &= \frac{1}{2i\pi} \oint_{\mathfrak{c}} \frac{1}{z - H_{\chi_i}} \left(\left(\rho_{\overline{Q_{\chi_i}}} - \nu_{\chi_i} \right) \star \frac{1}{|\cdot|} \right) \frac{1}{z - H_{\chi_i}} d\zeta, \\ Q_{2,i} &= \frac{1}{2i\pi} \oint_{\mathfrak{c}} \frac{1}{z - H_{\chi_i}} \left(\left(\rho_{\overline{Q_{\chi_i}}} - \nu_{\chi_i} \right) \star \frac{1}{|\cdot|} \right) \frac{1}{z - H_{\chi_i}} \left(\left(\rho_{\overline{Q_{\chi_i}}} - \nu_{\chi_i} \right) \star \frac{1}{|\cdot|} \right) \frac{1}{z - H_{\chi_i}} d\zeta \\ Q_{3,i} &= \frac{1}{2i\pi} \oint_{\mathfrak{c}} \frac{1}{z - H_{\overline{Q_{\chi_i}}}} \left(\left(\rho_{\overline{Q_{\chi_i}}} - \nu_{\chi_i} \right) \star \frac{1}{|\cdot|} \right) \frac{1}{z - H_{\chi_i}} \left(\left(\rho_{\overline{Q_{\chi_i}}} - \nu_{\chi_i} \right) \star \frac{1}{|\cdot|} \right) \frac{1}{z - H_{\chi_i}} \\ & \quad \cdot \left(\left(\rho_{\overline{Q_{\chi_i}}} - \nu_{\chi_i} \right) \star \frac{1}{|\cdot|} \right) \frac{1}{z - H_{\chi_i}} d\zeta. \end{aligned}$$

Following arguments similar to the ones used in the proof of [CDL08a, Proposition 2] we obtain that $(\rho_{\tilde{Q}_{\chi_i}} - \nu_{\chi_i}) \star \frac{1}{|\cdot|}$ belongs to $L^2(\mathbb{R}^3) + C'$, and we can conclude that $(1 - \Delta)Q_{\chi_i} \in \mathfrak{S}_2$. Remark that $V_{\chi_1} - V_{\chi_2} = (\chi_1^2 - \chi_2^2)(V_{\text{per},L} - V_{\text{per},R}) \in L^\infty(\mathbb{R}^3) \cap L^2(\mathbb{R}^3)$. By definition of Θ , by the Kato–Seiler–Simon inequality and use calculations similar to (3.98)

$$\begin{aligned} \left\| (V_{\chi_1} - V_{\chi_2}) \Theta \right\|_{\mathfrak{S}_1} &= \left\| (V_{\chi_1} - V_{\chi_2}) (Q_{\chi_1} - Q_{\chi_2} + \gamma_{\chi_1} - \gamma_{\chi_2}) \right\|_{\mathfrak{S}_1} \\ &\leq \left\| (V_{\chi_1} - V_{\chi_2}) (1 - \Delta)^{-1} \right\|_{\mathfrak{S}_2} \left(\left\| (1 - \Delta) (Q_{\chi_1} - Q_{\chi_2}) \right\|_{\mathfrak{S}_2} + \left\| (1 - \Delta) (\gamma_{\chi_1} - \gamma_{\chi_2}) \right\|_{\mathfrak{S}_2} \right) \\ &\leq \frac{1}{2\sqrt{\pi}} \left\| V_{\chi_1} - V_{\chi_2} \right\|_{L^2} \left(\left\| (1 - \Delta) (Q_{\chi_1} - Q_{\chi_2}) \right\|_{\mathfrak{S}_2} \right. \\ &\quad \left. + C \left\| (\chi_1^2 - \chi_2^2) (V_{\text{per},L} - V_{\text{per},R}) (1 - \Delta)^{-1} \right\|_{\mathfrak{S}_2} \right) < \infty, \end{aligned}$$

which proves that $(V_{\chi_1} - V_{\chi_2}) \Theta$ belongs to \mathfrak{S}_1 , hence

$$\text{Tr}_{\gamma_{\chi_2}} ((V_{\chi_2} - V_{\chi_1}) \Theta) = \text{Tr} ((V_{\chi_2} - V_{\chi_1}) \Theta).$$

On the other hand, by the definition of V_{χ_i} in (3.31) and ν_i in (3.33) for $i = 1, 2$, we deduce that

$$\text{Tr} ((V_{\chi_2} - V_{\chi_1}) \Theta) = D(\rho_\Theta, (\rho_{\chi_2} - \mu_{\chi_2}) - (\rho_{\chi_1} - \mu_{\chi_1})) = D(\rho_\Theta, \rho_{\chi_2} - \rho_{\chi_1} + \nu_{\chi_2} - \nu_{\chi_1}).$$

The above equation implies that the quantity (3.105) equals to 0. Hence, in view of (3.103) and (3.104),

$$\mathcal{E}_{\chi_2}(\Theta) - \kappa \text{Tr}_{\gamma_{\chi_2}}(\Theta) + D(\rho_\Theta, \rho_{Q_{\chi_2}}) = \mathcal{E}_{\chi_1}(\Theta) - \kappa \text{Tr}_{\gamma_{\chi_1}}(\Theta) + D(\rho_\Theta, \rho_{\tilde{Q}}) \equiv 0.$$

We conclude with (3.102) that

$$\mathcal{E}_{\chi_2}(\tilde{Q}) - \kappa \text{Tr}_{\gamma_{\chi_2}}(\tilde{Q}) \equiv \mathcal{E}_{\chi_2}(Q_{\chi_2}) - \kappa \text{Tr}_{\gamma_{\chi_2}}(Q_{\chi_2}).$$

Therefore \tilde{Q} is a minimizer of the problem (3.35) associated with the cut-off function χ_2 . From Theorem 3.15 we know that $\rho_{\tilde{Q}} \equiv \rho_{Q_{\chi_2}}$, which is equivalent to that $\rho_{Q_{\chi_2}} + \rho_{\chi_2} = \rho_{\chi_1} + \rho_{Q_{\chi_1}}$. By the arbitrariness of the choice of χ_1, χ_2 we deduce that $\rho_\chi + \rho_{Q_\chi}$ is independent of the cut-off function $\chi \in \mathcal{X}$.

CHAPTER 4

LATTICE DYNAMICS IN AN ADIABATIC BORN-OPPENHEIMER APPROXIMATION

This chapter describes the on-going work on lattice dynamics.

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4.1 Introduction

Research on atomic dynamics started from Einstein's observation of the Brownian motion in liquids [Ein05, Ein06] and his work on the heat capacity of solids [Ein07]. Latter on, Born and von Kàrmàn [BvK12, BvK13] focused on lattice vibrations, and their works laid the foundations for the modern theory of lattice dynamics.

It is well known that atomic vibrations in crystals play a key role in material features such as heat conductivity or defect dynamics (see [Dov93] and references therein). First-principle calculation methods nowadays allow the numerical simulation of many of these physical properties. Although based on the fundamental laws of quantum physics, these methods do not aim at solving by brute-force the many-body time-dependent Schrödinger equation which governs the dynamics of nuclei and electrons, as this task is well beyond the capabilities of today's computers. Instead, these methods provide numerical solutions of approximate models derived from the many-body time-dependent Schrödinger equation. The Born-Oppenheimer approximation [BO27, PLC⁺07], based on the smallness of mass ratios between electrons and nuclei, first allows to decouple electronic and nuclear dynamics. More precisely, in this approximation, nuclei obey an autonomous quantum Hamiltonian dynamics, in which the effective interatomic potential

is obtained by assuming that the electrons are in their ground state (which depends of the nuclear configuration via the Coulomb potential generated by the nuclei). This approximation can be justified for finite molecular systems by adiabatic theorems provided there is a uniform gap between the ground state and first excited state of potential energy surfaces (see [PST03, Teu03] and reference therein). By analogy, the Born-Oppenheimer approximation seems quite reasonable for insulating and semiconducting materials, while more questionable for metallic systems. A second approximation, almost always made in practice, consists in approximating the quantum Born-Oppenheimer nuclear dynamics by a classical one. From a mathematical viewpoint, this can be justified by a semiclassical approximation obtained by letting the Planck constant go to zero in the nuclear dynamics (see [Hag80] and reference therein). Lastly, the ground state electronic problem must itself be approximated, typically using Density Functional Theory (DFT). The resulting model (classical nuclei interacting via an effective many-body potential obtained by solving an electronic ground-state problem using DFT for each nuclear configuration) is often referred to as first-principle molecular dynamics. Note that Car-Parrinello molecular dynamics [CP85] is an approximation of first-principle molecular dynamics.

In this chapter we focus on first-principle molecular dynamics, and use the reduced Hartree-Fock (rHF) model to approximate electronic ground states. This model has already been discussed in Section 1.1 of Chapter 1. To illustrate the problems at hand, consider for simplicity a finite system with M nuclei and N electrons, and denote by $\mathbf{X}(t) = (X_1(t), \dots, X_M(t)) \in (\mathbb{R}^3)^M$ the positions of the M nuclei at time t and by $\mathcal{W} : (\mathbb{R}^3)^M \ni \mathbf{X} \mapsto \mathcal{W}(\mathbf{X}) \in \mathbb{R}$ the rHF potential energy surface. The force acting on the i^{th} nucleus at time t is

$$F_i(t) = -\nabla_{X_i} \mathcal{W}(\mathbf{X}(t)).$$

In practice, the forces can be computed using Density functional perturbation theory (DFPT) (see [BdGDCG01] and references therein). Global minimizers of \mathcal{W} correspond to the most stable configurations of the molecular system. Local, non-global minimizers correspond to metastable states and critical points with Morse index equal to one to transition states. Let \mathbf{X}^0 be a local minimizer. The vibration modes of the molecular system in configuration \mathbf{X}^0 are obtained by solving the secular equation

$$(\mathbf{D}^2 \mathcal{W}(\mathbf{X}^0)) \mathbf{Y} = \omega^2 \mathbf{M} \mathbf{Y} \quad (4.1)$$

where $\mathbf{D}^2 \mathcal{W}(\mathbf{X}^0) \in \mathbb{R}_{\text{sym}}^{3M \times 3M}$ and $\mathbf{M} \in \mathbb{R}_{\text{sym}}^{3M \times 3M}$ are respectively the stiffness and mass matrices of the molecular system. The former is the Hessian matrix of the potential energy surface \mathcal{W} at \mathbf{X}^0 , while the latter is the diagonal matrix containing the masses of the nuclei.

In a crystalline solid, the stiffness and mass matrices are infinite-dimensional but \mathcal{L} -translation invariant, where \mathcal{L} is the Bravais lattice of the crystal. The eigenvalues of the (discrete) Fourier transform of (4.1) are the phonon frequencies and are labeled by a wave-vector. Phonons are collective excitations of the crystal describing quantum harmonic lattice vibrations within the Born-Oppenheimer approximation [AM76, Sch08]. Anharmonic effects can be taken into account by perturbation theory (phonon-phonon scattering [AM76, Kit04]). Perturbation theory is also used to compute the effect of nuclear vibrations on electronic transport in semiconductors and metals (electron-phonon scattering, see [Giu17] and references therein).

In this chapter, we follow a different path and study the fully nonlinear (non-perturbative) rHF Born-Oppenheimer dynamics of classical nuclei in a crystal in the neighborhood of an equilibrium periodic configuration. Addressing the general case of arbitrary excitations of the nuclear configuration is quite challenging because it is not clear how to define a rHF (or *a fortiori* a Hartree-Fock or Kohn-Sham) ground state for generic nuclear displacements small enough in the $\ell^\infty(\mathcal{R})$ -norm, where \mathcal{R} is the crystal lattice. In numerical simulations, nuclear displacements usually have the periodicity of some supercell. The electronic problem then remains periodic and can be dealt with using Bloch theory. The alternative we consider in this work is to study the nonlinear dynamics of localized displacements, typically small in the $\ell^2(\mathcal{R})$ -norm. We rely on the previous works on the rHF ground-states of crystals with local defects [CDL08a, CE11] to compute the atomic forces in the deformed crystal. Our main result is the characterization of a Hilbert space

\mathcal{H} densely embedded in $\ell^2(\mathcal{R})$ and the definition of a classical Hamiltonian $H : \mathcal{H} \times \ell^2(\mathcal{R}) \rightarrow \mathbb{R}$. We show that if the initial data $(\mathbf{R}(0), \mathbf{P}(0))$ (atomic displacements and momenta) is small enough in $\mathcal{H} \times \ell^2(\mathcal{R})$, then the rHF Born-Oppenheimer molecular dynamics is well posed for short times.

This chapter is organized as follows: we start by considering a system with a finite number of nuclei and electrons in Section 4.2, and construct a mathematical framework for the classical nuclear Hamiltonian dynamics around a local minimum of the potential energy surface, where the electronic state is described by a rHF model. We then pass formally to the thermodynamic limit in this model and obtain a lattice dynamics around a periodic equilibrium configuration in Section 4.3. We prove the well-posedness of the so-obtained infinite-dimensional Hamiltonian dynamics in short time for a small initial data. Some on-going work and possible extensions are discussed in Section 4.4.

Let us conclude this section by mentioning other mathematical works on the dynamics of crystals with classical nuclei and quantum electrons. In the framework of the Schrödinger–Poisson model, the coupled electronic-nuclear dynamics has been studied in [KK17] for finite systems, and in [KK16, KK18] for perturbations around periodic configurations. In these works, electrons are described by a wavefunction evolving according to a nonlinear time-dependent Schrödinger equation. Let us also mention that for the electronic dynamics only (nuclei are fixed), the Cauchy problem of the time-dependent Hartree equation has been studied in [LS15] for a Fermi sea, with electrons driven by an external short-range potential. In [CS12], the authors have proved the local and global well-posedness of the Hartree dynamics in the rHF model for a small time-dependent nuclear perturbation.

4.2 Nuclear dynamics for finite systems in an adiabatic Born-Oppenheimer approximation

In order to motivate the model for lattice dynamics around periodic configurations introduced in Section 4.3, we first consider a neutral molecular system consisting of M smeared classical nuclei and N electrons. We denote by $(z_k)_{1 \leq k \leq M} \in (\mathbb{N}^*)^M$ the charges of the nuclei ($\sum_{k=1}^M z_k = N$), by $(m_k)_{1 \leq k \leq M} \in (\mathbb{R}_+^*)^M$ their masses, and by $\mathbf{X} = (X_k)_{1 \leq k \leq M} \in (\mathbb{R}^3)^M$ their positions. The nuclear charge distribution is represented by a smooth function

$$\mu_{\mathbf{X}}^{\text{fs}}(x) = \sum_{k=1}^M z_k m(x - X_k),$$

where the superscript "fs" stands for "finite system", and where $m \in C_c^\infty(\mathbb{R}^3)$ is a smooth radial nonnegative function supported in the ball $\mathfrak{B}_\eta = \{x \in \mathbb{R}^3 \mid |x| < \eta\}$ for some $\eta > 0$ and such that $\int_{\mathbb{R}^3} m = 1$.

The rHF Born–Oppenheimer energy surface. We start by recalling the rHF model for finite systems, which was already discussed in Section 1.1.2 of Chapter 1. Let us introduce the following set of admissible density matrices:

$$\mathcal{P}^{\text{fs}} := \left\{ \gamma \in \mathcal{S}(L^2(\mathbb{R}^3)) \mid 0 \leq \gamma \leq 1, \text{Tr}_{L^2(\mathbb{R}^3)}(\gamma) < \infty, \text{Tr}_{L^2(\mathbb{R}^3)}(|\nabla|\gamma|\nabla|) < \infty \right\}.$$

The rHF energy functional is defined for $\mathbf{X} \in (\mathbb{R}^3)^M$ and $\gamma \in \mathcal{P}^{\text{fs}}$ as:

$$\mathcal{E}^{\text{fs}}(\mathbf{X}, \gamma) = \text{Tr}_{L^2(\mathbb{R}^3)} \left(-\frac{1}{2} \Delta \gamma \right) + \frac{1}{2} D \left(\rho_\gamma - \mu_{\mathbf{X}}^{\text{fs}}, \rho_\gamma - \mu_{\mathbf{X}}^{\text{fs}} \right),$$

where $\text{Tr}_{L^2(\mathbb{R}^3)} \left(-\frac{1}{2} \Delta \gamma \right) := \frac{1}{2} \text{Tr}_{L^2(\mathbb{R}^3)} (|\nabla|\gamma|\nabla|)$ and $D(\cdot, \cdot)$ is the Coulomb energy

$$D(\rho_1, \rho_2) = 4\pi \int_{\mathbb{R}^3} \frac{\widehat{\rho}_1(\overline{k}) \widehat{\rho}_2(k)}{|k|^2} dk,$$

defined for ρ_1, ρ_2 in the Coulomb space

$$\mathcal{C} := \left\{ \rho \in \mathcal{S}'(\mathbb{R}^3) \mid \widehat{\rho} \in L_{\text{loc}}^1(\mathbb{R}^3), \frac{\widehat{\rho}(\cdot)}{|\cdot|} \in L^2(\mathbb{R}^3) \right\},$$

where $\widehat{\rho}$ is the Fourier transform of ρ . Endowed with the inner product $(\rho_1, \rho_2)_C := D(\rho_1, \rho_2)$, the Coulomb space \mathcal{C} is a Hilbert space. Its dual space \mathcal{C}' (Beppo-Levi space [CDL08a]) is:

$$\mathcal{C}' := \{V \in L^6(\mathbb{R}^3) \mid \nabla V \in (L^2(\mathbb{R}^3))^3\}.$$

Within the rHF approximation, the *Born–Oppenheimer energy surface* is defined as:

$$\forall \mathbf{X} \in (\mathbb{R}^3)^M, \quad \mathcal{W}^{\text{fs}}(\mathbf{X}) = \inf \left\{ \mathcal{E}^{\text{fs}}(\mathbf{X}, \gamma) \mid \gamma \in \mathcal{P}^{\text{fs}}, \text{Tr}_{L^2(\mathbb{R}^3)}(\gamma) = N \right\}. \quad (4.2)$$

It is known [Sol91] that for any $\mathbf{R} \in (\mathbb{R}^3)^N$, (4.2) has a minimizer, and that all minimizers share the same density. The latter property is due to the fact that the rHF model is strictly convex in the density.

Hamiltonian dynamics around a reference configuration. Let \mathbf{X}^0 be a (local) minimizer of $\mathbf{X} \mapsto \mathcal{W}^{\text{fs}}(\mathbf{X})$. Let γ^0 be a minimizer of (4.2) for $\mathbf{X} = \mathbf{X}^0$. We denote by $\rho^0 := \rho_{\gamma^0}$ the common density of the minimizers, by $V^0 := (\rho_{\gamma^0} - \mu_{\mathbf{X}^0}^{\text{fs}}) \star |\cdot|^{-1}$ the electrostatic potential generated by the electronic density ρ^0 and the nuclear density $\mu_{\mathbf{X}^0}^{\text{fs}}$, and by $H^0 := -\frac{1}{2}\Delta + V^0$ the corresponding rHF Hamiltonian. Assume that there is a gap between the N^{th} and $(N+1)^{\text{st}}$ eigenvalues of H^0 , and choose a Fermi level ϵ_F in this gap. Then, $\gamma^0 = \mathbb{1}_{(-\infty, \epsilon_F]}(H^0)$ is the unique minimizer of (4.2) for $\mathbf{X} = \mathbf{X}^0$ (it is a rank- N orthogonal projector). Using results from [CM14], it can be shown that for any $\mathbf{X} \in (\mathbb{R}^3)^M$ in the vicinity of \mathbf{X}^0 ,

- the minimization problem (4.2) admits a unique minimizer which we denote by $\gamma_{\mathbf{X}}$. In fact, $\gamma_{\mathbf{X}}$ is also the unique minimizer of the free energy $\mathcal{E}^{\text{fs}}(\mathbf{X}, \gamma) - \epsilon_F \text{Tr}_{L^2(\mathbb{R}^3)}(\gamma)$ on \mathcal{P}^{fs} ;
- the map $\mathbf{X} \mapsto \mathcal{W}^{\text{fs}}(\mathbf{X})$ is real-analytic.

Remark that \mathbf{X}^0 is an equilibrium configuration of \mathcal{W}^{fs} , and that the nuclear forces in the equilibrium configuration \mathbf{X}^0 vanish. More precisely, for all $1 \leq k \leq M$:

$$0 = -\nabla_{X_k} \mathcal{W}^{\text{fs}}(\mathbf{X}^0) = -\int_{\mathbb{R}^3} V^0(x) \nabla m(x - X_k^0) dx = \int_{\mathbb{R}^3} m(x - X_k^0) \nabla V^0(x) dx. \quad (4.3)$$

Let us write the nuclear dynamics around the equilibrium position \mathbf{X}^0 , as a preparation for the lattice dynamics around a periodic configuration considered in Section 4.3. Denoting respectively by $X_k(t) \in \mathbb{R}^3$ and $P_k(t) \in \mathbb{R}^3$ the position and momentum of the k -th nucleus at time t , the rHF Born–Oppenheimer nuclear dynamics around \mathbf{X}^0 is defined by: for $1 \leq k \leq M$,

$$\begin{cases} \frac{dX_k(t)}{dt} = \frac{P_k(t)}{m_k}, \\ \frac{dP_k(t)}{dt} = -\nabla_{X_k} \mathcal{W}^{\text{fs}}(\mathbf{X}(t)). \end{cases} \quad (4.4)$$

Reformulation of the dynamics. Given a generic state $(\mathbf{X}, \gamma) \in (\mathbb{R}^3)^M \times \mathcal{P}^{\text{fs}}$, we denote by (\mathbf{R}, Q) the deviation from the equilibrium state (\mathbf{X}^0, γ^0) , i.e.

$$\mathbf{X} = \mathbf{X}^0 + \mathbf{R} = (X_k^0 + R_k)_{1 \leq k \leq M}, \quad \gamma = \gamma^0 + Q.$$

Let us introduce the variation of nuclear density

$$\nu_{\mathbf{R}}^{\text{fs}} := \mu_{\mathbf{X}^0 + \mathbf{R}}^{\text{fs}} - \mu_{\mathbf{X}^0}^{\text{fs}} = \sum_{k=1}^M z_k (m(\cdot - X_k^0 - R_k) - m(\cdot - X_k^0)),$$

and its first order approximation

$$\nu_{1, \mathbf{R}}^{\text{fs}} := -\sum_{k=1}^M z_k \nabla m(\cdot - X_k^0) \cdot R_k.$$

The relative free energy of the system can be written as

$$\begin{aligned}
E^{\text{fs}}(\mathbf{R}, Q) &= \left(\mathcal{E}^{\text{fs}}(\mathbf{X}, \gamma) - \epsilon_{\text{F}} \text{Tr}_{L^2(\mathbb{R}^3)}(\gamma) \right) - \left(\mathcal{E}^{\text{fs}}(\mathbf{X}^0, \gamma^0) - \epsilon_{\text{F}} \text{Tr}_{L^2(\mathbb{R}^3)}(\gamma^0) \right) \\
&= \text{Tr}_{L^2(\mathbb{R}^3)} \left(-\frac{1}{2} \Delta (\gamma^0 + Q) \right) + \frac{1}{2} D \left(\rho_{\gamma^0+Q} - (\mu_{\mathbf{X}^0}^{\text{fs}} + \nu_{\mathbf{R}}), \rho_{\gamma^0+Q} - (\mu_{\mathbf{X}^0}^{\text{fs}} + \nu_{\mathbf{R}}^{\text{fs}}) \right) - \epsilon_{\text{F}} \text{Tr}_{L^2(\mathbb{R}^3)}(\gamma) \\
&\quad - \text{Tr}_{L^2(\mathbb{R}^3)} \left(-\frac{1}{2} \Delta \gamma^0 \right) + \frac{1}{2} D \left(\rho_{\gamma^0} - \mu_{\mathbf{X}^0}^{\text{fs}}, \rho_{\gamma^0} - \mu_{\mathbf{X}^0}^{\text{fs}} \right) - \epsilon_{\text{F}} \text{Tr}_{L^2(\mathbb{R}^3)}(\gamma^0) \\
&= \text{Tr}_{L^2(\mathbb{R}^3)} \left(-\frac{1}{2} \Delta Q \right) + D \left(\rho_{\gamma^0} - \mu_{\mathbf{X}^0}^{\text{fs}}, \rho_Q - \nu_{\mathbf{R}}^{\text{fs}} \right) + \frac{1}{2} D \left(\rho_Q - \nu_{\mathbf{R}}^{\text{fs}}, \rho_Q - \nu_{\mathbf{R}}^{\text{fs}} \right) - \epsilon_{\text{F}} \text{Tr}_{L^2(\mathbb{R}^3)}(Q) \\
&= \text{Tr}_{L^2(\mathbb{R}^3)} \left((H^0 - \epsilon_{\text{F}}) Q \right) + \frac{1}{2} D \left(\rho_Q - \nu_{\mathbf{R}}^{\text{fs}}, \rho_Q - \nu_{\mathbf{R}}^{\text{fs}} \right) - \int_{\mathbb{R}^3} V^0 \nu_{\mathbf{R}}^{\text{fs}} \\
&= \text{Tr}_{L^2(\mathbb{R}^3)} \left((H^0 - \epsilon_{\text{F}}) Q \right) + \frac{1}{2} D \left(\rho_Q - \nu_{\mathbf{R}}^{\text{fs}}, \rho_Q - \nu_{\mathbf{R}}^{\text{fs}} \right) - \int_{\mathbb{R}^3} V^0 \left(\nu_{\mathbf{R}}^{\text{fs}} - \nu_{1, \mathbf{R}}^{\text{fs}} \right), \tag{4.5}
\end{aligned}$$

where we have used (4.3) to obtain the last equality. Finally, the *relative Born–Oppenheimer free energy surface* is given by

$$W^{\text{fs}}(\mathbf{R}) := \mathcal{W}^{\text{fs}}(\mathbf{X}^0 + \mathbf{R}) - \mathcal{W}^{\text{fs}}(\mathbf{X}^0) = \inf \left\{ E^{\text{fs}}(\mathbf{R}, Q), Q + \gamma^0 \in \mathcal{P}^{\text{fs}} \right\}. \tag{4.6}$$

We observe that for \mathbf{R} small enough, the force on the k -th nucleus can be obtained by differentiating (4.6) as

$$\begin{aligned}
\forall 1 \leq k \leq M, \quad F_k^{\text{fs}}(\mathbf{R}) &:= -\nabla_{R_k} W^{\text{fs}}(\mathbf{R}) \\
&= z_k \int_{\mathbb{R}^3} m(\cdot - X_k^0 - R_k) \nabla V_{\mathbf{R}}^{\text{fs}} - z_k \int_{\mathbb{R}^3} V^0 (\nabla m(\cdot - X_k^0 - R_k) - \nabla m(\cdot - X_k^0)) \\
&= z_k \int_{\mathbb{R}^3} m(\cdot - X_k^0 - R_k) \left(\nabla V^0 + \nabla V_{\mathbf{R}}^{\text{fs}} \right), \tag{4.7}
\end{aligned}$$

where $V_{\mathbf{R}}^{\text{fs}} = (\rho_{\mathbf{R}} - \nu_{\mathbf{R}}^{\text{fs}}) \star |\cdot|^{-1}$, and $\rho_{\mathbf{R}}$ is the unique density of the minimizers $Q_{\mathbf{R}}$ of (4.6). If the state (\mathbf{X}^0, γ^0) is a global minimizer of \mathcal{E}^{fs} on $(\mathbb{R}^3)^M \times \mathcal{P}^{\text{fs}}$ (and not only a local one), it holds

$$\forall (\mathbf{R}, \gamma^0 + Q) \in (\mathbb{R}^3)^M \times \mathcal{P}^{\text{fs}}, \quad E^{\text{fs}}(\mathbf{R}, Q) \geq 0; \tag{4.8}$$

and therefore

$$\forall \mathbf{R} \in (\mathbb{R}^3)^M, \quad W^{\text{fs}}(\mathbf{R}) \geq 0. \tag{4.9}$$

In view of (4.9), we can define a Hamiltonian $H^{\text{fs}} : (\mathbb{R}^3)^M \times (\mathbb{R}^3)^M \rightarrow \mathbb{R}$ associated with the nuclear degree of freedom by summing up the kinetic energy of the nuclei and the relative Born–Oppenheimer energy surface, which serves as a potential energy driving the nuclear dynamics:

$$H^{\text{fs}}(\mathbf{R}, \mathbf{P}) = \sum_{k=1}^M \frac{|P_k|^2}{2m_k} + W^{\text{fs}}(\mathbf{R}). \tag{4.10}$$

The Born–Oppenheimer dynamics (4.4) around the local equilibrium configuration \mathbf{X}^0 can then be recast as

$$\begin{cases} \frac{dR_k(t)}{dt} = \nabla_{P_k} H^{\text{fs}}(\mathbf{R}(t), \mathbf{P}(t)) = \frac{P_k(t)}{m_k}, \\ \frac{dP_k(t)}{dt} = -\nabla_{R_k} H^{\text{fs}}(\mathbf{R}(t), \mathbf{P}(t)) = -\nabla_{R_k} W^{\text{fs}}(\mathbf{R}(t)). \end{cases} \tag{4.11}$$

4.3 Lattice dynamics around a periodic equilibrium configuration

In this section we generalize the nuclear dynamics for finite systems introduced in the previous section to lattice dynamics around a periodic equilibrium configuration. This is obtained by a formal thermodynamic limit of the model for finite systems. More precisely, we now assume that the reference equilibrium configuration is a perfect crystal, and we denote by \mathcal{L} its Bravais lattice and by z_k the nuclear charge of the nucleus located at equilibrium at the point $k \in \mathcal{R}$, where \mathcal{R} denotes the set of lattice sites (for convenience, we label the nuclei by the corresponding lattice points). We assume that the nuclear charge is modeled by a \mathcal{R} -periodic distribution:

$$\mu_{\text{per}}^0 = \sum_{k \in \mathcal{R}} z_k m(\cdot - k),$$

where we recall that $m \in C_c^\infty(\mathbb{R}^3)$ is a smooth radial nonnegative function supported in the ball $\mathfrak{B}_\eta = \{x \in \mathbb{R}^3 \mid |x| < \eta\}$ for some $\eta > 0$ and such that $\int_{\mathbb{R}^3} m = 1$. We assume that the minimal distance between the centers of two nuclei in the periodic lattice \mathcal{R} is $d_m \gg \eta$ for simplicity. As shown in [CLBL01, CLBL02, CDL08a], the rHF model for such a crystal is well posed and the ground-state density matrix γ_{per}^0 is unique (see also Section 1.2 of Chapter 1. We denote by ρ_{per}^0 the density of γ_{per}^0 , by V_{per}^0 the unique \mathcal{R} -periodic solution of the Poisson equation $-\Delta V_{\text{per}}^0 = 4\pi(\rho_{\text{per}}^0 - \mu_{\text{per}}^0)$ with zero average in unit cells of \mathcal{R} , and by

$$H_{\text{per}}^0 = -\frac{1}{2}\Delta + V_{\text{per}}^0$$

the rHF mean-field Hamiltonian of the perfect crystal. Recall that H_{per}^0 is an \mathcal{R} -periodic Schrödinger operator on $L^2(\mathbb{R}^3)$ with domain $H^2(\mathbb{R}^3)$. We also know that

$$\gamma_{\text{per}}^0 = \mathbb{1}_{(-\infty, \epsilon_F]}(H_{\text{per}}^0)$$

is a (infinite-rank) orthogonal projector on $L^2(\mathbb{R}^3)$. Similarly to (4.3), the fact that the \mathcal{R} -periodic nuclear configuration forms an equilibrium geometry implies that the force on each nucleus vanishes:

$$\forall k \in \mathcal{R}, \quad \int_{\mathbb{R}^3} m(\cdot - k) \nabla V_{\text{per}}^0 = - \int_{\mathbb{R}^3} V_{\text{per}}^0 \nabla m(\cdot - k) = 0. \quad (4.12)$$

From now on, we make the following assumption.

Assumption 4. *The reference perfect crystal is an insulator or a semiconductor, in the sense that the Fermi level ϵ_F lays in a spectral gap of H_{per}^0 : $d(\epsilon_F, \sigma(H_{\text{per}}^0)) > 0$.*

Defects induced by nuclear displacements. We denote by $\mathbf{R} = (R_k)_{k \in \mathcal{R}} \in (\mathbb{R}^3)^{\mathcal{R}}$ the nuclear displacement with respect to the perfect lattice, where $R_k \in \mathbb{R}^3$ denotes the displacement of the k -th nucleus with respect to its site in the \mathcal{R} -periodic configuration. The change of nuclear density is thus given by:

$$\nu_{\mathbf{R}}(x) := \sum_{k \in \mathcal{R}} z_k (m(x - (k + R_k)) - m(x - k)).$$

Remark that the function $\nu_{\mathbf{R}}$ can be considered as defects of the nuclear configuration with respect to the perfect crystal. This relates the study of lattice dynamics to works on local defects as considered in [CDL08a, CL10, CE11] and presented in Section 1.3.1 of Chapter 1. In particular, these works ensure that the rHF model for ground-state electronic structures of local defects in insulating systems is well-posed as soon as the nuclear charge distribution of the defect $\nu_{\mathbf{R}}$ belongs to the Hilbert space $\nu_{\mathbf{R}} \in v_c^{-1}(L^2(\mathbb{R}^3)) + \mathcal{C}$ (see [CL10, Theorem 1]), where $v_c(\rho) := \rho \star |\cdot|^{-1}$ (v_c is the Coulomb operator). In this study, we will consider a functional setting of lattice dynamics in which $\nu_{\mathbf{R}}(t)$ remains in $v_c^{-1}(L^2(\mathbb{R}^3)) + \mathcal{C}$ for all $t \geq 0$.

Functional setting. Introduce the space of square integrable displacements

$$\ell^2(\mathcal{R}) := \left\{ \mathbf{R} = (R_k)_{k \in \mathcal{R}} \in (\mathbb{R}^3)^{\mathcal{R}} \mid \sum_{k \in \mathcal{R}} |R_k|^2 < \infty \right\},$$

equipped with its natural inner product:

$$(\mathbf{R}, \mathbf{R}')_{\ell^2} := \sum_{k \in \mathcal{R}} R_k \cdot R'_k.$$

An admissible functional space of nuclear displacements is provided by the following result.

Lemma 4.1. *Consider the dense subspace of $\ell^2(\mathcal{R})$ defined by*

$$\mathcal{H} := \left\{ \mathbf{R} = (R_k)_{k \in \mathcal{R}} \in \ell^2(\mathcal{R}) \mid \nu_{1, \mathbf{R}} := - \sum_{k \in \mathcal{R}} z_k \nabla m(\cdot - k) \cdot R_k \in \mathcal{C} \right\}. \quad (4.13)$$

Endowed with the inner product defined by

$$(\mathbf{R}, \mathbf{R}')_{\mathcal{H}} := (\mathbf{R}, \mathbf{R}')_{\ell^2} + (\nu_{1, \mathbf{R}}, \nu_{1, \mathbf{R}'})_{\mathcal{C}},$$

the space \mathcal{H} is a Hilbert space. Moreover, for all $\mathbf{R} \in \mathcal{H}$ it holds $\nu_{\mathbf{R}} \in L^2(\mathbb{R}^3) \cap \mathcal{C}$, and $\nu_{\mathbf{R}} - \nu_{1, \mathbf{R}}$ belongs to $L^1(\mathbb{R}^3) \cap L^2(\mathbb{R}^3)$. In fact, there exists $C_1, C_2 \in \mathbb{R}_+$ such that

$$\forall \mathbf{R} \in \mathcal{H}, \quad \|\nu_{\mathbf{R}}\|_{\mathcal{C}} + \|\nu_{\mathbf{R}}\|_{L^2} \leq C_1 \|\mathbf{R}\|_{\mathcal{H}} (1 + \|\mathbf{R}\|_{\mathcal{H}}), \quad (4.14)$$

and

$$\forall \mathbf{R} \in \ell^2(\mathcal{R}), \quad \|\nu_{\mathbf{R}} - \nu_{1, \mathbf{R}}\|_{L^1} + \|\nu_{\mathbf{R}} - \nu_{1, \mathbf{R}}\|_{L^2} \leq C_2 \|\mathbf{R}\|_{\ell^2}^2. \quad (4.15)$$

The proof can be read in Section 4.5.1. Passing formally to the bulk limit in the Born-Oppenheimer rHF model for finite systems (4.6)-(4.10), and relying on the results in [CDL08a], we can henceforth define a rHF ground-state Born-Oppenheimer energy surface associated with the nuclear defect $\nu_{\mathbf{R}}$. The analogue of (4.6) is

$$W(\mathbf{R}) := \inf \left\{ E(\mathbf{R}, Q), Q \in \mathcal{K}_{\gamma_{\text{per}}^0} \right\}, \quad (4.16)$$

where

$$E(\mathbf{R}, Q) := \text{Tr}_0((H_{\text{per}}^0 - \varepsilon_{\text{F}})Q) + \frac{1}{2} D(\rho_Q - \nu_{\mathbf{R}}, \rho_Q - \nu_{\mathbf{R}}) - \int_{\mathbb{R}^3} V_{\text{per}}^0(\nu_{\mathbf{R}} - \nu_{1, \mathbf{R}}).$$

In this expression,

$$\begin{aligned} \text{Tr}_0((H_{\text{per}}^0 - \varepsilon_{\text{F}})Q) &:= \text{Tr}_{L^2(\mathbb{R}^3)} \left(|H_{\text{per}}^0 - \varepsilon_{\text{F}}|^{1/2} (Q^{++} - Q^{--}) |H_{\text{per}}^0 - \varepsilon_{\text{F}}|^{1/2} \right), \\ Q^{++} &:= (1 - \gamma_{\text{per}}^0) Q (1 - \gamma_{\text{per}}^0), \quad Q^{--} := \gamma_{\text{per}}^0 Q \gamma_{\text{per}}^0, \end{aligned}$$

and

$$\mathcal{K}_{\gamma_{\text{per}}^0} := \left\{ Q \in \mathcal{Q}_{\gamma_{\text{per}}^0} \mid -\gamma_{\text{per}}^0 \leq Q \leq 1 - \gamma_{\text{per}}^0 \right\},$$

where $\mathcal{Q}_{\gamma_{\text{per}}^0}$ is the Banach space of operators having finite γ_{per}^0 -trace and finite kinetic energies:

$$\begin{aligned} \mathcal{Q}_{\gamma_{\text{per}}^0} := \left\{ Q \in \mathfrak{S}_1^{\gamma_{\text{per}}^0}(L^2(\mathbb{R}^3)) \mid Q^* = Q, |\nabla|Q \in \mathfrak{S}_2(L^2(\mathbb{R}^3)), \right. \\ \left. |\nabla|Q^{++}|\nabla| \in \mathfrak{S}_1(L^2(\mathbb{R}^3)), |\nabla|Q^{--}|\nabla| \in \mathfrak{S}_1(L^2(\mathbb{R}^3)) \right\}, \end{aligned}$$

equipped with its natural norm

$$\|Q\|_{\mathcal{Q}_{\gamma_{\text{per}}^0}} := \|Q\|_{\mathfrak{S}_2} + \|Q^{++}\|_{\mathfrak{S}_1} + \|Q^{--}\|_{\mathfrak{S}_1} + \||\nabla|Q\|_{\mathfrak{S}_2} + \||\nabla|Q^{++}|\nabla|\|_{\mathfrak{S}_1} + \||\nabla|Q^{--}|\nabla|\|_{\mathfrak{S}_1}.$$

Recall that we have already introduced the convex set $\mathcal{K}_{\gamma_{\text{per}}^0}$ and the space $\mathcal{Q}_{\gamma_{\text{per}}^0}$ in Section 1.3.1 of Chapter 1.

Well-posedness of the rHF electronic problem. We have shown in Lemma 4.1 that the displacement $\mathbf{R} \in \mathcal{H}$ leads to admissible defect function $\nu(\mathbf{R})$. At this stage, we have to make the following assumption on the stability of the crystal. Remark that the condition (4.17) is the analogue of the inequality (4.8) for finite systems.

Assumption 5. *The point $\mathbf{R} = 0$ is a global minimum of the relative ground state energy $W(\mathbf{R})$ defined in (4.16). That is,*

$$\forall (\mathbf{R}, Q) \in \mathcal{H} \times \mathcal{K}_{\gamma_{\text{per}}^0}, \quad E(\mathbf{R}, Q) \geq E(\mathbf{0}, 0) = 0. \quad (4.17)$$

Under Assumption 5 the following inequality holds,

$$\forall \mathbf{R} \in \mathcal{H}, \quad W(\mathbf{R}) \geq 0. \quad (4.18)$$

We have the following result on the well-posedness of the rHF electronic problem given nuclear displacements \mathcal{R} in \mathcal{H} .

Lemma 4.2 (Well-posedness of the electronic problem for $\mathbf{R} \in \mathcal{H}$). *For any $\mathbf{R} \in \mathcal{H}$, the electronic problem (4.16) has a minimizer, and all the minimizers share the same density $\rho_{\mathbf{R}} \in L^2(\mathbb{R}^3) \cap \mathcal{C}$. In addition, the following properties hold: there exists $C \in \mathbb{R}_+$ such that, for all $\mathbf{R} \in \mathcal{H}$,*

$$\|\nabla V_{\mathbf{R}}\|_{L^2}^2 \leq 2 (\|\mathbf{R}\|_{\mathcal{H}}^2 + C\|\mathbf{R}\|_{\ell^2}^4), \quad (4.19)$$

where $V_{\mathbf{R}} = (\rho_{\mathbf{R}} - \nu_{\mathbf{R}}) \star |\cdot|^{-1} \in \mathcal{C}'$ is the rHF mean-field potential generated by the defect $\nu_{\mathbf{R}}$, and

$$\|\rho_{\mathbf{R}}\|_{L^2 \cap \mathcal{C}} \leq C \left(W(\mathbf{R})^{1/2} + W(\mathbf{R}) + \|\mathbf{R}\|_{\ell^2} + \|\mathbf{R}\|_{\ell^2}^2 \right). \quad (4.20)$$

The proof can be read in Section 4.5.2.

The Hamiltonian dynamics of nuclei. Consider the Hamiltonian $H : \mathcal{H} \times \ell^2(\mathcal{R}) \rightarrow \mathbb{R}_+$ defined by

$$\forall (\mathbf{R}, \mathbf{P}) \in \mathcal{H} \times \ell^2(\mathcal{R}), \quad H(\mathbf{R}, \mathbf{P}) = \sum_{k \in \mathcal{R}} \frac{|P_k|^2}{2m_k} + W(\mathbf{R}), \quad (4.21)$$

where we recall that $W(\mathbf{R})$ defined in (4.16) is the relative rHF ground-state Born-Oppenheimer energy surface. The function H admits partial derivatives with respect to the variables $R_k \in \mathbb{R}^3$ and $P_k \in \mathbb{R}^3$ for all $k \in \mathcal{R}$. Similarly to (4.7) for finite systems, for \mathbf{R} small enough, the force acting on nucleus k is

$$\begin{aligned} F_k(\mathbf{R}) &:= -(\nabla_{R_k} H)(\mathbf{R}, \mathbf{P}) = -\nabla_{R_k} W(\mathbf{R}) = -\int_{\mathbb{R}^3} (V_{\text{per}}^0 + V_{\mathbf{R}}) \nabla m(\cdot - k - R_k) \\ &= \int_{\mathbb{R}^3} m(\cdot - k - R_k) (\nabla V_{\text{per}}^0 + \nabla V_{\mathbf{R}}). \end{aligned}$$

We denote by $\mathbf{F}(\mathbf{R}) = (F_k(\mathbf{R}))_{k \in \mathcal{R}}$.

Lemma 4.3 (Bounds on the force). *For any $\mathbf{R} \in \mathcal{H}$, it holds that $\mathbf{F}(\mathbf{R}) \in \ell^2(\mathcal{R})$. Moreover, there exists a constant $C \in \mathbb{R}_+$ independent of \mathbf{R} such that*

$$\forall \mathbf{R} \in \mathcal{H}, \quad \|\mathbf{F}(\mathbf{R})\|_{\ell^2} \leq C\|\mathbf{R}\|_{\ell^2} (1 + \|\mathbf{R}\|_{\mathcal{H}} + \|\mathbf{R}\|_{\ell^2}^2). \quad (4.22)$$

The proof can be read in Section 4.5.3. This allows us to define the rHF Born-Oppenheimer lattice dynamics, which is an infinite-dimensional Hamiltonian dynamics:

$$\forall k \in \mathcal{R}, \quad \begin{cases} \frac{dR_k(t)}{dt} = \nabla_{P_k} H(\mathbf{R}(t), \mathbf{P}(t)) = \frac{P_k(t)}{m_k}, \\ \frac{dP_k(t)}{dt} = -\nabla_{R_k} H(\mathbf{R}(t), \mathbf{P}(t)) = -\nabla_{R_k} W(\mathbf{R}(t)) = F_k(\mathbf{R}(t)). \end{cases} \quad (4.23)$$

Denoting by $\mathbf{Y}(t) = (\mathbf{R}(t), \mathbf{P}(t))$, the Hamiltonian dynamics (4.23) can be written as

$$\frac{d\mathbf{Y}(t)}{dt} = \mathbf{N}(\mathbf{Y}(t)), \quad (4.24)$$

with $\mathbf{N}(\mathbf{Y}) := (M^{-1}\mathbf{P}, \mathbf{F}(\mathbf{R}))$ for $\mathbf{Y} = (\mathbf{R}, \mathbf{P})$ and $M := (m_k)_{k \in \mathcal{R}}$. We consider the norm

$$\|\mathbf{Y}\|_{\mathcal{H} \times \ell^2(\mathcal{R})} := \left(\|\mathbf{R}\|_{\mathcal{H}}^2 + \|\mathbf{P}\|_{\ell^2(\mathcal{R})}^2 \right)^{1/2}.$$

We have the following result on the local well-posedness of the Hamiltonian dynamics (4.24) for a small initial data.

Proposition 4.4 (local well-posedness of Hamiltonian dynamics). *There exists a positive constant α such that for any $\varepsilon \in (0, \alpha)$, there exists $\tau(\varepsilon, \alpha) > 0$ depending only on ε and α such that for any initial condition of the Hamiltonian dynamics (4.24) satisfying*

$$\|\mathbf{Y}(0)\|_{\mathcal{H} \times \ell^2(\mathcal{R})} \leq \alpha - \varepsilon, \quad (4.25)$$

the equation (4.24) has a unique solution $\mathbf{Y} \in C^1([0, \tau(\varepsilon, \alpha)], \mathcal{H} \times \ell^2(\mathcal{R}))$.

The proof can be read in Section 4.5.5. The condition (4.25) on the initial data guarantees that the Fermi level ε_F is not an eigenvalue of the mean-field Hamiltonian, which guarantees that the Hellmann–Feynman expression of the force term is correct, and that the forces are Lipschitz continuous.

4.4 Perspectives

We discuss here the two obstacles for proving the global existence and uniqueness of the Hamiltonian dynamics, and also hint at some on-going work. The existence and uniqueness for initial data which are not small (condition (4.25) is no longer satisfied), and/or for long time requires a perturbation analysis of the rHF model when the Fermi level is ε_F occupied. For finite systems, the situation of fractional occupations has already been studied in [CM14]. One should be able to adapt results in [CM14] to our problem. Additionally, for the global existence, one should prove local Lipschitz continuity of the force term $\mathbf{F}(\mathbf{R})$ for the whole space \mathcal{H} . The main ingredient is to extend the technical estimate (4.42) to all $\alpha > 0$. This requires results on the linear response theory around a generic potential $V_{\text{per}}^0 + V_{\mathbf{R}} \in \mathcal{C}'$ for $\mathbf{R} \in \mathcal{H}$, while only results on the linear response around a periodic configuration V_{per}^0 are known in the rHF model [CL10].

4.5 Proofs of the results

4.5.1 Proof of Lemma 4.1

Let us first show that \mathcal{H} is a Hilbert space. It suffices to verify that \mathcal{H} is complete. Consider a Cauchy sequence $(\mathbf{R}_n)_{n \in \mathbb{N}^*}$ in \mathcal{H} . It is easy to see that there exists $\tilde{\mathbf{R}}$ in $\ell^2(\mathcal{R})$ such that $\mathbf{R}_n \xrightarrow[n \rightarrow \infty]{} \tilde{\mathbf{R}}$ in $\ell^2(\mathcal{R})$, and $w \in L^2(\mathbb{R}^3)$ such that $|\xi|^{-1} \hat{\nu}_{1, \mathbf{R}_n}(\xi) \xrightarrow[n \rightarrow \infty]{} \hat{w}(\xi)$ in $L^2(\mathbb{R}^3)$. Let us show that $\hat{w}(\xi) = |\xi|^{-1} \hat{\nu}_{1, \tilde{\mathbf{R}}}(\xi)$. Introduce the discrete Fourier transform \mathfrak{F} which is a unitary operator from $\ell^2(\mathcal{R})$ to $L^2_{\text{per}}(\Gamma^*)$:

$$\forall \phi = (\phi_k)_{k \in \mathcal{R}} \in \ell^2(\mathcal{R}), \quad \mathfrak{F}\phi_k(\xi) := \sum_{k \in \mathcal{R}} e^{-ik\xi} \phi_k,$$

with its inverse

$$\forall \psi \in L^2_{\text{per}}(\Gamma^*), \quad (\mathfrak{F}^{-1}\phi)(k) := \int_{\Gamma^*} e^{ik\xi} \psi(\xi) d\xi.$$

Then,

$$|\xi|^{-1}\widehat{\nu}_{1,\mathbf{R}_n}(\xi) = -i\widehat{m}(\xi)|\xi|^{-1}\xi \cdot \left(\sum_{k \in \mathcal{R}} e^{-ik\xi} R_{n,k} z_k \right) = -i\widehat{m}(\xi)|\xi|^{-1}\xi \cdot \mathfrak{F}(z \odot \mathbf{R}_n)(\xi),$$

where $z := (z_k)_{k \in \mathcal{R}}$ and $z \odot \mathbf{R} := (z_\ell R_\ell)_{\ell \in \mathcal{R}}$. The fact that $\mathbf{R}_n \xrightarrow[n \rightarrow \infty]{} \widetilde{\mathbf{R}}$ in $\ell^2(\mathcal{R})$ and $z \in \ell^\infty(\mathcal{R})$ implies that

$$z \odot \mathbf{R}_n \xrightarrow[n \rightarrow \infty]{} z \odot \widetilde{\mathbf{R}} \text{ in } \ell^2(\mathcal{R}),$$

and therefore

$$\mathfrak{F}(z \odot \mathbf{R}_n) \xrightarrow[n \rightarrow \infty]{} \mathfrak{F}(z \odot \widetilde{\mathbf{R}}) \text{ in } L^2_{\text{per}}(\Gamma^*).$$

As $\widehat{m}(\xi)|\xi|^{-1}\xi$ belongs to $L^\infty(\mathbb{R}^3)$, we obtain that

$$|\xi|^{-1}\widehat{\nu}_{1,\mathbf{R}_n}(\xi) \xrightarrow[n \rightarrow \infty]{} |\xi|^{-1}\widehat{\nu}_{1,\widetilde{\mathbf{R}}}(\xi) \text{ in } L^2_{\text{loc}}(\mathbb{R}^3).$$

By the uniqueness of the limit in $L^2_{\text{loc}}(\mathbb{R}^3)$ we conclude that $|\xi|^{-1}\widehat{\nu}_{1,\widetilde{\mathbf{R}}}(\xi) = \widehat{w}(\xi) \in L^2(\mathbb{R}^3)$. This shows that \mathcal{H} is complete.

Let us now prove the remaining statements of the lemma. First of all, since the nuclear distributions do not overlap in the equilibrium configuration, we have

$$\begin{aligned} \|\nu_{1,\mathbf{R}}\|_{L^2}^2 &= \int_{\mathbb{R}^3} \left| \sum_{k \in \mathcal{R}} z_k \nabla m(x-k) \cdot R_k \right|^2 dx \leq \sum_{k,l \in \mathcal{R}} z_k z_l \left(\int_{\mathbb{R}^3} |\nabla m(x-k)| |\nabla m(x-l)| dx \right) |R_k| |R_l| \\ &= \sum_{k \in \mathcal{R}} z_k^2 \left(\int_{\mathbb{R}^3} |\nabla m(x-k)|^2 dx \right) |R_k|^2 \leq \left(\max_{k \in \mathcal{R}} z_k^2 \right) \|\nabla m\|_{L^2}^2 \|\mathbf{R}\|_{\ell^2}^2. \end{aligned}$$

Therefore,

$$\forall \mathbf{R} \in \ell^2(\mathcal{R}), \quad \|\nu_{1,\mathbf{R}}\|_{L^2} \leq \left(\max_{k \in \mathcal{R}} z_k \right) \|\nabla m\|_{L^2} \|\mathbf{R}\|_{\ell^2}. \quad (4.26)$$

The linear map $\mathbf{R} \mapsto \nu_{1,\mathbf{R}}$ is thus continuous from \mathcal{H} to $L^2(\mathbb{R}^3) \cap \mathcal{C}$. Let us next show that $\nu_{\mathbf{R}}$ belongs to $L^2(\mathbb{R}^3) \cap \mathcal{C}$. It holds

$$(\nu_{\mathbf{R}} - \nu_{1,\mathbf{R}})(x) = \sum_{k \in \mathbf{R}} z_k (m(x-k-R_k) - m(x-k) + \nabla m(x-k) \cdot R_k). \quad (4.27)$$

By the fundamental theorem of calculus, it holds,

$$m(x-k-R_k) - m(x-k) = - \int_0^1 \nabla m(x-k-tR_k) \cdot R_k dt. \quad (4.28)$$

Therefore,

$$\begin{aligned} m(x-k-R_k) - m(x-k) + \nabla m(x-k) \cdot R_k &= \int_0^1 (\nabla m(x-k) - \nabla m(x-k-tR_k)) \cdot R_k dt \\ &= \int_0^1 \int_0^1 t R_k^T \text{Hess}(m)(x-k-stR_k) R_k ds dt. \end{aligned}$$

where $\text{Hess}(m) \in C_c^\infty(\mathbb{R}^3; \mathbb{R}^{3 \times 3})$ stands for the Hessian of m . Therefore,

$$\begin{aligned} &\|m(\cdot-k-R_k) - m(\cdot-k) + \nabla m(\cdot-k) \cdot R_k\|_{L^1(\mathbb{R}^3)} \\ &\leq \int_0^1 \int_0^1 t \left(\int_{\mathbb{R}^3} \|\text{Hess}(m)(x-k-stR_k)\|_2 dx \right) |R_k|^2 ds dt \leq \frac{1}{2} \|\text{Hess}(m)\|_{L^1(\mathbb{R}^3)} |R_k|^2, \end{aligned}$$

where $\|\cdot\|_2$ is the matrix norm associated with the Euclidean scalar product on \mathbb{R}^3 . Similarly,

$$\|m(\cdot - k - R_k) - m(\cdot - k) + \nabla m(\cdot - k) \cdot R_k\|_{L^\infty(\mathbb{R}^3)} \leq \frac{1}{2} \|\text{Hess}(m)\|_{L^\infty(\mathbb{R}^3)} |R_k|^2.$$

Hence by interpolation, for all $1 \leq p \leq +\infty$,

$$\|m(\cdot - k - R_k) - m(\cdot - k) + \nabla m(\cdot - k) \cdot R_k\|_{L^p(\mathbb{R}^3)} \leq \frac{1}{2} \|\text{Hess}(m)\|_{L^p(\mathbb{R}^3)} |R_k|^2. \quad (4.29)$$

In view of (4.27) and (4.29), it follows that for $1 \leq p \leq +\infty$ and $p' = p/(p-1)$:

$$\forall \mathbf{R} \in \ell^2(\mathcal{R}), \quad \|\nu_{\mathbf{R}} - \nu_{1,\mathbf{R}}\|_{L^p} \leq \frac{1}{2} \left(\max_{k \in \mathcal{R}} z_k \right) \|\text{Hess}(m)\|_{L^1(\mathbb{R}^3)}^{1/p} \|\text{Hess}(m)\|_{L^\infty(\mathbb{R}^3)}^{1/p'} \|\mathbf{R}\|_{\ell^2}^2. \quad (4.30)$$

Therefore (4.15) holds. Since $L^{6/5}(\mathbb{R}^3) \hookrightarrow \mathcal{C}$, there exists $C \in \mathbb{R}_+$ such that

$$\forall \mathbf{R} \in \ell^2(\mathcal{R}), \quad \|\nu_{\mathbf{R}} - \nu_{1,\mathbf{R}}\|_{\mathcal{C}} \leq C \|\mathbf{R}\|_{\ell^2}^2.$$

Therefore,

$$\forall \mathbf{R} \in \mathcal{H}, \quad \|\nu_{\mathbf{R}}\|_{\mathcal{C}} \leq \|\nu_{1,\mathbf{R}}\|_{\mathcal{C}} + \|\nu_{\mathbf{R}} - \nu_{1,\mathbf{R}}\|_{\mathcal{C}} \leq \|\nu_{1,\mathbf{R}}\|_{\mathcal{C}} + C \|\mathbf{R}\|_{\ell^2}^2 \leq \|\mathbf{R}\|_{\mathcal{H}} + C \|\mathbf{R}\|_{\mathcal{H}}^2, \quad (4.31)$$

and by (4.26) and (4.30),

$$\forall \mathbf{R} \in \mathcal{H}, \quad \|\nu_{\mathbf{R}}\|_{L^2} \leq \|\nu_{1,\mathbf{R}}\|_{L^2} + \|\nu_{\mathbf{R}} - \nu_{1,\mathbf{R}}\|_{L^2} \leq C (\|\mathbf{R}\|_{\ell^2} + \|\mathbf{R}\|_{\ell^2}^2) \leq C (\|\mathbf{R}\|_{\mathcal{H}} + \|\mathbf{R}\|_{\mathcal{H}}^2).$$

In particular, this implies that $\nu_{\mathbf{R}}$ belongs to $L^2(\mathbb{R}^3) \cap \mathcal{C}$ for all $\mathbf{R} \in \mathcal{H}$ and (4.14) is satisfied.

4.5.2 Proof of Lemma 4.2

Since $\nu_{\mathbf{R}} \in L^2(\mathbb{R}^3) \cap \mathcal{C}$ for any $\mathbf{R} \in \mathcal{H}$ by Lemma 4.1, the result of [CL10, Theorem 1] ensures that the electronic problem (4.16) admits a minimizer and that all the minimizers share the same density $\rho_{\mathbf{R}}$. Let us prove the remaining statements in Lemma 4.2. First, $\text{Tr}_0((H_{\text{per}}^0 - \varepsilon_{\text{F}})Q_{\mathbf{R}}) \geq 0$ and $D(\rho_{\mathbf{R}} - \nu_{\mathbf{R}}, \rho_{\mathbf{R}} - \nu_{\mathbf{R}}) \geq 0$. As $Q_{\mathbf{R}}$ minimizes E and 0 is an admissible state, we obtain that, for any $\mathbf{R} \in \mathcal{H}$,

$$\begin{aligned} & \frac{1}{2} D(\nu_{\mathbf{R}}, \nu_{\mathbf{R}}) - \int_{\mathbb{R}^3} V_{\text{per}}^0(\nu_{\mathbf{R}} - \nu_{1,\mathbf{R}}) = E(\mathbf{R}, 0) \\ & \geq E(\mathbf{R}, Q_{\mathbf{R}}) = \text{Tr}_0((H_{\text{per}}^0 - \varepsilon_{\text{F}})Q_{\mathbf{R}}) + \frac{1}{2} D(\rho_{\mathbf{R}} - \nu_{\mathbf{R}}, \rho_{\mathbf{R}} - \nu_{\mathbf{R}}) - \int_{\mathbb{R}^3} V_{\text{per}}^0(\nu_{\mathbf{R}} - \nu_{1,\mathbf{R}}) \\ & \geq \frac{1}{2} D(\rho_{\mathbf{R}} - \nu_{\mathbf{R}}, \rho_{\mathbf{R}} - \nu_{\mathbf{R}}) - \int_{\mathbb{R}^3} V_{\text{per}}^0(\nu_{\mathbf{R}} - \nu_{1,\mathbf{R}}). \end{aligned}$$

This implies that

$$D(\rho_{\mathbf{R}} - \nu_{\mathbf{R}}, \rho_{\mathbf{R}} - \nu_{\mathbf{R}}) \leq D(\nu_{\mathbf{R}}, \nu_{\mathbf{R}}). \quad (4.32)$$

Hence in view of (4.31), it holds,

$$\begin{aligned} \|V_{\mathbf{R}}\|_{\mathcal{C}'}^2 &= \|\nabla V_{\mathbf{R}}\|_{L^2}^2 = \|\rho_{\mathbf{R}} - \nu_{\mathbf{R}}\|_{\mathcal{C}}^2 = D(\rho_{\mathbf{R}} - \nu_{\mathbf{R}}, \rho_{\mathbf{R}} - \nu_{\mathbf{R}}) \\ &\leq D(\nu_{\mathbf{R}}, \nu_{\mathbf{R}}) = \|\nu_{\mathbf{R}}\|_{\mathcal{C}}^2 \leq 2 (\|\mathbf{R}\|_{\mathcal{H}}^2 + C \|\mathbf{R}\|_{\ell^2}^4), \end{aligned} \quad (4.33)$$

which proves (4.19). It also follows from (4.15) and (4.30) that

$$\left| \int_{\mathbb{R}^3} V_{\text{per}}^0(\nu_{\mathbf{R}} - \nu_{1,\mathbf{R}}) \right| \leq \|V_{\text{per}}^0\|_{L^\infty} \|\nu_{\mathbf{R}} - \nu_{1,\mathbf{R}}\|_{L^1} \leq \frac{1}{2} \left(\max_{k \in \mathcal{R}} z_k \right) \|\text{Hess}(m)\|_{L^1} \|V_{\text{per}}^0\|_{L^\infty} \|\mathbf{R}\|_{\ell^2}^2. \quad (4.34)$$

Therefore,

$$\begin{aligned} W(\mathbf{R}) &= E(\mathbf{R}, Q_{\mathbf{R}}) = \text{Tr}_0 \left((H_{\text{per}}^0 - \varepsilon_F) Q_{\mathbf{R}} \right) + \frac{1}{2} D(\rho_{\mathbf{R}} - \nu_{\mathbf{R}}, \rho_{\mathbf{R}} - \nu_{\mathbf{R}}) - \int_{\mathbb{R}^3} V_{\text{per}}^0(\nu_{\mathbf{R}} - \nu_{1, \mathbf{R}}) \\ &\geq \text{Tr}_0 \left((H_{\text{per}}^0 - \varepsilon_F) Q_{\mathbf{R}} \right) + \frac{1}{2} D(\rho_{\mathbf{R}} - \nu_{\mathbf{R}}, \rho_{\mathbf{R}} - \nu_{\mathbf{R}}) - \frac{1}{2} \max_{k \in \mathcal{R}} z_k \|\text{Hess}(m)\|_{L^1} \|V_{\text{per}}^0\|_{L^\infty} \|\mathbf{R}\|_{\ell^2}^2. \end{aligned}$$

This implies that

$$0 \leq \text{Tr}_0 \left((H_{\text{per}}^0 - \varepsilon_F) Q_{\mathbf{R}} \right) \leq W(\mathbf{R}) + \frac{1}{2} \max_{k \in \mathcal{R}} z_k \|\text{Hess}(m)\|_{L^1} \|V_{\text{per}}^0\|_{L^\infty} \|\mathbf{R}\|_{\ell^2}^2. \quad (4.35)$$

By [CDL08a, Corollary 2] it follows from Assumption 4 that there exists $c > 0$ such that for all $Q \in \mathcal{Q}_{\gamma_{\text{per}}^0}$,

$$\begin{aligned} \text{Tr}_0 \left((H_{\text{per}}^0 - \varepsilon_F) Q \right) \\ \geq c \left(\|Q^{++}\|_{\mathfrak{S}_1} + \|Q^{--}\|_{\mathfrak{S}_1} + \|\nabla|Q^{++}| \nabla\|_{\mathfrak{S}_1} + \|\nabla|Q^{--}| \nabla\|_{\mathfrak{S}_1} + \|Q\|_{\mathfrak{S}_2}^2 + \|\nabla|Q|\|_{\mathfrak{S}_2}^2 \right). \end{aligned}$$

On the other hand, there exists $C \in \mathbb{R}_+$ such that (see [CDL08a, Proposition 1]) for all $Q \in \mathcal{Q}_{\gamma_{\text{per}}^0}$,

$$\|\rho_Q\|_{L^2 \cap \mathcal{C}} \leq C \|Q\|_{\mathcal{Q}_{\gamma_{\text{per}}^0}}.$$

In view of (4.35) and the above inequality, there exists $C \in \mathbb{R}_+$ such that

$$\forall \mathbf{R} \in \mathcal{H}, \quad \|\rho_{\mathbf{R}}\|_{L^2 \cap \mathcal{C}} \leq C \left(W(\mathbf{R})^{1/2} + W(\mathbf{R}) + \|\mathbf{R}\|_{\ell^2} + \|\mathbf{R}\|_{\ell^2}^2 \right),$$

which leads to (4.20).

4.5.3 Proof of Lemma 4.3

To establish the estimates in Lemma 4.3, we first introduce the maximum number of overlapping nuclei in the configuration \mathbf{R} , *i.e.*

$$C_{\#}(\mathbf{R}) := \sup_{k \in \mathcal{R}} \#\left\{ j \in \mathcal{R} \setminus \{k\} \mid |(k + R_k) - (j + R_j)| < 2\eta \right\}, \quad (4.36)$$

where we recall that $\eta > 0$ is the common radius of the smeared nuclei.

Lemma 4.5. *The following estimate holds:*

$$\forall \mathbf{R} \in \ell^2(\mathcal{R}), \quad C_{\#}(\mathbf{R}) \leq 2 \left(\frac{d_m}{2} - 2\eta \right)^{-2} \|\mathbf{R}\|_{\ell^2}^2, \quad (4.37)$$

where recall that $d_m \gg \eta$ is the minimal distance of the center of two nuclei in the \mathcal{R} -periodic lattice.

The proof of this lemma can be read in Section 4.5.4. Remark that one can obtain a bound of $C_{\#}(\mathbf{R})$ by $\|\mathbf{R}\|_{\ell^2}^{6/5}$ instead of $\|\mathbf{R}\|_{\ell^2}^2$ in (4.37), but the proof of the former is more complicated, while the exponent is not significant in this study.

To prove (4.22), we first rewrite $F_k(\mathbf{R})$ using (4.12) as

$$\begin{aligned} F_k(\mathbf{R}) &= \int_{\mathbb{R}^3} m(\cdot - k - R_k) (\nabla V_{\text{per}}^0 + \nabla V_{\mathbf{R}}) \\ &= \int_{\mathbb{R}^3} (m(\cdot - k - R_k) - m(\cdot - k)) \nabla V_{\text{per}}^0 + \int_{\mathbb{R}^3} m(\cdot - k - R_k) \nabla V_{\mathbf{R}}. \end{aligned}$$

From (4.28) we obtain that

$$\|m(\cdot - k - R_k) - m(\cdot - k)\|_{L^2(\mathbb{R}^3)} \leq \|\nabla m\|_{L^2(\mathbb{R}^3)} |R_k|,$$

from which, together with (4.19) and (4.37) we deduce

$$\begin{aligned}
\|\mathbf{F}(\mathbf{R})\|_{\ell^2}^2 &\leq 2 \sum_{k \in \mathcal{R}} \left| \int_{\mathbb{R}^3} (m(\cdot - k - R_k) - m(\cdot - k)) \nabla V_{\text{per}}^0 \right|^2 + 2 \sum_{k \in \mathcal{R}} \left| \int_{\mathbb{R}^3} m(\cdot - k - R_k) \nabla V_{\mathbf{R}} \right|^2 \\
&\leq 4 \|\nabla V_{\text{per}}^0\|_{L_{\text{unif}}^2}^2 \sum_{k \in \mathcal{R}} \|m(\cdot - k - R_k) - m(\cdot - k)\|_{L^2}^2 + 2 \|m\|_{L^2}^2 \sum_{k \in \mathcal{R}} \int_{k+R_k+B_\eta} |\nabla V_{\mathbf{R}}|^2 \\
&\leq 4 \|\nabla V_{\text{per}}^0\|_{L_{\text{unif}}^2}^2 \|\nabla m\|_{L^2}^2 \|\mathbf{R}\|_{\ell^2}^2 + 2 \|m\|_{L^2}^2 C_{\#}(\mathbf{R}) \|\nabla V_{\mathbf{R}}\|_{L^2}^2 \\
&\leq C \|\mathbf{R}\|_{\ell^2}^2 + C \|\mathbf{R}\|_{\ell^2}^2 (\|\mathbf{R}\|_{\mathcal{H}}^2 + C \|\mathbf{R}\|_{\ell^2}^4) \\
&\leq C \|\mathbf{R}\|_{\ell^2}^2 (1 + \|\mathbf{R}\|_{\mathcal{H}}^2 + \|\mathbf{R}\|_{\ell^2}^4),
\end{aligned}$$

which leads to (4.22).

4.5.4 Proof of Lemma 4.5

First of all, note that if $\|\mathbf{R}\|_{\ell^2} \leq d_m/2 - \eta$, there are no overlapping nuclei since $\|\mathbf{R}\|_{\ell^\infty} \leq \|\mathbf{R}\|_{\ell^2}$, hence $C_{\#}(\mathbf{R}) \equiv 0$. We next consider the case when $\|\mathbf{R}\|_{\ell^2} > d_m/2 - \eta$. We denote by $k^* \in \mathcal{R}$ the lattice site at which the maximum in the definition (4.36) is attained, by $D_j := k^* + R_{k^*} - j$ and by \mathcal{D}_{k^*} the set of elements j such that

$$|D_j - R_j| < 2\eta. \quad (4.38)$$

By definition, $C_{\#}(\mathbf{R})$ is the cardinality of the set \mathcal{D}_{k^*} .

Assume that $C_{\#}(\mathbf{R}) \geq 2$, otherwise the result is trivial. Denote by $a \in \mathcal{D}_{k^*}$ and $b \in \mathcal{D}_{k^*}$ the minimum and the second minimum of $|D_j|$, that is

$$|D_a| = \min_{j \in \mathcal{D}_{k^*}} |D_j|, \quad |D_b| = \min_{j \in \mathcal{D}_{k^*} \setminus \{a\}} |D_j|.$$

For simplicity, we further assume that the minimum is attained only by a , and $|D_b| > |D_a|$. We shall remove this assumption at the end of the proof. Let us show that $|D_b| > d_m/2$: when $|D_a| \geq d_m/2$ this trivially holds. If $|D_a| < d_m/2$, noting that $D_b = D_a + a - b$, the triangle inequality for Euclidean space leads to

$$|D_b| + |D_a| \geq |a - b| \geq d_m,$$

which implies that $|D_b| > d_m/2$. Therefore in view of (4.38), it holds

$$\forall j \in \mathcal{D}_{k^*} \setminus \{a\}, \quad 0 < \frac{d_m}{2} - 2\eta < |D_j| - 2\eta \leq |R_j|.$$

This implies that

$$(C_{\#}(\mathbf{R}) - 1) \left(\frac{d_m}{2} - 2\eta \right)^2 < \sum_{j \in \mathcal{D}_{k^*} \setminus \{a\}} |R_j|^2 \leq \|\mathbf{R}\|_{\ell^2}^2.$$

As we have assumed that $\|\mathbf{R}\|_{\ell^2} > d_m/2 - \eta > d_m/2 - 2\eta$, the above inequality implies that

$$C_{\#}(\mathbf{R}) < \left(\frac{d_m}{2} - 2\eta \right)^{-2} \left(\|\mathbf{R}\|_{\ell^2}^2 + \left(\frac{d_m}{2} - 2\eta \right)^2 \right) \leq 2 \left(\frac{d_m}{2} - 2\eta \right)^{-2} \|\mathbf{R}\|_{\ell^2}^2. \quad (4.39)$$

When there are two or more points that minimize $\min_{j \in \mathcal{D}_{k^*}} |D_j|$ (that is, $|D_a| = |D_b|$), we obtain by a reasoning similar to the one above, that

$$\min_{j \in \mathcal{D}_{k^*}} |D_j| \geq \frac{d_m}{2},$$

and so

$$C_{\#}(\mathbf{R}) \leq \left(\frac{d_m}{2} - 2\eta \right)^{-2} \left(\sum_{j \in \mathcal{D}_{k^*}} |R_j|^2 \right) \leq \left(\frac{d_m}{2} - 2\eta \right)^{-2} \|\mathbf{R}\|_{\ell^2}^2. \quad (4.40)$$

The inequality (4.37) then follows from (4.39) and (4.40).

4.5.5 Proof of Proposition 4.4

First of all, let us show that $\mathbf{N}(\cdot)$ is a map from $\mathcal{H} \times \ell^2(\mathcal{R})$ to $\ell^2(\mathcal{R}) \times \ell^2(\mathcal{R})$. By (4.22), it holds,

$$\begin{aligned} \|\mathbf{N}(\mathbf{Y})\|_{\ell^2(\mathcal{R}) \times \ell^2(\mathcal{R})} &\leq \left(\frac{1}{\min_{k \in \mathcal{R}} m_k^2} \|\mathbf{P}\|_{\ell^2(\mathcal{R})}^2 + \|\mathbf{F}(\mathbf{R})\|_{\ell^2(\mathcal{R})}^2 \right)^{1/2} \\ &\leq \left(\frac{1}{\min_{k \in \mathcal{R}} m_k^2} \|\mathbf{P}\|_{\ell^2(\mathcal{R})}^2 + (C \|\mathbf{R}\|_{\mathcal{H}} (1 + \|\mathbf{R}\|_{\ell^2} + \|\mathbf{R}\|_{\mathcal{H}}^2))^2 \right)^{1/2}. \end{aligned}$$

There exists therefore a constant $C_{\mathbf{N},b} \in \mathbb{R}_+$ such that, for any $\mathbf{Y} \in \mathcal{H} \times \ell^2(\mathcal{R})$,

$$\|\mathbf{N}(\mathbf{Y})\|_{\ell^2(\mathcal{R}) \times \ell^2(\mathcal{R})} \leq C_{\mathbf{N},b} \left(\|\mathbf{Y}\|_{\mathcal{H} \times \ell^2(\mathcal{R})} + \|\mathbf{Y}\|_{\mathcal{H} \times \ell^2(\mathcal{R})}^3 \right). \quad (4.41)$$

The local well-posedness of the Hamiltonian dynamics relies on the local Lipschitz continuity of $\mathbf{N}(\cdot)$, which is a direct consequence of the local Lipschitz continuity of the force term $\mathbf{F}(\cdot)$. Simple calculations show that the latter property follows from the following lemma.

Lemma 4.6. *There exist $\alpha > 0$ and $C_\alpha \in \mathbb{R}_+$ depending only on α such that, for any \mathbf{R} and $\tilde{\mathbf{R}}$ belonging to \mathcal{H} with $\|\mathbf{R}\|_{\mathcal{H}}, \|\tilde{\mathbf{R}}\|_{\mathcal{H}} \leq \alpha$, it holds*

$$\|\rho_{\mathbf{R}} - \rho_{\tilde{\mathbf{R}}}\|_{\mathcal{C}} \leq C_\alpha \|\nu_{\mathbf{R}} - \nu_{\tilde{\mathbf{R}}}\|_{\mathcal{C}}. \quad (4.42)$$

The proof of this result can be read in Section 4.5.6. The following lemma can then be obtained (see Section 4.5.7 for the proof).

Lemma 4.7 (local Lipschitz continuity of the force \mathbf{F}). *There exists a constant $\tilde{C}_\alpha \in \mathbb{R}_+$ (depending on the constant α given in Lemma 4.6), such that for all $\mathbf{R}, \tilde{\mathbf{R}} \in \mathcal{H}$ with $\|\mathbf{R}\|_{\mathcal{H}}, \|\tilde{\mathbf{R}}\|_{\mathcal{H}} \leq \alpha$,*

$$\|\mathbf{F}(\mathbf{R}) - \mathbf{F}(\tilde{\mathbf{R}})\|_{\ell^2(\mathcal{R})} \leq \tilde{C}_\alpha \|\mathbf{R} - \tilde{\mathbf{R}}\|_{\mathcal{H}}. \quad (4.43)$$

The local Lipschitz regularity of \mathbf{N} is a direct consequence of Lemma 4.7:

$$\begin{aligned} \|\mathbf{N}(\mathbf{Y}) - \mathbf{N}(\tilde{\mathbf{Y}})\|_{\ell^2(\mathcal{R}) \times \ell^2(\mathcal{R})} &\leq \left(\frac{1}{\min_{k \in \mathcal{R}} m_k^2} \|\mathbf{P} - \tilde{\mathbf{P}}\|_{\ell^2(\mathcal{R})}^2 + \|\mathbf{F}(\mathbf{R}) - \mathbf{F}(\tilde{\mathbf{R}})\|_{\ell^2(\mathcal{R})}^2 \right)^{1/2} \\ &\leq \left(\frac{1}{\min_{k \in \mathcal{R}} m_k^2} \|\mathbf{P} - \tilde{\mathbf{P}}\|_{\ell^2(\mathcal{R})}^2 + \tilde{C}_\alpha^2 \|\mathbf{R} - \tilde{\mathbf{R}}\|_{\mathcal{H}}^2 \right)^{1/2} \\ &\leq C_{\mathbf{N}}(\alpha) \|\mathbf{Y} - \tilde{\mathbf{Y}}\|_{\mathcal{H} \times \ell^2(\mathcal{R})}, \end{aligned}$$

where

$$C_{\mathbf{N}}(\alpha) = \max \left(\frac{1}{\min_{k \in \mathcal{R}} m_k^2}, \tilde{C}_\alpha^2 \right)^{1/2}.$$

By the Cauchy–Lipschitz theorem the Hamiltonian dynamics (4.24) is locally well-posed for any initial condition $\mathbf{Y}(0)$ such that $\|\mathbf{Y}(0)\|_{\mathcal{H} \times \ell^2(\mathcal{R})} < \alpha$.

4.5.6 Proof of Lemma 4.6

We prove the result by a linear response expansion of the rHF minimizer based on results obtained in [CL10]. In view of (4.33) and [CL10, Lemma 2], there exists $\beta > 0$ such that if $\|\mathbf{V}_{\mathbf{R}}\|_{\mathcal{C}'} \leq \beta$, then

$$\epsilon_F \notin \sigma(H_{\text{per}}^0 + V_{\mathbf{R}}), \quad Q_{\mathbf{R}} := \mathbf{1}_{(-\infty, \epsilon_F]}(H_{\text{per}}^0 + V_{\mathbf{R}}) - \mathbf{1}_{(-\infty, \epsilon_F]}(H_{\text{per}}^0) \in \mathcal{Q}_{\gamma_{\text{per}}^0}. \quad (4.44)$$

Using again (4.33), we next observe that

$$\|V_{\mathbf{R}}\|_{\mathcal{C}'} \leq \|\nu_{\mathbf{R}}\|_{\mathcal{C}} \leq \sqrt{2} (\|\mathbf{R}\|_{\mathcal{H}}^2 + C\|\mathbf{R}\|_{\ell^2}^4)^{1/2} \leq \sqrt{2} (\alpha^2 + C\alpha^4)^{1/2} := \beta(\alpha).$$

Therefore there exists $\alpha > 0$ such that (4.44) holds. Consider the following expansion:

$$Q_{\mathbf{R}} = Q_{1,V_{\mathbf{R}}} + Q_{2,V_{\mathbf{R}}} + Q_{3,V_{\mathbf{R}}}, \quad (4.45)$$

where, by denoting \mathfrak{C} a smooth curve in the complex plan enclosing the spectrum of H_{per}^0 below ϵ_F ,

$$Q_{1,V_{\mathbf{R}}} := \frac{1}{2i\pi} \oint_{\mathfrak{C}} (z - H_{\text{per}}^0)^{-1} V_{\mathbf{R}} (z - H_{\text{per}}^0)^{-1} dz,$$

$$Q_{2,V_{\mathbf{R}}} := \frac{1}{2i\pi} \oint_{\mathfrak{C}} (z - H_{\text{per}}^0)^{-1} \left(V_{\mathbf{R}} (z - H_{\text{per}}^0)^{-1} \right)^2 dz,$$

and

$$Q_{3,V_{\mathbf{R}}} := \frac{1}{2i\pi} \oint_{\mathfrak{C}} (z - H_{\text{per}}^0 - V_{\mathbf{R}})^{-1} \left(V_{\mathbf{R}} (z - H_{\text{per}}^0)^{-1} \right)^3 dz.$$

Recall that v_c denotes the Coulomb operator ($v_c(\rho) := \rho \star |\cdot|^{-1}$), which is an isometry from \mathcal{C} to \mathcal{C}' [CL10]. Note also that the rHF mean-field potential generated by the defect $V_{\mathbf{R}} = v_c(\rho_{\mathbf{R}} - \nu_{\mathbf{R}})$ belongs to \mathcal{C}' by the results of Lemma 4.2. The linear response operator on \mathcal{C} is defined as [CL10, Equation (21)]

$$\forall \varrho \in \mathcal{C}, \quad \mathcal{L}(\varrho) := -\rho_{Q_{1,v_c(\varrho)}}.$$

Hence, in view of (4.45),

$$\rho_{\mathbf{R}} = -\mathcal{L}(\rho_{\mathbf{R}} - \nu_{\mathbf{R}}) + \rho_{Q_{2,V_{\mathbf{R}}}} + \rho_{Q_{3,V_{\mathbf{R}}}}.$$

The operator \mathcal{L} is a bounded nonnegative self-adjoint operator on \mathcal{C} and $1 + \mathcal{L}$ is invertible and bicontinuous on \mathcal{C} [CL10, Proposition 2]. The above equality can be recast as

$$\rho_{\mathbf{R}} = \frac{\mathcal{L}}{1 + \mathcal{L}} \nu_{\mathbf{R}} + \frac{1}{1 + \mathcal{L}} \rho_{Q_{2,V_{\mathbf{R}}}} + \frac{1}{1 + \mathcal{L}} \rho_{Q_{3,V_{\mathbf{R}}}}. \quad (4.46)$$

Therefore,

$$\rho_{\mathbf{R}} - \rho_{\tilde{\mathbf{R}}} = \frac{\mathcal{L}}{1 + \mathcal{L}} (\nu_{\mathbf{R}} - \nu_{\tilde{\mathbf{R}}}) + \frac{1}{1 + \mathcal{L}} (\rho_{Q_{2,V_{\mathbf{R}}}} - \rho_{Q_{2,V_{\tilde{\mathbf{R}}}}}) + \frac{1}{1 + \mathcal{L}} (\rho_{Q_{3,V_{\mathbf{R}}}} - \rho_{Q_{3,V_{\tilde{\mathbf{R}}}}}). \quad (4.47)$$

On the other hand, for all $k \geq 1$, the k -linear map

$$\begin{aligned} \mathcal{Q}_k : (\mathcal{C}')^k &\mapsto \mathcal{Q}_{\gamma_{\text{per}}^0} \\ (V_1, V_2, \dots, V_k) &\mapsto \frac{1}{2i\pi} \oint_{\mathfrak{C}} (z - H_{\text{per}}^0)^{-1} V_1 (z - H_{\text{per}}^0)^{-1} V_2 (z - H_{\text{per}}^0)^{-1} \dots V_k (z - H_{\text{per}}^0)^{-1} dz, \end{aligned} \quad (4.48)$$

is continuous [CL10, Lemma 3]. In particular, there exists a constant $C_k \in \mathbb{R}_+$ such that

$$\forall (V_1, \dots, V_k) \in (\mathcal{C}')^k, \quad \|\mathcal{Q}_k(V_1, V_2, \dots, V_k)\|_{\mathcal{Q}_{\gamma_{\text{per}}^0}} \leq C_k \|V_1\|_{\mathcal{C}'} \|V_2\|_{\mathcal{C}'} \dots \|V_k\|_{\mathcal{C}'}. \quad (4.49)$$

Therefore, as

$$\begin{aligned} Q_{2,V_{\mathbf{R}}} - Q_{2,V_{\tilde{\mathbf{R}}}} &= \frac{1}{2i\pi} \oint_{\mathfrak{C}} (z - H_{\text{per}}^0)^{-1} (V_{\mathbf{R}} - V_{\tilde{\mathbf{R}}}) (z - H_{\text{per}}^0)^{-1} V_{\mathbf{R}} (z - H_{\text{per}}^0)^{-1} dz \\ &\quad + \frac{1}{2i\pi} \oint_{\mathfrak{C}} (z - H_{\text{per}}^0)^{-1} V_{\tilde{\mathbf{R}}} (z - H_{\text{per}}^0)^{-1} (V_{\mathbf{R}} - V_{\tilde{\mathbf{R}}}) (z - H_{\text{per}}^0)^{-1} dz, \end{aligned}$$

the bound (4.49) and [CDL08a, Proposition 1] lead to

$$\left\| \rho_{Q_2, V_{\mathbf{R}}} - \rho_{Q_2, V_{\tilde{\mathbf{R}}}} \right\|_{\mathcal{C}} \leq C \left\| Q_2, V_{\mathbf{R}} - Q_2, V_{\tilde{\mathbf{R}}} \right\|_{\mathcal{Q}_{\gamma_{\text{per}}^0}} \leq C (\|V_{\mathbf{R}}\|_{\mathcal{C}'} + \|V_{\tilde{\mathbf{R}}}\|_{\mathcal{C}'}) \|V_{\mathbf{R}} - V_{\tilde{\mathbf{R}}}\|_{\mathcal{C}'} \quad (4.50)$$

Similarly,

$$\begin{aligned} Q_{3, V_{\mathbf{R}}} - Q_{3, V_{\tilde{\mathbf{R}}}} &= \frac{1}{2i\pi} \oint_{\mathcal{C}} (z - H_{\mathbf{R}})^{-1} (V_{\mathbf{R}} - V_{\tilde{\mathbf{R}}}) (z - H_{\tilde{\mathbf{R}}})^{-1} \left(V_{\tilde{\mathbf{R}}} (z - H_{\text{per}}^0)^{-1} \right)^3 dz \\ &\quad + \frac{1}{2i\pi} \oint_{\mathcal{C}} (z - H_{\mathbf{R}})^{-1} (V_{\mathbf{R}} - V_{\tilde{\mathbf{R}}}) (z - H_{\text{per}}^0)^{-1} \left(V_{\tilde{\mathbf{R}}} (z - H_{\text{per}}^0)^{-1} \right)^2 dz \\ &\quad + \frac{1}{2i\pi} \oint_{\mathcal{C}} (z - H_{\mathbf{R}})^{-1} V_{\mathbf{R}} (z - H_{\text{per}}^0)^{-1} (V_{\mathbf{R}} - V_{\tilde{\mathbf{R}}}) (z - H_{\text{per}}^0)^{-1} V_{\tilde{\mathbf{R}}} (z - H_{\text{per}}^0)^{-1} dz \\ &\quad + \frac{1}{2i\pi} \oint_{\mathcal{C}} \left((z - H_{\mathbf{R}})^{-1} V_{\mathbf{R}} \right)^2 (z - H_{\text{per}}^0)^{-1} (V_{\mathbf{R}} - V_{\tilde{\mathbf{R}}}) (z - H_{\text{per}}^0)^{-1} dz. \end{aligned}$$

A bound similar to (4.50) holds in view of (4.48):

$$\begin{aligned} \left\| \rho_{Q_3, V_{\mathbf{R}}} - \rho_{Q_3, V_{\tilde{\mathbf{R}}}} \right\|_{\mathcal{C}} &\leq C \left\| Q_3, V_{\mathbf{R}} - Q_3, V_{\tilde{\mathbf{R}}} \right\|_{\mathcal{Q}_{\gamma_{\text{per}}^0}} \\ &\leq C (\|V_{\mathbf{R}}\|_{\mathcal{C}'}^2 + \|V_{\tilde{\mathbf{R}}}\|_{\mathcal{C}'}^2 + \|V_{\tilde{\mathbf{R}}}\|_{\mathcal{C}'}^3) \|V_{\mathbf{R}} - V_{\tilde{\mathbf{R}}}\|_{\mathcal{C}'}. \end{aligned} \quad (4.51)$$

Gathering (4.33), (4.47), (4.50) and (4.51), and relying on the boundedness of \mathcal{L} and $(1 + \mathcal{L})^{-1}$ on \mathcal{C} , there exist constants $C_1, C_2 \in \mathbb{R}_+$ such that for all $\|\mathbf{R}\|_{\mathcal{H}}, \|\tilde{\mathbf{R}}\|_{\mathcal{H}} \leq \alpha$,

$$\begin{aligned} \|\rho_{\mathbf{R}} - \rho_{\tilde{\mathbf{R}}}\|_{\mathcal{C}} &\leq C_1 \|\nu_{\mathbf{R}} - \nu_{\tilde{\mathbf{R}}}\|_{\mathcal{C}} \\ &\quad + C (\|V_{\mathbf{R}}\|_{\mathcal{C}'} + \|V_{\tilde{\mathbf{R}}}\|_{\mathcal{C}'} + \|V_{\mathbf{R}}\|_{\mathcal{C}'}^2 + \|V_{\tilde{\mathbf{R}}}\|_{\mathcal{C}'}^3) \|V_{\mathbf{R}} - V_{\tilde{\mathbf{R}}}\|_{\mathcal{C}'} \\ &\leq C_1 \|\nu_{\mathbf{R}} - \nu_{\tilde{\mathbf{R}}}\|_{\mathcal{C}} \\ &\quad + C (\|\nu_{\mathbf{R}}\|_{\mathcal{C}} + \|\nu_{\tilde{\mathbf{R}}}\|_{\mathcal{C}} + \|\nu_{\mathbf{R}}\|_{\mathcal{C}}^2 + \|\nu_{\tilde{\mathbf{R}}}\|_{\mathcal{C}}^3) \|\nabla V_{\mathbf{R}} - \nabla V_{\tilde{\mathbf{R}}}\|_{L^2} \\ &\leq C_1 \|\nu_{\mathbf{R}} - \nu_{\tilde{\mathbf{R}}}\|_{\mathcal{C}} + C_2 (\beta(\alpha) + \beta^3(\alpha)) \|\rho_{\mathbf{R}} - \nu_{\mathbf{R}} - \rho_{\tilde{\mathbf{R}}} + \nu_{\tilde{\mathbf{R}}}\|_{\mathcal{C}} \\ &\leq C_1 \|\nu_{\mathbf{R}} - \nu_{\tilde{\mathbf{R}}}\|_{\mathcal{C}} + C_2 (\beta(\alpha) + \beta^3(\alpha)) (\|\rho_{\mathbf{R}} - \rho_{\tilde{\mathbf{R}}}\|_{\mathcal{C}} + \|\nu_{\mathbf{R}} - \nu_{\tilde{\mathbf{R}}}\|_{\mathcal{C}}). \end{aligned}$$

It is easy to see that for $\alpha > 0$ sufficiently small so that $0 < C_2 (\beta(\alpha) + \beta^3(\alpha)) < 1$, it holds

$$\|\rho_{\mathbf{R}} - \rho_{\tilde{\mathbf{R}}}\|_{\mathcal{C}} \leq C_{\alpha} \|\nu_{\mathbf{R}} - \nu_{\tilde{\mathbf{R}}}\|_{\mathcal{C}}, \quad (4.52)$$

with

$$0 \leq C_{\alpha} := \frac{C_1 + C_2 (\beta(\alpha) + \beta^3(\alpha))}{1 - C_2 (\beta(\alpha) + \beta^3(\alpha))} < +\infty.$$

This allows to conclude that (4.42) holds.

4.5.7 Proof of Lemma 4.7

Consider $\mathbf{R}, \tilde{\mathbf{R}} \in \mathcal{H}$ with $\|\mathbf{R}\|_{\mathcal{H}}, \|\tilde{\mathbf{R}}\|_{\mathcal{H}} \leq \alpha$. By calculations similar to the ones in the proof of Lemma 4.3,

$$\begin{aligned}
\|\mathbf{F}(\mathbf{R}) - \mathbf{F}(\tilde{\mathbf{R}})\|_{\ell^2}^2 &\leq 2 \sum_{k \in \mathcal{R}} \left| \int_{\mathbb{R}^3} (\nabla V_{\text{per}}^0 + \nabla V_{\mathbf{R}}) \left(m(\cdot - k - R_k) - m(\cdot - k - \tilde{R}_k) \right) \right|^2 \\
&\quad + 2 \sum_{k \in \mathcal{R}} \left| \int_{\mathbb{R}^3} (\nabla V_{\mathbf{R}} - \nabla V_{\tilde{\mathbf{R}}}) m(\cdot - k - \tilde{R}_k) \right|^2 \\
&\leq \left(4 \|\nabla V_{\text{per}}^0\|_{L_{\text{unif}}^2}^2 + 2 \|\nabla V_{\mathbf{R}}\|_{L^2}^2 \right) \sum_{k \in \mathcal{R}} \|m(\cdot - k - R_k) - m(\cdot - k - \tilde{R}_k)\|_{L^2}^2 \\
&\quad + 2 \|m\|_{L^2}^2 \sum_{k \in \mathcal{R}} \int_{k + \tilde{R}_k + B_\eta} |\nabla V_{\mathbf{R}} - \nabla V_{\tilde{\mathbf{R}}}|^2 \\
&\leq 4 \|m\|_{L^2}^2 \left(\|\nabla V_{\text{per}}^0\|_{L_{\text{unif}}^2}^2 + \|\nabla V_{\mathbf{R}}\|_{L^2}^2 \right) \|\mathbf{R} - \tilde{\mathbf{R}}\|_{\ell^2}^2 + 2 \|m\|_{L^2}^2 C_{\#}(\tilde{\mathbf{R}}) \|\nabla V_{\mathbf{R}} - \nabla V_{\tilde{\mathbf{R}}}\|_{L^2}^2.
\end{aligned} \tag{4.53}$$

In view of (4.42), the last term of the above equation can be estimated as

$$\begin{aligned}
\|\nabla V_{\mathbf{R}} - \nabla V_{\tilde{\mathbf{R}}}\|_{L^2}^2 &\leq \|\rho_{\mathbf{R}} - \rho_{\tilde{\mathbf{R}}} - \nu_{\mathbf{R}} + \nu_{\tilde{\mathbf{R}}}\|_{\mathcal{C}}^2 \leq 2(1 + C_{\alpha}^2) \|\nu_{\mathbf{R}} - \nu_{\tilde{\mathbf{R}}}\|_{\mathcal{C}}^2 \\
&\leq 4(1 + C_{\alpha}^2) \left(\|\nu_{\mathbf{R}} - \nu_{1, \mathbf{R}} - \nu_{\tilde{\mathbf{R}}} + \nu_{1, \tilde{\mathbf{R}}}\|_{\mathcal{C}}^2 + \|\mathbf{R} - \tilde{\mathbf{R}}\|_{\mathcal{H}}^2 \right).
\end{aligned} \tag{4.54}$$

On the other hand,

$$\begin{aligned}
&\nu_{\mathbf{R}} - \nu_{1, \mathbf{R}} - \nu_{\tilde{\mathbf{R}}} + \nu_{1, \tilde{\mathbf{R}}} \\
&= \sum_{k \in \mathbf{R}} z_k \left(m(\cdot - k - R_k) - m(\cdot - k - \tilde{R}_k) + \nabla m(\cdot - k) \cdot (R_k - \tilde{R}_k) \right) \\
&= \sum_{k \in \mathbf{R}} z_k \int_0^1 \left(-\nabla m(\cdot - k - R_k + t(R_k - \tilde{R}_k)) + \nabla m(\cdot - k) \right) \cdot (R_k - \tilde{R}_k) dt \\
&= - \sum_{k \in \mathbf{R}} z_k \int_0^1 \int_0^1 \left(-R_k + t(R_k - \tilde{R}_k) \right)^T \text{Hess}(m) \left(\cdot - k + s \left(-R_k + t(R_k - \tilde{R}_k) \right) \right) (R_k - \tilde{R}_k) ds dt.
\end{aligned}$$

Therefore by similar arguments leading to (4.29) as well as the Cauchy-Schwarz inequality, it holds

$$\begin{aligned}
\|\nu_{\mathbf{R}} - \nu_{1, \mathbf{R}} - \nu_{\tilde{\mathbf{R}}} + \nu_{1, \tilde{\mathbf{R}}}\|_{L^1(\mathbb{R}^3)} &\leq \|\text{Hess}(m)\|_{L^1(\mathbb{R}^3)} \sum_{k \in \mathbf{R}} z_k \int_0^1 \left| -R_k + t(R_k - \tilde{R}_k) \right| |R_k - \tilde{R}_k| dt \\
&\leq \|\text{Hess}(m)\|_{L^1(\mathbb{R}^3)} \sum_{k \in \mathbf{R}} z_k |R_k| |R_k - \tilde{R}_k| + \frac{1}{2} \|\text{Hess}(m)\|_{L^1(\mathbb{R}^3)} \sum_{k \in \mathbf{R}} z_k |R_k - \tilde{R}_k|^2 \\
&\leq \left(\max_{k \in \mathcal{R}} z_k \right) \|\text{Hess}(m)\|_{L^1(\mathbb{R}^3)} \left(\|\mathbf{R}\|_{\ell^2} \|\mathbf{R} - \tilde{\mathbf{R}}\|_{\ell^2} + \frac{1}{2} \|\mathbf{R} - \tilde{\mathbf{R}}\|_{\ell^2}^2 \right).
\end{aligned}$$

Similarly,

$$\|\nu_{\mathbf{R}} - \nu_{1, \mathbf{R}} - \nu_{\tilde{\mathbf{R}}} + \nu_{1, \tilde{\mathbf{R}}}\|_{L^{\infty}(\mathbb{R}^3)} \leq \left(\max_{k \in \mathcal{R}} z_k \right) \|\text{Hess}(m)\|_{L^{\infty}(\mathbb{R}^3)} \left(\|\mathbf{R}\|_{\ell^2} \|\mathbf{R} - \tilde{\mathbf{R}}\|_{\ell^2} + \frac{1}{2} \|\mathbf{R} - \tilde{\mathbf{R}}\|_{\ell^2}^2 \right).$$

By interpolation and remarking that $L^{6/5}(\mathbb{R}^3) \hookrightarrow \mathcal{C}$, there exists therefore a constant $C \in \mathbb{R}_+$ such that

$$\|\nu_{\mathbf{R}} - \nu_{1, \mathbf{R}} - \nu_{\tilde{\mathbf{R}}} + \nu_{1, \tilde{\mathbf{R}}}\|_{\mathcal{C}} \leq C \left(\|\mathbf{R}\|_{\ell^2} + \frac{1}{2} \|\mathbf{R} - \tilde{\mathbf{R}}\|_{\ell^2} \right) \|\mathbf{R} - \tilde{\mathbf{R}}\|_{\ell^2}. \tag{4.55}$$

In view of (4.19), (4.37), (4.54), and (4.55), there exists a positive constant \tilde{C}_α depending only on α such that the estimate (4.53) leads to

$$\begin{aligned} \|\mathbf{F}(\mathbf{R}) - \mathbf{F}(\tilde{\mathbf{R}})\|_{\ell^2}^2 &\leq 4\|m\|_{H^1}^2 \left(\|\nabla V_{\text{per}}^0\|_{L_{\text{unif}}^2}^2 + 2(\|\mathbf{R}\|_{\mathcal{H}}^2 + C\|\mathbf{R}\|_{\ell^2}^4) \right) \|\mathbf{R} - \tilde{\mathbf{R}}\|_{\ell^2}^2 \\ &\quad + 4C\|m\|_{L^2}^2 \|\tilde{\mathbf{R}}\|_{\ell^2}^2 (1 + C_\alpha) \left(C \left(\|\mathbf{R}\|_{\ell^2} + \frac{1}{2} \|\mathbf{R} - \tilde{\mathbf{R}}\|_{\ell^2} \right)^2 \|\mathbf{R} - \tilde{\mathbf{R}}\|_{\ell^2}^2 + \|\mathbf{R} - \tilde{\mathbf{R}}\|_{\mathcal{H}}^2 \right) \\ &\leq \tilde{C}_\alpha^2 \|\mathbf{R} - \tilde{\mathbf{R}}\|_{\mathcal{H}}^2. \end{aligned}$$

This finally allows to conclude that (4.43) holds.

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