Mean–field stability for the junction of semi-infinite systems

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Abstract

Junction appears naturally when one studies the surface states or transport properties of quasi 1D materials such as carbon nanotubes, polymers and quantum wires. These materials can be seen as 1D systems embedded in the 3D space. Moreover, topological edge states of 2D materials are recently the center topics in condensed matter physics. These 2D materials possess periodicity in one direction, can therefore be modeled as the junction of quasi 1D semi-infinite system with the vacuum when studying the edge states. In this article we first establish a mean–field description (of reduced Hartree–Fock type) for the 1D periodic system in the 3D space and prove the ground state energy is always non-positive under some symmetry condition. The junction system is described by two different semi-infinite 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 the junction system, and the uniqueness of ground state electronic density. We finally give a brief discussion of extension to the junctions of 2D materials at the end of the article.

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1 Introduction

Atomic junctions appear when studying the surface states of one-dimensional (1D) crystal [1, 51], quantum thermal transport in nanostructures [55], and the p-n junctions [3, 47] which are the foundation of the modern semiconductor electronic devices. Furthermore, electronic transport in carbon nanotubes [39] and in molecular wires [46], which recently attracts wide interests, 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 give rise to attentions on 2D materials, see [27] and references therein. These 2D materials often possess periodicity in one dimension, can therefore be reduced to quasi 1D semi-infinite materials (junction with the vacuum) by momentum representation in the periodic direction when studying edge states properties (see [28, 2] and references therein).

Real world materials are often described by periodic systems [13, 11] or ergodically periodic [12] in mathematical modeling. In this paper we consider a junction of two different periodic quasi 1D systems without any assumption on the commensurability of periods, hence the junction system does not possess any translation-invariant symmetry. Generally speaking, there are two regimes for the junction of two different semi-infinite periodic systems: when the chemical potentials of the underlying periodic systems are separated by some occupied bands (non-equilibrium regime, see Fig. 3), and when the chemical potential are in a common spectral gap (equilibrium regime, see Fig. 4). The non-equilibrium regime models a persistent (non-perturbative) current in the junction system [6, 7, 8, 16], 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.

In this article we only consider the equilibrium regime while giving a quick comment on the non-equilibrium regime in Section 3.2, as the non-equilibrium regime requires different techniques. We establish a mean-field model to describe the junction of two different semi-infinite quasi 1D periodic systems (see Fig. 2) in the 3D space with Coulomb interactions, under the framework of the reduced Hartree–Fock [52] description. We prove that the ground state of the junction system exists. This approach is extended to junction of 2D materials in Section 4. Let us mention another approach [5] when defining the ground state energy of non-periodic system of particles.

This non-linear model can be employed to describe the junction of two nanotubes, or a more realistic model of the junction of two 1D crystals for electronic structure calculations, and 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 [40, 9] formalism for the electronic (thermal) transport which is based on the lead-devise-lead description, can be seen as the junction of two different semi-infinite systems (leads) with different chemical (thermal) potentials, and the devise as a perturbation of this junction. Remark also that p-n junction of the carbon nanotubes without external battery [42, 41] correspond to the equilibrium regime, and thus can be described by the model. Furthermore, our model can also be easily adapted to describe 1D dislocation problems in the 3D space under the rHF description, while the linear 1D dislocation problems have been studied in [36, 37] and some generalizations have been provided for higher dimensional systems [18, 30, 31].

Let us emphasize that we do not assume any commensurability of periods for the two semi-infinite systems, therefore the junction system does not possess any translation-invariant symmetry. From mathematical point of view, the usual Bloch decomposition of periodic system [48, 13, 11] is not applicable for the junction system. The main idea is to establish a well-suited reference system based on the linear combination of periodical systems, and
use perturbative techniques which has been widely used for the mean-field type model [26, 23, 25, 11, 20] to justify the construction. Let us also mention the work of Thomas–Fermi type model [4] for polymers, which is also modeled as a 1D periodic system in the 3D space.

The paper is organized as follows. In Section 2 we construct the rHF model for a 1D periodic system in the 3D space, which is a building block for the junction system. Remark that this is different from [13, 11] as the system is periodic only in the $x$-direction, hence the unit cell is unbounded. In Section 2.1 we introduce mathematical preliminaries for the construction. In Section 2.2, we define a periodic rHF energy functional and show that the ground state exists and the ground state electronic density is unique. We also prove that under certain symmetry assumptions on the nuclear density, the ground state energy is always non-positive. In Section 3.1 we give a rigorous mathematical description of the junction system, and define a reference system which is a linear combination of underlying periodic systems in Section 3.2. We show that the essential spectrum of the reference Hamiltonian is the union of those of underlying periodic systems, and the electronic density associated with the reference system is close to the linear combination of the underlying periodical electronic densities, and the difference of which decays exponentially fast. This justifies the choice of reference system. In Section 3.3 we define the difference of the junction system and the reference system as a perturbative system, and associate it with a minimization problem. In Section 3.4 we show that the perturbative system admits a ground state and has unique ground state electronic density, following the idea developed in [11]. Furthermore, we prove that the ground state electronic density of the junction system is unique and is independent of the choice of the reference state, showing the validity of our approach. In Section 4 we briefly discuss the extension to 2D materials.

## 2 Mean–field stability for the quasi 1D system: a reduced Hartree–Fock approach

In this section, we give a mathematical description of a 1D periodic system in the 3D space in the framework of the reduced Hartree-Fock (rHF) approach, and prove the existence of the ground state (stability of the system). The 1D periodic system is described by atoms arranged periodically alongside the $x$-axis (see for example Fig. 1) with electrons occupying the 3D space. Once again this is different from classical results in [13, 11] as the unit cell of the 1D periodic system is a unbounded domain. In Section 2.1, we introduce some mathematical preliminaries such as the partial Bloch decomposition, a 3D Green’s function which is periodic only in the $x$-direction, a mixed Fourier transform and the kinetic as well as Coulomb energy space. In Section 2.2 we construct a periodic rHF energy functional for the 1D system in the 3D space and prove the mean–field stability.

Let us first introduce some notation. Unless otherwise specified, the functions on $\mathbb{R}^d$ considered in this article are complex-valued. Elements of $\mathbb{R}^3$ are denoted by $x = (x, r)$, where $x \in \mathbb{R}$ and $r = (y, z) \in \mathbb{R}^2$. For a given separable Hilbert space $\mathcal{H}$, we denote by $\mathcal{L}(\mathcal{H})$ the space of bounded (linear) operators acting on $\mathcal{H}$, by $\mathcal{S}(\mathcal{H})$ the space of bounded self-adjoint operators acting on $\mathcal{H}$, and by $\mathcal{S}_p(\mathcal{H})$ the Schatten class of operators acting on $\mathcal{H}$ for $1 \leq p < \infty$: a compact operator $A$ belongs to $\mathcal{S}_p(\mathcal{H})$ if and only if $\|A\|_{\mathcal{S}_p} := (\text{Tr}(\|A\|^p))^{1/p} < \infty$. Operators in $\mathcal{S}_1(\mathcal{H})$ and $\mathcal{S}_2(\mathcal{H})$ are respectively called trace-class and Hilbert–Schmidt. If $A \in \mathcal{S}_1(\mathcal{L}^2(\mathbb{R}^d))$, there exists a unique function $\rho_A \in \mathcal{L}^1(\mathbb{R}^d)$ such that

$$\forall \phi \in \mathcal{L}^\infty(\mathbb{R}^d), \quad \text{Tr}(A\phi) = \int_{\mathbb{R}^d} \rho_A\phi.$$

The function $\rho_A$ is called the density of the operator $A$. If the integral kernel $A(r, r')$ of $A$ is continuous on $\mathbb{R}^d \times \mathbb{R}^d$, then $\rho_A(r) = A(r, r)$ for all $r \in \mathbb{R}^d$. This relation still stands in some weaker sense for a generic trace-class operator.

An operator $A \in \mathcal{L}(\mathcal{L}^2(\mathbb{R}^d))$ is called locally trace-class if the operator $\rho A\phi$ is trace-class for any $\phi \in C_0^\infty(\mathbb{R}^d)$. The density of a locally trace-class operator $A \in \mathcal{L}(\mathcal{L}^2(\mathbb{R}^d))$ is the unique function $\rho_A \in \mathcal{L}^1_{\text{loc}}(\mathbb{R}^d)$ such that

$$\forall \phi \in C_0^\infty(\mathbb{R}^d), \quad \text{Tr}(A\phi) = \int_{\mathbb{R}^d} \rho_A\phi.$$
Let $\mathcal{S}(\mathbb{R}^d)$ be the Schwartz space of rapidly decreasing functions on $\mathbb{R}^d$, and $\mathcal{S}'(\mathbb{R}^d)$ the space of tempered distributions on $\mathbb{R}^d$. We denote by $\hat{\phi}$ (resp. $\check{\phi}$) the Fourier transform (resp. inverse Fourier transform) on $\mathcal{S}'(\mathbb{R}^d)$, with the following normalization:

$$\forall \phi \in L^1(\mathbb{R}^d), \quad \hat{\phi}(\zeta) := \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} \phi(x) e^{-i\zeta x} \, dx, \quad \check{\phi}(x) := \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} \phi(\zeta) e^{i\zeta x} \, d\zeta.$$

The normalization ensures that the Fourier transform defines a unitary operator on $L^2(\mathbb{R}^d)$.

### 2.1 Preliminary settings

We first introduce a decomposition of the operator which is $\mathbb{Z}$-translation invariant in the $x$-direction based on 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 the density matrices and Coulomb interactions for the 1D system in the 3D space.

**Bloch transform in the $x$-direction.** For $k \in \mathbb{Z}$, we denote by $\tau_k^x$ the translation operator in the $x$-direction acting on $L^2_{\text{loc}}(\mathbb{R}^3)$

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

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

$$L^p_{\text{per}, x}(\Gamma) := \left\{ u \in L^p_{\text{loc}}(\mathbb{R}^3) \mid \|u\|_{L^p(\Gamma)} < +\infty, \tau_k^x u = u, \forall k \in \mathbb{Z} \right\},$$

$$H^1_{\text{per}, x}(\Gamma) := \left\{ u \in L^2_{\text{per}, x}(\Gamma) \mid \nabla u \in L^2_{\text{per}, x}(\Gamma) \right\}.$$

Let us also introduce the following constant fiber direct integral of Hilbert spaces [48]:

$$L^2(\Gamma^*; L^2_{\text{per}, x}(\Gamma)) := \bigoplus_{\xi \in \Gamma^*} L^2_{\text{per}, x}(\Gamma) \frac{d\xi}{2\pi},$$

in which the base $\Gamma^* := [-\pi, \pi] \times \{0\} = [-\pi, \pi).$ We introduce the partial Bloch transform $\mathcal{B}$, which is a unitary operator from $L^2(\mathbb{R}^3)$ to $L^2(\Gamma^*; L^2_{\text{per}, x}(\Gamma))$, defined on the dense subspace of $C_c^\infty(\mathbb{R}^3)$ of $L^2(\mathbb{R}^3)$:

$$\forall (x, r) \in \Gamma, \xi \in \Gamma^*, \quad (\mathcal{B} \phi)(\xi, x, r) := \sum_{k \in \mathbb{Z}} e^{-i(x+k)\xi} \phi(x+k, r).$$

Its inverse is given by

$$\forall k \in \mathbb{Z}, \quad \text{for a.a. } (x, r) \in \Gamma, \quad \left( \mathcal{B}^{-1} f \right)(x+k, r) := \int_{\Gamma^*} e^{i(k+x)\xi} f(\xi, x, r) \frac{d\xi}{2\pi}.$$

The partial Bloch transform has the property that any operator $A$ on $L^2(\mathbb{R}^3)$ which commutes with $\tau_k^x$ 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 $A \in \mathcal{L}(\Gamma^*; \mathcal{L}(L^2_{\text{per}, x}(\Gamma)))$ such that for all $u \in L^2(\mathbb{R}^3)$,

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

Hence we use the following notation for the decomposition of an operator $A$ which is $\mathbb{Z}$-translation invariant in the $x$-direction

$$A = \mathcal{B}^{-1} \left( \int_{\Gamma^*} A_\xi \frac{d\xi}{2\pi} \right) \mathcal{B}.$$
In addition, \( \|A\|_{L^2(\mathbb{R}^3)} = \|A_\xi\|_{L^2(\mathbb{R}^3)} \|\xi\|_{L^p(\Gamma^*)}. \) In particular, if \( A \) is positive and locally trace-class, then for almost all \( \xi \in \Gamma^* \), \( A_\xi \) is locally trace-class. The densities of these operators are related by the formula

\[
\rho_A(x) = \frac{1}{2\pi} \int_{\Gamma^*} \rho_{A_\xi}(x) \, d\xi.
\]

If \( A \) is a (not necessarily bounded) self-adjoint operator such that \( \tau_k^\xi (A + i)^{-1} = (A + i)^{-1} \tau_k^\xi \) for all \( k \in \mathbb{Z} \), then \( A \) is decomposed by \( \mathcal{U} \) (see [48, Theorem XIII.84 and XIII.85]). In particular, denoting by \( \Delta \) the Laplace operator acting on \( L^2(\mathbb{R}^3) \), the kinetic energy operator \([11, 13]\) \(-\frac{1}{2} \Delta \) on \( L^2(\mathbb{R}^3) \) is decomposed by \( \mathcal{B} \) as follows:

\[
-\frac{1}{2} \Delta = \mathcal{B}^{-1} \left( \int_{\Gamma^*} -\frac{1}{2} \Delta \xi \frac{d\xi}{2\pi} \right) \mathcal{B}, \quad -\Delta \xi = (-i\nabla \xi)^2 = (i\partial_x - \xi)^2 - \Delta_x,
\]

where \( \Delta_x \) 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 \( r \)-direction. Denote by \( \mathcal{S}_{\text{per},x}(\Gamma) \) the space of functions that are \( C^\infty \) on \( \mathbb{R}^3 \) and \( \Gamma \)-periodic, decaying faster than any power of \( |r| \) when \( |r| \) 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:

\[
\forall \phi \in \mathcal{S}_{\text{per},x}(\Gamma), \forall (n, k) \in \mathbb{Z} \times \mathbb{R}^2, \quad \mathcal{F}\phi(n, k) := \frac{1}{2\pi} \int_{\Gamma} \phi(x, r) e^{-i(2\pi nx + kr)} \, dx \, dr.
\]

Its inverse is given by

\[
\mathcal{F}^{-1} \psi(x, r) := \frac{1}{2\pi} \sum_{n \in \mathbb{Z}} \int_{\mathbb{R}^2} \psi(n, k) e^{i(2\pi nx + kr)} \, dk.
\]

Note that \( \mathcal{F} \) can be extended from \( \mathcal{S}'_{\text{per},x}(\Gamma) \) to \( \mathcal{S}'(\mathbb{R}^3) \). It is also easy to verify 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:

\[
\forall f, g \in L^2_{\text{per},x}(\Gamma), \quad \int_{\Gamma} \mathcal{F}(f)(x, r) g(x, r) \, dx \, dr = \sum_{n \in \mathbb{Z}} \left( \mathcal{F} f(n, k) \mathcal{F} g(n, k) \right) \, dk.
\]

Moreover, it is easy to verify that for \( f, g \in L^2_{\text{per},x}(\Gamma) \),

\[
\mathcal{F} (f \star_{\Gamma} g) = 2\pi (\mathcal{F} f) (\mathcal{F} g),
\]

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 [49] for the operator \(-i\nabla_\xi = (-i\partial_x + \xi, -i\partial_r)\) for all \( \xi \in \Gamma^* \), which will be repeatedly used in the proofs.

**Lemma 2.1.** Fix \( \xi \in \Gamma^* \). Let \( 2 \leq p \leq +\infty \) and \( f, g \in L^p_{\text{per},x}(\Gamma) \). Then

\[
\|f(-i\nabla_\xi)g\|_{\mathcal{E}_p(L^p_{\text{per},x}(\Gamma))} \leq (2\pi)^{-2/p} \|g\|_{L^p_{\text{per},x}(\Gamma)} \left( \sum_{n \in \mathbb{Z}} \| f((2\pi n + \xi, \cdot)) \|_{L^p(\mathbb{R}^2)} \right)^{1/p},
\]

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 5.1.
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 \([4, 45]\):

**Definition 2.2** (Periodic Green’s function). For \( (x, r) \in \mathbb{R}^3 \), the periodic Green’s function is defined as

\[
G(x, r) = -2 \log(|r|) + \tilde{G}(x, r), \quad \tilde{G}(x, r) := 4 \sum_{n \geq 1} K_0(2\pi n |r|) \cos(2\pi nx),
\]

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 (2.7).

**Lemma 2.3.**

1. The Green’s function \( G(x, r) \) defined in (2.7) satisfies the following Poisson’s equation:

\[
-\Delta G(x, r) = 4\pi \sum_{n \in \mathbb{Z}} \delta_{(x, r) = (n, 0)} \in \mathcal{S}'(\mathbb{R}^3),
\]

where \( \delta_n \in \mathcal{S}'(\mathbb{R}^d) \) is the Dirac distribution at point \( a \in \mathbb{R}^d \). Moreover \( G \in \mathcal{S}'_{\text{per}, x}(\Gamma) \) and

\[
\mathcal{F}(G)(n, k) = \frac{2}{4\pi^2 n^2 + |k|^2} \in \mathcal{S}'(\mathbb{R}^3).
\]

2. The function \( \tilde{G} \) defined in (2.7) belongs to \( L^p_{\text{per}, x}(\Gamma) \) for \( 1 \leq p < 2 \) and satisfies \( \int \tilde{G} = 0 \). Moreover, there exist positive constants \( d_1 \) and \( d_2 \) such that when \( |r| \to +\infty \), \(|\tilde{G}(|\cdot| r)| \leq d_1 \frac{e^{-2|x|}}{\sqrt{|r|}} \), and when \( |r| \to 0 \), \(|\tilde{G}(|\cdot| r)| \leq \frac{d_2}{|r|} \)

uniformly with respect to \( x \). Furthermore, the function \( \tilde{G}(x, r) \) can also be written as

\[
\tilde{G}(x, r) = \sum_{n \in \mathbb{Z}} \left( \frac{1}{\sqrt{(x-n)^2 + |r|^2}} - \int_{-1/2}^{1/2} \frac{1}{\sqrt{(x-y-n)^2 + |r|^2}} dy \right).
\]

The proof of this lemma can be read in Section 5.2.

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. \([11, 20, 10]\)). Recall that for a finite system with \( N \) electrons, a density matrix is a trace-class self-adjoint operator \( \gamma \in \mathcal{S}(L^2(\mathbb{R}^3)) \cap \mathcal{G}_1(L^2(\mathbb{R}^3)) \) 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 \( \gamma \) is given by \( \text{Tr}(-\frac{1}{2} \Delta \gamma) = \frac{1}{2} \text{Tr}(\langle \nabla |\gamma| \nabla \rangle) \) (see \([13, 11]\)).

Consider a 1D periodic system in the 3D space, where atoms are arranged periodically in the \( x \)-direction with unit cell \( \Gamma \) and first Brillouin zone \( \Gamma^* \). The nuclear density of this 1D periodic crystal is \( \mathbb{Z} \)-translation invariant in the \( x \)-direction. Since the rHF model is strictly convex in the density \([52]\), we do not expect any spontaneous symmetry breaking. Therefore the electronic state of this 1D system will be described by a one-body density matrix which commutes with the translations \( \{ \tau_k \}_{k \in \mathbb{Z}} \), hence is decomposed by the partial Bloch transform \( \mathcal{B} \). In view of the decomposition (2.2), we define the following admissible set of the one-body density matrices, which guarantees that the number of electrons per unit cell and the kinetic energy per unit cell are finite:

\[
P_{\text{per}, x} := \left\{ \gamma \in \mathcal{S}(L^2(\mathbb{R}^3)) \left| 0 \leq \gamma \leq 1, \forall k \in \mathbb{Z}, \tau_k^x \gamma = \gamma \tau_k^x, \int_{\Gamma^*} \text{Tr}_{L^2_{\text{per}, x}} \left( \sqrt{1 - \Delta_k \gamma} \sqrt{1 - \Delta_k} \right) d\xi < \infty \right\},
\]

where

\[
\gamma = \mathcal{B}^{-1} \left( \int_{\Gamma^*} \gamma \frac{d\xi}{2\pi} \right) \mathcal{B},
\]
For any $\gamma \in P_{\text{per}, x}$, it is easy to see that $\rho_\gamma \in L^1_{\text{per}, x}(\Gamma)$. Moreover, it can also be deduced from [13, Equation (4.42)] a Hoffmann-Ostenhof [35] type inequality:
\[
\int_\Gamma |\nabla \sqrt{\rho_\gamma}|^2 \leq \int_{\Gamma^*} \text{Tr}_{L^2_{\text{per}, x}} (-\Delta \gamma, \xi) \frac{d\xi}{2\pi}.
\] (2.12)
Therefore $\sqrt{\rho_\gamma}$ is in $H^1_{\text{per}, x}(\Gamma)$ hence in $L^6_{\text{per}, x}(\Gamma)$ by Sobolev embeddings, hence $\rho_\gamma \in L^p_{\text{per}, x}(\Gamma)$ 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:
\[
D(f, g) := \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{f(x)g(x')}{|x-x'|} \, dx \, dx' = 4\pi \int_{\mathbb{R}^3} \frac{\mathcal{F}(f)(k)\mathcal{F}(g)(k)}{|k|^2} \, dk.
\]
In order to describe Coulomb interactions in the reciprocal space for the 1D periodic system in the 3D space, we gather the results obtained in (2.4), (2.5) and (2.8), and define the Coulomb interaction energy per unit cell for charge densities $f, g$ belonging to $\mathcal{S}_{\text{per}, x}(\Gamma)$ as:
\[
D_\Gamma(f, g) := 4\pi \sum_{n \in \mathbb{Z}} \int_{\mathbb{R}^2} \frac{\mathcal{S}(f)(n, k)\mathcal{S}(g)(n, k)}{|k|^2 + 4\pi^2n^2} \, dk.
\] (2.13)
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
\[
\mathcal{C}_\Gamma := \left\{ f \in \mathcal{S}'_{\text{per}, x}(\Gamma) \, | \, \forall n \in \mathbb{Z}, \mathcal{S}(f)(n, \cdot) \in L^1_{\text{loc}}(\mathbb{R}^2), D_\Gamma(f, f) < +\infty \right\},
\] (2.14)
which is a Hilbert space endowed with the inner product $D_\Gamma(\cdot, \cdot)$.

Remark 2.4. Remark that the charge densities in $\mathcal{C}_\Gamma$ are neutral in some weak sense. For $f \in \mathcal{C}_\Gamma \cap L^1_{\text{per}, x}(\Gamma)$, the condition $\int_{\mathbb{R}^2} \left| \mathcal{S}(f)(0,k) \right|^2 \frac{dk}{|k|^2} < +\infty$ implies that $\mathcal{S}(f)(0,0) = \int_{\Gamma} f(x, r) \, dx \, dr = 0$.

2.2 Reduced Hartree-Fock description for a 1D periodic system in the 3D space

Based on the kinetic energy space and Coulomb interactions defined in the previous section, in this section we construct a rHF energy functional for the 1D system in the 3D space which is 1-periodic only in the $x$-direction. We show that the ground state of the quasi 1D system is given by the solution of some minimization problem. Denoting by $Z > 0$ the total charge of the nuclei in each unit cell, we model the nuclear density of the quasi 1D system by a smooth function which is 1-periodic in the $x$-direction:
\[
\mu_{\text{per}}(x, r) = \sum_{n \in \mathbb{Z}} Z \, m(x - n, r),
\]
where $m(x, r)$ is a non-negative $C^C(\Gamma)$ function such that $\int_{\mathbb{R}^3} m = 1$. Hence $\int_{\Gamma} \mu_{\text{per}} = Z$. For any trial density matrix $\gamma$ which commutes with the translation $\tau^x$ in the $x$-direction, we define the periodic rHF energy functional for the quasi 1D system associated with the nuclear density $\mu_{\text{per}}$ as:
\[
\mathcal{E}_{\text{per}, x}(\gamma, \mu_{\text{per}}) := \frac{1}{2\pi} \int_{\Gamma^*} \text{Tr}_{L^2_{\text{per}, x}(\Gamma)} \left( -\frac{1}{2} \Delta_x \gamma \xi \right) \, d\xi + \frac{1}{2} D_\Gamma \left( \rho_\gamma - \mu_{\text{per}}, \rho_\gamma - \mu_{\text{per}} \right).
\] (2.15)
Let us introduce the following set of admissible density matrices for the rHF energy functional, which guarantees that the kinetic energy and Coulomb interaction energy per-unit cell are finite:
\[
\mathcal{F}_\Gamma := \{ \gamma \in P_{\text{per}, x} \mid \rho_\gamma - \mu_{\text{per}} \in \mathcal{C}_\Gamma \}.\]
where $P_{\text{per},x}$ is the kinetic energy space defined in (2.10) and $C_\Gamma$ is the Coulomb space defined in (2.14). Let us also introduce a class of nuclear densities with an extra symmetry condition in the $r$-direction:

$$
\mu_{\text{per},\text{sym}}(x, r) = \sum_{n \in \mathbb{Z}} Z m_{\text{sym}}(x - n, r),
$$

where $m_{\text{sym}}(x, r)$ is a non-negative $C^\infty_\Gamma$ function such that $\int_{\mathbb{R}^3} m_{\text{sym}} = 1$ and

$$
\int_{\Gamma} r m_{\text{sym}}(x, r) \, dx \, dr = 0.
$$

(2.16)

See Fig. 1 for an example of the nuclear density $\mu_{\text{per},\text{sym}}$. In the following we shall see that the condition (2.16) is sufficient to obtain a mean-field potential which tends to 0 in the $r$-direction. In the real world many materials satisfy the condition (2.16): nanotubes, polymers with rotational symmetry in the $r$-direction. As a matter of fact, if the $x$-averaged nuclear density $\int_{-1/2}^{1/2} m_{\text{sym}}(x, r) \, dx$ is invariant under the action of an element of the 2D orthogonal group, then the condition (2.16) is always satisfied.

We also introduce the following admissible set associated with the nuclear density $\mu_{\text{per},\text{sym}}$:

$$
\mathcal{F}_{\Gamma, \text{sym}} := \{ \gamma \in P_{\text{per},x} | \rho_{\gamma} - \mu_{\text{per},\text{sym}} \in C_\Gamma \} \subset \mathcal{F}_{\Gamma}.
$$

**Lemma 2.5.** The set $\mathcal{F}_{\Gamma}$ and $\mathcal{F}_{\Gamma, \text{sym}}$ are not empty. For any $\gamma \in \mathcal{F}_{\Gamma}$,

$$
\int_{\Gamma} \rho_{\gamma} = \int_{\Gamma} \mu_{\text{per}}.
$$

(2.17)

The proof can be read in Section 5.3. The periodic rHF ground state energy (per unit cell) of the quasi 1D crystal can then be written as minimization problems depending on admissible sets:

$$
I_{\text{per}} = \inf \{ \mathcal{E}_{\text{per},x}(\gamma, \mu_{\text{per}}); \gamma \in \mathcal{F}_{\Gamma} \},
$$

(2.18)

$$
I_{\text{per},\text{sym}} = \inf \{ \mathcal{E}_{\text{per},x}(\gamma, \mu_{\text{per},\text{sym}}); \gamma \in \mathcal{F}_{\Gamma, \text{sym}} \}.
$$

(2.19)

The minimization problem similar to (2.18) under the Thomas-Fermi type models has been studied in [4], where they have proved the uniqueness of the minimizers, and justified the model by a thermodynamic limit argument. For a 3D periodic crystal, the minimization problem (2.18) has been examined in [13], where authors have proved the existence of minimizers and the uniqueness of the density of the minimizers. The characterization of the minimizers is given in [11, Theorem 1]: it has been shown that the minimizer is unique and is a spectral projector satisfying a self-consistent equation. The following theorem provides similar results for the quasi 1D system: we show that the minimizer of (2.18) (resp. of (2.19)) exists, and the density of the minimizers are unique. Furthermore, for the minimization problem (2.19) which has some symmetry assumption on the nuclear density, we prove that the ground state energy of the quasi 1D system is always non-positive. This coincides with the physical reality: additional symmetry condition on the nuclear density is sufficient to guarantee that the mean-field potential tends to 0 in the $r$-direction. Therefore the electrons can escape to infinity in the $r$-direction if the ground state energy is positive, decreasing the energy of the system. Hence the ground state energy of the 1D system should be non-positive. Furthermore, we are able to characterize the unique minimizer as a spectral projector of the mean-field Hamiltonian.
Theorem 2.6 (Existence of rHF ground state with smeared nuclear). The minimization problem (2.18) admits a minimizer with density belonging to $L^p_{\text{per}, x}(\Gamma)$ for $1 \leq p \leq 3$. Besides, all the minimizers share the same density.

Theorem 2.7 (Existence of rHF ground state with smeared nuclear with symmetry). The minimization problem (2.19) admits a minimizer $\gamma_{\text{per}}$ with density $\rho_{\gamma_{\text{per}}} \in L^p_{\text{per}, x}(\Gamma)$ for $1 \leq p \leq 3$. Besides, all the minimizers share the same density. Moreover, we have

1. (Spectral properties of the mean-field Hamiltonian.) The mean-field potential

$$V_{\text{per, sym}} = (\rho_{\gamma_{\text{per}}} - \mu_{\text{per, sym}}) \ast_G$$

belongs to $H^2_{\text{per}, x}(\Gamma)$, hence in $L^p_{\text{per}, x}(\Gamma)$ for $2 \leq p \leq +\infty$. Moreover, $V_{\text{per, sym}}$ is continuous and tends to zero in the $r$-direction. The mean-field Hamiltonian

$$H_{\text{per}} = \mathcal{B}^{-1} \left( \int_{\Gamma^*} H_{\text{per}, \xi} \frac{d\xi}{2\pi} \right) \mathcal{B} = \frac{1}{2} \Delta + V_{\text{per, sym}}, \quad H_{\text{per}, \xi} := -\frac{1}{2} \Delta_\xi + V_{\text{per, sym}} \quad (2.20)$$

is a self-adjoint operator acting on $L^2(\mathbb{R}^3)$ with domain $H^2(\mathbb{R}^3)$ and form domain $H^1(\mathbb{R}^3)$. Denote by $\sigma(A) = \sigma_{\text{disc}}(A) \cup \sigma_{\text{ess}}(A)$ the spectrum of $A$, where $\sigma_{\text{disc}}(A)$ (resp. $\sigma_{\text{ess}}(A)$) denotes the discrete (resp. essential) spectrum of $A$. For all $\xi \in \Gamma^*$, there exists $N_H \in \mathbb{N}^*$ which can be finite or infinite, and a sequence $\{\lambda_n(\xi)\}_{1 \leq n \leq N_H}$ 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:

$$\sigma(H_{\text{per}}) = \sigma_{\text{ess}}(H_{\text{per}}) = \bigcup_{\xi \in \Gamma^*} \sigma(H_{\text{per}, \xi}). \quad (2.21)$$

In particular, $[0, +\infty) \subset \sigma_{\text{ess}}(H_{\text{per}})$.

2. (Ground state energy is always non-positive.) The energy level counting function

$$\kappa \leq 0, \quad F(\kappa) : \kappa \mapsto \frac{1}{|\Gamma^*|} \int_{\Gamma^*} \text{Tr}_{L^2_{\text{per}, x}(\Gamma)} \left( 1_{(-\infty, \kappa]}(H_{\text{per}, \xi}) \right) d\xi = \frac{1}{|\Gamma^*|} \sum_{n=1}^{N_H} \int_{\Gamma^*} 1_{(\lambda_n(\xi) \leq \kappa)} d\xi$$

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

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

which means that there are always enough negative energy levels for the electrons, hence the ground state energy of the 1D system in the 3D space is always non-positive.

3. (Unique minimizer is a spectral projector.) There exists $\epsilon_F \leq 0$ called Fermi level such that $F(\epsilon_F) = Z$, which can be interpreted as the Lagrange multiplier associated with the charge neutrality condition (2.17). The minimizer of the problem (2.19) is unique and satisfies the following self-consistent equation:

$$\gamma_{\text{per}} = 1_{(-\infty, \epsilon_F]}(H_{\text{per}}) = \mathcal{B}^{-1} \left( \int_{\Gamma^*} \gamma_{\text{per}, \xi} \frac{d\xi}{2\pi} \right) \mathcal{B}, \quad \gamma_{\text{per}, \xi} := 1_{(-\infty, \epsilon_F]}(H_{\text{per}, \xi}). \quad (2.22)$$

4. (Integrability of the mean-field potential) There exist positive constants $C_{\epsilon_F}$ and $\alpha_{\epsilon_F}$ which depend on the Fermi level $\epsilon_F$ such that

$$0 \leq \rho_{\gamma_{\text{per}}}(x, r) \leq C_{\epsilon_F} e^{-\alpha_{\epsilon_F} |r|}. \quad (2.23)$$

Furthermore, the mean-field potential $V_{\text{per, sym}}$ belongs to $L^p_{\text{per}, x}(\Gamma)$ for $1 < p \leq +\infty$. 


The proof of Theorem 2.6 and Theorem 2.7 can be read in Section 5.4.

Remark 2.8. The unit cell of the 1D system in the 3D space is an unbounded domain \( \Gamma \), hence 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 \([13, 11]\).

Remark 2.9. The condition (2.16) is probably a sufficient but not necessary condition for the non-positivity of the ground state energy and the characterization of the minimizers. The main difficult is to control the decay of the mean-field potential \( V_{\text{per, sym}} \) in the \( r \)-direction by just controlling the nuclear density \( \mu_{\text{per, sym}} \), given that the Green’s function defined in (2.7) has log-growth in the \( r \)-direction. Furthermore, different decay scenarios of \( V_{\text{per, sym}} \) in the \( r \)-direction lead to different characterizations of the spectrum of the Hamiltonian \( H_{\text{per}} \): if \( V_{\text{per, sym}} \) is bounded from below, and is positive while has log-growth when \( |r| \to \infty \), one can show that the spectrum of \( H_{\text{per,} \xi} \) is purely discrete and the spectrum of \( H_{\text{per}} \) may have a band structure and the ground state energy of the system can be positive; while if we have \( \int_{\Gamma} |r| \rho_{\text{per, sym}}(x, r) \, dx \, dr < +\infty \), then \( V_{\text{per, sym}} \) tends to 0 when \( |r| \to \infty \), one can have similar results as in Theorem 2.7. However, none of these above statements can be trivially obtained.

### 3 Mean-field stability for the junction of two semi-infinite quasi 1D systems

In this section, we construct a rHF model for the junction of two different semi-infinite 1D periodic systems in the 3D space. The junction system is described by periodic nuclei satisfying the symmetry condition (2.16) 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\)). 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 the perturbative approach when treating infinitely extended systems \([24, 23, 26, 25, 11]\), the idea is to find an appropriate reference state which is close enough to the actual one. Section 3.1 gives a mathematical description of the junction system. Section 3.2 is devoted to a rigorous construction of a reference density matrix, which is a spectral projector of the linear combination of Hamiltonians of periodic systems. We show in particular that the electronic density associated with this reference state is close to the linear combination of periodical densities. In Section 3.3 we construct the perturbative state, which encodes the non-linear effects due to electron-electron interactions in the rHF approximation, and associated the ground state energy of this perturbative state to some minimization problem in Section 3.4, which proves the mean-field stability of the junction system. In particular, we show that the electronic density of the junction system is the sum of the reference state density and the perturbative density, and is independent of the choice of the reference state. This justifies the construction.

#### 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 \( \Gamma_L := \left[ -\frac{a_L}{2}, \frac{a_L}{2} \right] \times \mathbb{R}^2 \) and \( \Gamma_R := \left[ -\frac{a_R}{2}, \frac{a_R}{2} \right] \times \mathbb{R}^2 \) with their duals \( \Gamma^*_L := \left[ -\frac{\pi}{a_L}, \frac{\pi}{a_L} \right] \) and \( \Gamma^*_R := \left[ -\frac{\pi}{a_R}, \frac{\pi}{a_R} \right] \). We consider nuclear densities with symmetry condition (2.16): let \( m_L(x, r) \) and \( m_R(x, r) \) be non-negative \( C^\infty_c \) functions with supports respectively in \( \Gamma_L \) and \( \Gamma_R \) such that \( \int_{\mathbb{R}^3} m_L = 1 \) and \( \int_{\mathbb{R}^3} m_R = 1 \). Moreover,

\[
\int_{\Gamma_L} rm_L(x, r) \, dx \, dr = 0, \quad \int_{\Gamma_R} rm_R(x, r) \, dx \, dr = 0.
\]

Denote 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

\[
\mu_{\text{per,} L}(x, r) := \sum_{n_L \in Z_L} Z_L m_L(x - n_L, r), \quad \mu_{\text{per,} R}(x, r) := \sum_{n_R \in Z_R} Z_R m_R(x - n_R, r).
\]

(3.1)
The periodic Green’s functions with period \( \Gamma_L \) and \( \Gamma_R \) are separately
\[
G_{a_L}(x, r) = a_L^{-1} G \left( \frac{x}{a_L}, r \right), \quad G_{a_R}(x, r) = a_R^{-1} G \left( \frac{x}{a_R}, r \right),
\]
where \( G(\cdot) \) is the periodic Green’s function defined in (2.7). According to the results of Theorem 2.7, the following self-consistent equations uniquely define the ground states density matrices associated with the periodic nuclear densities \( \rho_{\text{per},L} \) and \( \rho_{\text{per},R} \):
\[
\gamma_{\text{per},L} := \mathbf{1}_{(-\infty,0]}(H_{\text{per},L}), \quad H_{\text{per},L} := -\frac{\Delta}{2} + V_{\text{per},L}, \quad V_{\text{per},L} := (\rho_{\text{per},L} - \mu_{\text{per},L}) \ast \gamma_{\text{per},L},
\]
\[
\gamma_{\text{per},R} := \mathbf{1}_{(-\infty,0]}(H_{\text{per},R}), \quad H_{\text{per},R} := -\frac{\Delta}{2} + V_{\text{per},R}, \quad V_{\text{per},R} := (\rho_{\text{per},R} - \mu_{\text{per},R}) \ast \gamma_{\text{per},R},
\]
where the non-positive constants \( \epsilon_L \) and \( \epsilon_R \) are the chemical potentials of the quasi 1D systems. The junction of the quasi 1D systems is described by considering the following nuclear density configuration (see Fig.2)
\[
\mu_j(x, r) := \mathbf{1}_{x \leq 0} \cdot \mu_{\text{per},L}(x, r) + \mathbf{1}_{x > 0} \cdot \mu_{\text{per},R}(x, r) + v(x, r), \quad (3.2)
\]
where \( v(x, r) \in L^p(\mathbb{R}^3) \) for \( 1 < p \leq +\infty \), which describes the local perturbation induced by the junction. Once one

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

sets the nuclear configuration (3.2), electrons are allowed to move in the 3D space. The infinite rHF energy functional for the junction system associated with a test density matrix \( \gamma_j \) formally reads
\[
\mathcal{E}(\gamma_j) = \text{Tr} \left( -\frac{1}{2} \Delta \gamma_j \right) + \frac{1}{2} D(\rho_{\gamma_j} - \mu_j, \rho_{\gamma_j} - \mu_j), \quad (3.3)
\]
where
\[
D(f, g) := \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{f(x)g(y)}{|x - y|} \, dx \, dy = \frac{1}{4\pi} \int_{\mathbb{R}^3} \frac{\hat{f}(k)\hat{g}(k)}{k^2} \, dk
\]
describing the whole space Coulomb interactions. Let us also introduce the Coulomb space \( \mathcal{C} \) and its dual \( \mathcal{C}' \) (Beppo-Levi space [11]):
\[
\mathcal{C} := \left\{ \rho \in \mathcal{S}'(\mathbb{R}^3) \mid D(\rho, \rho) < \infty \right\}, \quad \mathcal{C}' := \left\{ V \in L^6(\mathbb{R}^3) \mid \nabla V \in \left( L^2(\mathbb{R}^3) \right)^3 \right\}. \quad (3.4)
\]
Remark that the ground state energy of the junction system is infinite and there is no periodicity in this lattice, hence usual techniques which essentially consist in considering the energy per unit volume [13, 11] are not applicable. The idea is to find 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 [26, 23, 25, 11] in different contexts. The next section is devoted to the rigorous mathematical construction of the reference state and its rHF energy functional.

### 3.2 Reference state for the junction system

In this section, we construct a reference state as the spectral projector of a reference Hamiltonian with 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 periodical 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 $x \in \mathbb{R}^3$, introduce:

$$
\mathcal{X} := \{ \chi \in C^2(\mathbb{R}^3) \mid 0 \leq \chi \leq 1; \chi(x) = 1 \text{ if } x \in \left(-\infty, -\frac{a_L}{2}\right] \times \mathbb{R}^2; \chi(x) = 0 \text{ if } x \in \left[\frac{a_R}{2}, +\infty\right) \times \mathbb{R}^2 \}. \quad (3.5)
$$

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 3.4 that the choice of $\chi \in \mathcal{X}$ is irrelevant. By Theorem 2.7 and the definition of $\chi$ we know that $V_\chi$ belonging to $L^p_{\text{loc}}(\mathbb{R}, L^p(\mathbb{R}^3))$ for $1 < p \leq \infty$ is continuous in all directions and tends to zero in the $r$-direction. Since the periodical potentials $V_{\text{per},L}$ and $V_{\text{per},R}$ satisfy the Poisson’s equations with periodic boundary conditions in the $x$-direction, this implies that $V_\chi$ satisfies the following Poisson’s equation

$$
-\Delta V_\chi = 4\pi \left(\chi^2(\rho_{\text{per},L} - \mu_{\text{per},L}) + (1 - \chi^2)(\rho_{\text{per},R} - \mu_{\text{per},R}) + \eta_\chi\right),
$$

where $\eta_\chi$ defined as follows has compact support in the $x$-direction:

$$
\eta_\chi := -\frac{1}{4\pi} \left(\partial_x^2(\chi^2) (V_{\text{per},L} - V_{\text{per},R}) + 2\partial_x(\chi^2)\partial_x (V_{\text{per},L} - V_{\text{per},R})\right). \quad (3.7)
$$

In order to guarantee that the perturbative state has finite Coulomb interactions, we need $\eta_\chi$ to lie in the Coulomb space $C$. A sufficient condition is that $\eta_\chi$ belongs to $L^{6/5}(\mathbb{R}^3)$. This motivates the following $L^p$-estimate on $\eta_\chi$.

**Lemma 3.1.** The function $\eta_\chi$ defined in (3.7) belongs to $L^p(\mathbb{R}^3)$ for $1 < p < 6$.

The proof can be read in Section 5.6. By the Kato–Rellich theorem (see for example [29, Theorem 9.10]), there exists a unique self-adjoint operator

$$
H_\chi := -\frac{1}{2}\Delta + V_\chi
$$

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 $H_\chi$ 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. Note that this is a
priori not obvious as the cut-off function $\chi$ 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 [17, 31] are not applicable in our situation since the junction surface is not compact.

**Proposition 3.2** (Spectral property of the reference state $H_\chi$). For any $\chi \in \mathcal{X}$, the essential spectrum of $H_\chi$ defined in (3.8) satisfies

$$\sigma_{\text{ess}}(H_\chi) = \sigma_{\text{ess}}(H_{\text{per},L}) \cup \sigma_{\text{ess}}(H_{\text{per},R}), \quad [0, +\infty) \subset \sigma_{\text{ess}}(H_\chi).$$

In particular, this implies that $\sigma_{\text{ess}}(H_\chi)$ does not depend on the shape of the cut-off function $\chi \in \mathcal{X}$ defined in (3.5).

The proof relies on explicit constructions of Weyl sequences associated with $H_\chi$, and can be read in Section 5.7.

**Reference state as a spectral projector.** Before going straightly to the construction of reference state, let us discuss the choice of different regimes of junction system. From **Theorem 2.7** we know that the chemical potentials (Fermi levels) $\epsilon_L$ and $\epsilon_R$ are non-positive. Denote by the energy interval $I_{\epsilon_F} := [\min(\epsilon_L, \epsilon_R), \max(\epsilon_L, \epsilon_R)]$. In view of Proposition 3.2, the non-equilibrium regime (Fig. 3) corresponds to the fact

$$\sigma_{\text{ess}}(H_\chi) \cap I_{\epsilon_F} \neq \emptyset.$$ 

In this regime, steady state current may occur and the Landauer-Büttiker conductance can be calculated [6, 7, 8]. When $\mu_{\text{per},L}$ and $\mu_{\text{per},R}$ are identical, the junction system becomes periodic with different chemical potentials $\epsilon_L$ and $\epsilon_R$, in this case the Thouless conductance [6] can be defined and is given by

$$C_T \left| \frac{\sigma_{\text{ess}}(H_\chi) \cap I_{\epsilon_F}}{|I_{\epsilon_F}|} \right| > 0,$$

with $C_T$ some positive constant. It is not the objective of this article to discuss the steady state current, where the system is not at equilibrium. Let us consider the equilibrium regime (see Fig. 4) with the following assumption.

**Assumption 1.** The chemical potential $\epsilon_L$ and $\epsilon_R$ are in a common spectral gap $(\Sigma_a, \Sigma_b)$ (equilibrium regime, see Fig. 4), where $\Sigma_a$ is the maximum of the filled bands of $H_{\text{per},L}$ and $H_{\text{per},R}$, and $\Sigma_b$ is the minimum of the unfilled bands of $H_{\text{per},L}$ and $H_{\text{per},R}$.

Assumption 1 guarantees that the Fermi level of the junction system lies in a spectral gap of $H_\chi$ in view of Proposition 3.2, which is a common hypothesis [11, 23, 25] for 3D periodic insulating and semi-conducting systems. We make this assumption for simplicity, remark that with approaches proposed in [19, 20, 10] we can extend the results to metallic junction systems provides that the junction system is in its ground state and no steady state current occurs.

![Figure 5: Spectrum of $H_{\text{per},L}$, $H_{\text{per},R}$ and $H_\chi$ below 0.](image)
Remark that the chemical potential of the junction system is in the interval \( I_{\epsilon_F} \) with possible bounded states. Let us without loss of generality choose the Fermi level \( \epsilon_F = \max(\epsilon_I, \epsilon_R) = \sup I_{\epsilon_F} \) and define the reference state \( \gamma_x \) as the spectral projector associated with the states of \( H_\chi \) below \( \epsilon_F \):

\[
\gamma_x := \mathbb{1}_{(-\infty, \epsilon_F)}(H_\chi).
\] (3.9)

Remark that there can be discrete spectra of \( H_\chi \) in the gap \( (\Sigma_a, \Sigma_b) \) possibly accumulating at \( \Sigma_a \) and \( \Sigma_b \), and \( \epsilon_F \) can also be an eigenvalue of \( H_\chi \). The definition of (3.9) however excludes the possible bounded states with energy \( \epsilon_F \).

The following proposition shows that the density \( \rho_x \) of \( \gamma_x \) 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 of which decays exponentially in the \( x \)-direction as \( |x| \to \infty \).

**Proposition 3.3 (Exponential decay of density).** Under Assumption 1, the spectral projector \( \gamma_x \) is locally trace class with its density \( \rho_x \) well defined in \( L^1_{\text{loc}}(\mathbb{R}^3) \). Moreover,

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

Furthermore, denote by \( w_a \) the characteristic function of the unit cube centered at \( a \in \mathbb{R}^3 \). For any \( \alpha = (\alpha_x, 0, 0) \in \mathbb{R}^3 \) such that the support of \( w_a \) is either in \((-\infty, \alpha_x/2) \times \mathbb{R}^2 \) or \([\alpha_x/2, +\infty) \times \mathbb{R}^2 \), there exist positive constants \( C \) and \( t \) such that

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

The proof can be read in Section 5.9.

**Fictitious nuclear density of the reference state.** The density \( \rho_x \) associated with \( \gamma_x \) is fixed once the Fermi level \( \epsilon_F \) is chosen. We can therefore define a fictitious nuclear density \( \mu_x \) by imposing that the total electronic density \( \rho_x - \mu_x \) generates the potential \( V_x \). More precisely, in view of the Poisson’s equation (3.6), the fictitious nuclear density \( \mu_x \) is given by

\[
- \Delta V_x = 4\pi (\rho_x - \mu_x), \quad \mu_x := \rho_x - \left( \chi^2 (\rho_{\text{per},L} - \mu_{\text{per},L}) + (1 - \chi^2) (\rho_{\text{per},R} - \mu_{\text{per},R}) + \eta_x \right).
\] (3.10)

Let us emphasize that the Poisson’s equation (3.10) is defined on the whole space \( \mathbb{R}^3 \), which does not have any periodicity in the \( x \)-direction.

**The nuclear density of the junction is the fictitious nuclear density plus a perturbation.** In view of the definition (3.10) of fictitious nuclear density \( \mu_x \), it is natural to treat the difference between the real nuclear density of the junction system \( \mu_J \) and the fictitious nuclear density \( \mu_x \) as a perturbation. Note that this idea is similar to the definition of the defect state in [11] for the defect in crystals, and the polarization of the vacuum in the Bogoliubov–Dirac–Fock model [26, 23, 25]. Introduce

\[
\nu_x := \mu_J - \mu_x = (1_{\chi \leq 0} - \chi^2) (\mu_{\text{per},L} - \mu_{\text{per},R}) + (\chi^2 \rho_{\text{per},L} + (1 - \chi^2) \rho_{\text{per},R} - \rho_x) + \eta_x + v.
\] (3.11)

In view of Lemma 3.1 and Proposition 3.3, together with the fact that \((1_{\chi \leq 0} - \chi^2) (\mu_{\text{per},L} - \mu_{\text{per},R})\) has compact support and \(v\) belongs to \( L^r(\mathbb{R}^3) \) for \( 1 \leq r \leq +\infty \), it is easy to see that \( \nu_x \in L^p(\mathbb{R}^3) \) for \( 1 < p \leq 2 \). In particular, \( \nu_x \) belongs to \( L^{6/5}(\mathbb{R}^3) \) hence is in the Coulomb space \( C \) defined in (3.4).
3.3 Definition of the perturbative state

In this section we define a perturbative state associated with the perturbative density \( \nu_\gamma \) following the ideas developed in [11]. We formally derive the rHF energy difference between the junction state \( \gamma_J \) and the reference state \( \gamma_\chi \) by writing \( \gamma_J = \gamma_\chi + Q \) with \( Q \) being a trial density state. In view of \eqref{3.12}, we formally have

\[
\mathcal{E}(\gamma_J) - \mathcal{E}(\gamma_\chi) \stackrel{\text{formally}}{=} \text{Tr} \left( \frac{1}{2} \Delta (\gamma_\chi + Q) \right) + \frac{1}{2} D(\rho_J - \mu_J, \rho_J - \mu_J) - \text{Tr} \left( \frac{1}{2} \Delta \gamma_\chi \right) \\
- \frac{1}{2} D(\rho_\chi - \mu_\chi, \rho_\chi - \mu_\chi) = \text{Tr} \left( \frac{1}{2} \Delta Q \right) + D(\rho_\chi - \mu_\chi, \rho_\chi) \\
- D(\rho_Q, \nu_\chi) + \frac{1}{2} D(\rho_Q, \rho_Q) - D(\rho_\chi - \mu_\chi, \nu_\chi) + \frac{1}{2} D(\nu_\chi, \nu_\chi) \\
= \text{Tr} (H_\chi Q) - D(\rho_Q, \nu_\chi) + \frac{1}{2} D(\rho_Q, \rho_Q) - D(\rho_\chi - \mu_\chi, \nu_\chi) + \frac{1}{2} D(\nu_\chi, \nu_\chi).
\]

\eqref{3.12}

We next give a mathematical definition of the terms in \eqref{3.12}. We expect \( Q \) to be a perturbation of the reference state \( \gamma_\chi \). More precisely, we expect \( Q \) to be Hilbert-Schmidt. This is usually called the “Shale-Stinespring” condition [50], see [43, 53] for a detailed discussion. Moreover, we also expect the kinetic energy of \( \gamma_\chi \) to be finite. Let \( \Pi \) be an orthogonal projector on the Hilbert space \( \mathfrak{H} \) such that both \( \Pi_1 := 1 - \Pi \) have infinite rank. A self-adjoint compact operator \( A \) on \( \mathfrak{H} \) is said to be \( \Pi \)-trace class if \( A \in \mathcal{S}_2 (\mathfrak{H}) \) and both \( \Pi_1 A \Pi_1 \) and \( \Pi_2 A \Pi_2 \) are in \( \mathcal{S}_1 (\mathfrak{H}) \). For an operator \( A \) we define its \( \Pi \)-trace

\[
\text{Tr}_\Pi (A) := \text{Tr} (\Pi A \Pi) + \text{Tr} (\Pi_1 A \Pi_1),
\]

denote by \( \mathcal{S}_1^\Pi (\mathfrak{H}) \) the associated set of \( \Pi \)-trace class operators. Since reference state \( \gamma_\chi \) defined in \eqref{3.9} is an orthogonal projector on \( L^2 (\mathbb{R}^3) \), we can define associated \( \gamma_\chi \)-trace class operators. For any trial density matrix \( Q \), let us denote by \( Q^+ := \gamma_\chi Q \gamma_\chi \) and \( Q^- := \gamma_\chi Q^* \gamma_\chi \) introduce a Banach space of operators with finite \( \gamma_\chi \)-trace and finite kinetic energy as follows:

\[
Q_\chi := \{ Q \in \mathcal{S}_1^\gamma (L^2 (\mathbb{R}^3)) \mid Q_* = Q, |Q| \in \mathcal{S}_2 (L^2 (\mathbb{R}^3)), |\nabla|Q^+ \nabla| \in \mathcal{S}_1 (L^2 (\mathbb{R}^3)), |\nabla|Q^- \nabla| \in \mathcal{S}_1 (L^2 (\mathbb{R}^3)) \}.
\]

equipped with its natural norm

\[
\| Q \|_{Q_\chi} := \| Q \|_{\mathcal{S}_2} + \| Q^+ \|_{\mathcal{S}_1} + \| Q^- \|_{\mathcal{S}_1} + \| \nabla Q \|_{\mathcal{S}_1} + \| \nabla Q^+ \|_{\mathcal{S}_1} + \| \nabla Q^- \|_{\mathcal{S}_1}.
\]

By construction \( \text{Tr}_{Q_\chi} (Q) = \text{Tr} (Q^+) + \text{Tr} (Q^-) \). For \( Q \) to be an admissible perturbation of the reference state \( \gamma_\chi \), the Pauli’s principle requires that \( 0 \leq \gamma_\chi + Q \leq 1 \). Let us introduce the following convex set of admissible perturbative states:

\[
K_\chi := \{ Q \in Q_\chi \mid -\gamma_\chi \leq Q \leq 1 - \gamma_\chi \}.
\]

Remark that \( K_\chi \) is not empty since it contains at least \( 0 \). Remark also that \( K_\chi \) is the convex hull of states in \( Q_\chi \) of the special form \( \gamma - \gamma_\chi \), where \( \gamma \) is an orthogonal projector [11]. Furthermore, for any \( Q \in K_\chi \), a simple algebraic calculation gives that

\[
Q^+ \geq 0, \quad Q^- \leq 0, \quad 0 \leq Q^2 \leq Q^+ - Q^-.
\]

As mentioned in the previous section, the Fermi level \( \epsilon_F \) can be a discrete spectrum of \( H_\chi \). Assume that there exists \( N \in \mathbb{N}^* \) such that \( \epsilon_F \in (\Sigma_{N, \chi}, \Sigma_{N+1, \chi}) \), where \( \Sigma_{N, \chi} \leq \Sigma_{N+1, \chi} \) are two discrete spectra of \( H_\chi \) in the gap \( (\Sigma_a, \Sigma_b) \), and let \( \Sigma_{N, \chi} = \Sigma_a \) and \( \Sigma_{N+1, \chi} = \Sigma_b \) whenever the existence of each is not guaranteed in the gap \( (\Sigma_a, \Sigma_b) \). For any \( \kappa \in (\Sigma_{N, \chi}, \epsilon_F) \), let us introduce the following rHF kinetic energy of a state \( Q \in Q_\chi \) as

\[
\text{Tr}_{Q_\chi} (H_\chi Q) := \text{Tr} \left( |H_\chi - \kappa|^{1/2} (Q^+ - Q^-) |H_\chi - \kappa|^{1/2} \right) + \kappa \text{Tr}_{\gamma_\chi} (Q).
\]
A result of [11, Corollary 1] shows that the above expression is independent of $\kappa \in (\Sigma_{\mathcal{N}, \chi}, \epsilon_F)$. In view of (3.12) we introduce the following minimization problem
\[
E_{\kappa, \chi} = \inf_{Q \in \mathcal{X}} \{ \mathcal{E}_\chi(Q) - \kappa \text{Tr}_{\gamma_\chi}(Q) \},
\] (3.13)
where
\[
\mathcal{E}_\chi(Q) := \text{Tr}_{\gamma_\chi}(H_Q) - D(\rho_\chi, \nu_\chi) + \frac{1}{2} D(\rho_\chi, \rho_\chi).
\] (3.14)

### 3.4 Properties of the junction system

The following result shows that the minimization problem (3.13) is well posed and admits minimizers.

**Proposition 3.4. (Existence of the perturbative ground state)** Assume that Assumption 1 holds. Then there exist minimizers for the problem (3.13). There may be several minimizers, but they all share the same density. Moreover, any minimizer $Q_\chi$ of (3.13) satisfies the following self-consistent equation:
\[
\begin{cases}
\overline{Q}_\chi = \mathbb{1}_{(-\infty, \epsilon_F)}(H_{\overline{Q}_\chi}) - \gamma_\chi + \delta, \\
H_{\overline{Q}_\chi} = H_\chi + (\rho_{\overline{Q}_\chi} - \nu_\chi) * | |^{-1},
\end{cases}
\] (3.15)
where $\delta$ is a finite-rank self-adjoint operator satisfying $0 \leq \delta \leq 1$ and $\text{Ran}(\delta) \subseteq \text{Ker}(H_{\overline{Q}_\chi} - \epsilon_F)$.

The proof is a direct adaptations of several results obtained in [11], see a short summary in Section 5.10 for the completeness of the article. The result of Proposition 3.4 can be interpreted as follows: given a cut-off function $\chi$ belonging to the class $\mathcal{X}$ defined in (3.5), we can construct a reference state $\gamma_\chi$ and a perturbative ground state $Q_\chi$, the sum of which forms the real junction ground state.

However it is artificial to introduce cut-off functions $\chi$ since there are arbitrarily many possible choices. Even more, the final 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 cut-off function $\chi$ belonging to $\mathcal{X}$.

**Theorem 3.5 (Independence of the reference state and uniqueness of ground state density).** The ground state density of the junction system with nuclear density defined in (3.2) 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 $\chi$, where $\rho_\chi$ is the density associated with the spectral projector $\gamma_\chi$ defined in (3.9), and $\rho_{Q_\chi}$ is the unique density associated with the solution $Q_\chi$ of the minimization problem (3.15).

The proof can be read in Section 5.11.

### 4 Extension to junctions of 2D materials: a brief discussion

Assume that the periods of 2D materials are commensurate in the $y$-direction with period $L_y > 0$ but not necessarily commensurate in the $x$-direction, see Fig 6 for illustration. Remark that semi-infinite 2D materials are special cases of this, as it can be modeled as the junction with vacuum occupying other half space. Following similar ideas developed in Section 2.1 and writing $\Gamma_{L_y} := \mathbb{R} \times L_y \mathbb{S}_1 = \mathbb{R} \times [-L_y/2, L_y/2]$ and $\Gamma_{L_y}^* = \left[ -\frac{\pi}{L_y}, \frac{\pi}{L_y} \right]$, the following decomposition holds:
\[
L^2(\mathbb{R}^2) = \int_{\Gamma_{L_y}^*} L^2_{\text{per}, y}(\Gamma_{L_y}) dq.
\]

The partial Bloch transform $\mathcal{B}_y$ can be defined from dense subspace $C_c^\infty(\mathbb{R}^2)$ of $L^2(\mathbb{R}^2)$ to $L^2 \left( \Gamma_{L_y}^* ; L^2_{\text{per}, y}(\Gamma_{L_y}) \right)$
\[
\forall (x, y) \in \Gamma_{L_y}, \; q \in \Gamma_{L_y}^*, \quad (\mathcal{B}_y \phi)_q(x, y) := \sum_{k \in L_y \mathbb{Z}} e^{-i(y+q)k} \phi(x, y + k).
\]
Figure 6: Junction of 2D materials which are commensurate in the $y$-direction. The unit cell of the total junction system is a cylinder $\Gamma_{L_y}$.

Its inverse is given by

$$\forall k \in L_y \mathbb{Z}, \text{ for a.a. } (x, y) \in \Gamma_{L_y}, \quad (\mathcal{B}_y^{-1} f_k)(x, y + k) := \frac{1}{|\Gamma_{L_y}^*|} \int_{\Gamma_{L_y}^*} e^{i(k \cdot x + y)} f_k(x, y) \, dq.$$  

Under $\mathcal{B}_y$, the (negative) Laplace operator on $L^2(\mathbb{R}^2)$ is decomposed as

$$\frac{1}{2} \Delta = \mathcal{B}_y^{-1} \left( \frac{1}{|\Gamma_{L_y}^*|} \int_{\Gamma_{L_y}^*} \frac{1}{2} \Delta_q dq \right) \mathcal{B}_y, \quad -\Delta_q = -\partial_x^2 + (i \partial_y - q)^2,$$

with $-\Delta_q$ acting on $L^2_{\text{per},y}(\Gamma_{L_y})$. Given $q \in \Gamma_{L_y}^*$, the junction problem follows exactly the same construction of Section 3 by replacing the space from $\mathbb{R}^3$ to the cylinder $\Gamma_{L_y}$. The latter construction is much more simpler as the cylinder is compact in its radius direction, meaning that the cut-off functions used to construct the reference Hamiltonian are periodic in $y$-direction, hence compact in the radius direction. This simplifies the proofs of Proposition 3.2.

With a little bit of abuse, let us still use the same notations as in Section 3. We can construct a reference Hamiltonian $H_{\chi}$ and spectral projector $\gamma_{\chi}$ which is $L_y \mathbb{Z}$-translation invariant in the $y$-direction with $\chi$ being $L_y \mathbb{Z}$-periodic in the $y$-direction. Moreover, $H_{\chi}$ is decomposed by $\mathcal{B}_y$

$$H_{\chi} = \mathcal{B}_y^{-1} \left( \frac{1}{|\Gamma_{L_y}^*|} \int_{\Gamma_{L_y}^*} H_{\chi,q} dq \right) \mathcal{B}_y, \quad H_{\chi,q} = -\partial_x^2 + (i \partial_y - q)^2 + V_{\chi},$$

$$\gamma_{\chi} = \mathcal{B}_y^{-1} \left( \frac{1}{|\Gamma_{L_y}^*|} \int_{\Gamma_{L_y}^*} \gamma_{\chi,q} dq \right) \mathcal{B}_y, \quad \gamma_{\chi,q} = 1_{(-\infty, \epsilon F)}(H_{\chi,q}).$$

A direction adaptation of Proposition 3.2 we obtain that

$$\forall q \in \Gamma_{L_y}^*, \quad \sigma_{\text{ess}}(H_{\chi,q}) = \sigma_{\text{ess}}(H_{\text{per},L,q}) \cup \sigma_{\text{ess}}(H_{\text{per},R,q}),$$

where $H_{\text{per},L,q}$ (resp. $H_{\text{per},R,q}$) are $\mathcal{B}_y$-decomposed $H_{\text{per},L}$ (resp. $H_{\text{per},R}$). Remark that by [48, Theorem XIII.85]

$$\sigma_{\text{ess}}(H_{\text{per},L}) \cup \sigma_{\text{ess}}(H_{\text{per},R}) \subseteq \sigma_{\text{ess}}(H_{\chi}). \quad (4.1)$$
Remark that the strictly equality of the above expression is hardly possible 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 $H_\chi$. Using same techniques in [10] when defining extended defects in the Fermi sea, we can define a new class of perturbations $Q = \mathcal{S}^{-1}_y \left( \int_{\Lambda^+_y} Q_y \frac{d\mu}{2\pi} \right) \mathcal{S}_y$ in suitable class and follow the same procedure in the quasi 1D case to prove the existence of mean–field ground state.

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5 Proof of the results

In order to simplify the notations, from Section 5.1 to Section 5.6 when treating the quasi 1D periodic system let us denote by $\mathcal{S}_p$ the Schatten class $\mathcal{S}_p(L^2_{\text{per},x}(\Gamma))$ for $1 \leq p \leq +\infty$. Unless otherwise specified, start from Section 5.7 we use $\mathcal{S}_p$ instead of $\mathcal{S}_p(L^2(\mathbb{R}^3))$ for the proofs of the junction system.

First of all, let us recall the following Kato-Seiler-Simon (KSS) inequality:

**Lemma 5.1.** ([49, Lemma 2.1]) Let $2 \leq p \leq \infty$. For $g, f$ belonging to $L^p(\mathbb{R}^3)$, the following inequality holds

$$
\|f(-i\nabla)g(x)\|_{\mathcal{S}_p(L^2(\mathbb{R}^3))} \leq (2\pi)^{-3/p}\|g\|_{L^p(\mathbb{R}^3)}\|f\|_{L^p(\mathbb{R}^3)}.
$$

(5.1)

**5.1 Proof of Lemma 2.1**

The proof is an easy adaptation of the proof of the classical Kato–Seiler–Simon inequality (5.1) by replacing the Fourier transform with the mixed Fourier transform $\mathcal{F}$. Let us prove separately (2.6) for $p = 2$ and $p = +\infty$ and conclude by an interpolation argument. We use the following kernel representation during the proofs. For $x = (x, r)$ and $y = (y, r')$ belonging to $\Gamma$, symbolic calculus shows that the Schwartz kernel $K_{f,\xi}((x, r), (y, r'))$ of the operator $f(-i\nabla_\xi)$ acting on $L^2_{\text{per},x}(\Gamma)$ formally reads

$$
K_{f,\xi}((x, r), (y, r')) = \frac{1}{4\pi^2} \left( \mathcal{F}^{-1} \circ \tau^x_\xi f \right) ((x - y), (r - r'))
$$

(5.2)

$$
= \frac{1}{4\pi^2} \sum_{n \in \mathbb{Z}} \int_{\mathbb{R}^2} e^{i(2\pi n (x - y) + k \cdot (r - r'))} f(2\pi n + \xi, k) \, dk.
$$

Let $p = 2$. In view of the isometry identity (2.4), the convolution equality (2.5) and the kernel representation (5.2), the following estimate holds

$$
\|f(-i\nabla_\xi)g\|_{\mathcal{S}_2}^2 = \frac{1}{4\pi^2} \int_{\Gamma \times \Gamma} \left| \left( \mathcal{F}^{-1} \circ \tau^x_\xi f \right) (x - y)g(y) \right|^2 \, dx \, dy
$$

$$
\leq \frac{1}{4\pi^2} \int_{\Gamma} |g(y)|^2 \left( \int_{\Gamma} \left| \left( \mathcal{F}^{-1} \circ \tau^x_\xi f \right) (x - y) \right|^2 \, dx \right) \, dy
$$

$$
= \frac{1}{4\pi^2} \int_{\Gamma} |g(y)|^2 \sum_{n \in \mathbb{Z}} \left( \int_{\mathbb{R}^2} |f(2\pi n + \xi, k)|^2 \, dk \right) \, dy
$$

$$
= \frac{1}{4\pi^2} \|g\|_{L^2_{\text{per},x}(\Gamma)}^2 \sum_{n \in \mathbb{Z}} \|f(2\pi n + \xi, \cdot)\|_{L^2(\mathbb{R}^2)}^2,
$$

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which proves (2.6) for \( p = 2 \). Now let \( p = +\infty \), it suffices to prove that for any \( \phi \in L^2_{\text{per},x}(\Gamma) \),

\[
\| f(-i\nabla_\xi)g\phi \|_{L^2_{\text{per},x}(\Gamma)} \leq \| g\|_{L^\infty(\mathbb{R})} \sup_{n \in \mathbb{Z}} \| f \left( (2\pi n + \xi, \cdot) \right) \|_{L^\infty(\mathbb{R})} \| \phi \|_{L^2_{\text{per},x}(\Gamma)}.
\]

Follow similar arguments as when \( p = 2 \), by the isometry of \( L^2 \) norm (2.4) we obtain that

\[
\| f(-i\nabla_\xi)g\phi \|_{L^2_{\text{per},x}(\Gamma)}^2 = \sum_{n \in \mathbb{Z}} \int_{\mathbb{R}} |\mathcal{F}(g\phi) (n, k)|^2 |f \left( (2\pi n + \xi + k, \cdot) \right)|^2 \, dk
\leq \sup_{n \in \mathbb{Z}} \| f \left( (2\pi n + \xi, \cdot) \right) \|_{L^\infty(\mathbb{R})}^2 \| g\phi \|_{L^2_{\text{per},x}(\Gamma)}^2
\leq \| g\|_{L^\infty(\mathbb{R})}^2 \sup_{n \in \mathbb{Z}} \| f \left( (2\pi n + \xi, \cdot) \right) \|_{L^\infty(\mathbb{R})}^2 \| \phi \|_{L^2_{\text{per},x}(\Gamma)}^2.
\]

We thus have proved the results when \( p = +\infty \). Therefore, following the same interpolation arguments as in [49, Lemma 2.1] we obtain the desired result for \( 2 < p < +\infty \).

### 5.2 Proof of Lemma 2.3

For \( n \in \mathbb{Z} \), let us consider the 2D equation:

\[-\Delta_r G_n + 4\pi^2 n^2 G_n = 2\pi \delta_{r=0} \quad \text{in } \mathcal{S}'(\mathbb{R}^2).\]

It is well known (see for example [44, 38]) that the solution of the above equation is

\[G_n(|r|) = \begin{cases} -\log(|r|), & n \equiv 0, \\ K_0 \left( 2\pi |n||r| \right), & |n| \geq 1, \end{cases}\]

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 \( G(x, r) \) defined in (2.7) can be rewritten as

\[G(x, r) = 2 \sum_{n \in \mathbb{Z}} e^{2\pi nx} G_n(r) \in \mathcal{S}'_{\text{per},x}(\Gamma).\]

Applying the Laplace operator to both sides,

\[-\Delta G(x, r) = 4\pi \sum_{n \in \mathbb{Z}} e^{2\pi nx} \delta_{r=0} \in \mathcal{S}'_{\text{per},x}(\Gamma).\]

Taking the Fourier transform \( \mathcal{F} \) on both sides of the above equation we obtain that

\[\mathcal{F} G(n, k) = \frac{2}{4\pi^2 n^2 + |k|^2} \in \mathcal{S}'(\mathbb{R})\]

On the other hand, by the Poisson summation formula \( \sum_{n \in \mathbb{Z}} \delta_{x=n} = \sum_{n \in \mathbb{Z}} e^{2\pi nx} \in \mathcal{S}(\mathbb{R}) \), we conclude that the Green’s function \( G(x, r) \) defined in (2.7) satisfies

\[-\Delta G(x, r) = 4\pi \sum_{n \in \mathbb{Z}} \delta_{(x, r)=(n, 0)}.\]

Let us now give some estimate on \( \tilde{G} \) defined in (2.7). Note that there exist two positive constants \( C_0 \) and \( C_1 \) such that [34]

\[0 \leq K_0(\alpha) \leq \begin{cases} C_0 |\log(\alpha)|, & \text{when } \alpha \leq 2\pi, \\ C_1 e^{-\alpha (\pi/2\alpha)^{1/2}}, & \text{when } \alpha > 2\pi. \end{cases}\]
For \(|r| > 1\), it holds that

\[
|\tilde{G}(x, r)| \leq 2C_1 \sum_{n=1}^{\infty} \frac{e^{-2\pi n|r|}}{\sqrt{|r|}} \leq \frac{2C_1}{1 - e^{-2\pi}} \frac{e^{-2\pi |r|}}{|r|}.
\] (5.3)

For \(|r| \leq 1\) fixed, there exists \(N \geq 1\) such that \(N \leq \frac{1}{|r|} < N + 1\). In particular, for \(n > N + 1\) we have \(2\pi n |r| > 2\pi\).

There exists therefore a positive constant \(C\) such that

\[
|\tilde{G}(x, r)| \leq 4C_0 \sum_{n=1}^{N} \log(2\pi n |r|) + 2C_1 \sum_{n=N+1}^{\infty} \frac{e^{-2\pi n |r|}}{\sqrt{|r|}} \leq 4C_0 \left( \int_1^{2\pi} \log(2\pi t |r|) \, dt \right) + 2C_1 \int_{2\pi}^{\infty} e^{-t} \, dt
\]

\[
= \frac{4C_0}{|r|} \left( |\log(2\pi) - 1| - |r| \log(2\pi |r|) \right) + 2C_1 e^{-2\pi} \leq \frac{C}{|r|}.
\] (5.4)

Together with (5.3) we deduce that \(\tilde{G}(x, r) \in L^p_{\text{per}, x}(\Gamma)\) for \(1 \leq p < 2\). Consider, for \(r \neq 0\),

\[
\tilde{G}(x, r) = \sum_{n \in \mathbb{Z}} \left( \frac{1}{\sqrt{(x-n)^2 + |r|^2}} - \int_{-1/2}^{1/2} \frac{1}{\sqrt{(x-y-n)^2 + |r|^2}} \, dy \right).
\]

Note that \(\forall r \in \mathbb{R}^2 \setminus \{0\}, \int_{-1/2}^{1/2} \tilde{G}(x, r) \, dx \equiv 0\). A result of [4, Equation (1.8)] gives

\[-\Delta (\tilde{G}(x, r) - 2 \log(|r|)) = 4\pi \sum_{k \in \mathbb{Z}} \delta_{(x=k, r=0)} \in \mathcal{S}'(\mathbb{R}^3),\]

with \(\tilde{G}(x, r) = O(\frac{1}{|r|})\) when \(|r| \to \infty\) by [4, Lemma 2.2]. Denoting by \(u(x, r) = \tilde{G}(x, r) - \tilde{G}(x, r)\), we therefore obtain that \(-\Delta u(x, r) \equiv 0\). As \(u(x, r)\) belongs to \(L^1_{\text{loc}}(\mathbb{R}^3)\), by Weyl’s lemma for the Laplace equation we obtain that \(u(x, r)\) is \(C^\infty(\mathbb{R}^3)\). On the other hand, by the decay properties of \(\tilde{G}\) and \(\tilde{G}\), we deduce that \(|u(\cdot, r)| \to 0\) when \(|r| \to \infty\) uniformly in \(x\), hence by the maximum modulus principle for harmonic functions we can conclude that \(u \equiv 0\), hence \(\tilde{G}(x, r) = \tilde{G}(x, r)\).

### 5.3 Proof of Lemma 2.5

We prove this lemma by an explicit construction of a density matrix that belongs to \(\mathcal{F}_{\Gamma, \text{sym}} \subseteq \mathcal{F}_{\Gamma}\). Consider a cut-off function \(\varrho \in C_c(\Gamma)\) such that \(0 \leq \varrho \leq 1\) and \(\int_{\Gamma} \varrho^2 = 1\). Let \(\varrho_{\text{per}} = \sum_{n \in \mathbb{N}} \rho(\cdot - n)\). Let \(\omega \geq 0\) be a parameter to be precised later. Define

\[
\gamma_\omega = \varrho^{-1} \left( \int_{\Gamma^*} \gamma_{\omega, \xi} \frac{d\xi}{2\pi} \right) \varrho, \quad \gamma_{\omega, \xi} = A_{\omega, \xi} A_{\omega, \xi}^*, \quad A_{\omega, \xi} := \mathbb{1}_{[0, \omega]}(-\Delta_{\xi}) \varrho_{\text{per}}.
\] (5.5)

It is easy to see that \(0 \leq \gamma_\omega \leq 1\), and that \(\forall k \in \mathbb{Z}, \tau_{\xi} \gamma_{\omega} = \gamma_{\omega} \tau_{\xi}^{\mathbb{Z}}\) by construction. Let us prove that the kinetic energy per unit cell of \(\gamma_\omega\) is finite. Denote by \(F_{\xi}(n, k) = \sqrt{(2\pi n + \xi)^2 + k^2}\). By the Kato–Seiler–Simon type inequality (2.6) it is easy to see that

\[
\int_{\Gamma^*} \, \text{Tr}_{L^2_{\text{per}, x}} \left( \sqrt{1 - \Delta_{\xi}} \gamma_{\omega, \xi} \sqrt{1 - \Delta_{\xi}} \right) \, d\xi \leq \frac{1}{4\pi^2} \int_{\Gamma^*} \varrho_{\text{per}} \left( \sum_{n \in \mathbb{Z}} \left\| \sqrt{1 + F_{\xi}^2(n, \cdot)} \mathbb{1}_{[0, \omega]} \left( F_{\xi}^2(n, \cdot) \right) \right\|_{L^2(\mathbb{R}^2)}^2 \right) \, d\xi < +\infty.
\]

Hence \(\gamma_{\omega}\) belongs to \(\mathcal{P}_{\text{per}, x}\). Let us now show that there exists \(\omega_{\ast} \geq 0\) such that \(\rho_{\omega_{\ast}, \text{sym}} = \mu_{\text{per}, \text{sym}} \in \mathcal{C}_{\Gamma}\). It is easy to see that the density \(\rho_{\omega_{\ast}}\) is smooth and compactly supported in \(\Gamma\) by definition. Moreover, in view of the kernel representation (5.2), the kernel \(K_{\omega, \xi}\) of the operator \(A_{\omega, \xi}\) is

\[
K_{\omega, \xi} \left( (x, r), (y, r') \right) = \frac{1}{4\pi^2} \sum_{n \in \mathbb{Z}} \int_{\mathbb{R}^2} e^{i(2\pi n(x-y) + k(r-r'))} \mathbb{1}_{[0, \omega]} \left( F_{\xi}^2(n, k) \right) \varrho_{\text{per}}(y, r') \, dk.
\]
Remark that the non-negative function $\omega \rightarrow \int_{[0,\omega]} \left( \sum_{n\in \mathbb{Z}} \int_{[0,\infty]} \left( F^2_n(n,k) \right) dk \right) d\xi$ is monotonic non-decreasing in $\omega$, which equals to 0 when $\omega = 0$ and tends to $+\infty$ when $\omega \to +\infty$. Hence there exists $\omega^* > 0$ such that

$$\int_{\Gamma} \rho_{\omega^*} = \frac{1}{2\pi} \int_{[0,\omega^*]} \| A_{\omega^*,\xi} \|_{L^2}^2 d\xi = \frac{1}{2\pi} \int_{[0,\omega^*]} \| K_{A,\xi} \|_{L^2_{per,x}(\Gamma)}^2 d\xi$$

$$= \frac{1}{(2\pi)^3} \int_{\Gamma^*} \int_{\Gamma^*} \int_{\mathbb{R}^2} \sum_{n\in \mathbb{Z}} \left( F^2_n(n,k) \right) \rho_{per}(y,r) dy dr dk d\xi$$

$$= \frac{1}{(2\pi)^3} \int_{\Gamma^*} \left( \sum_{n\in \mathbb{Z}} \int_{[0,\omega^*]} \left( F^2_n(n,k) \right) dk \right) d\xi = \int_{\Gamma} \mu_{per,sym} > 0. \tag{5.6}$$

This condition is equivalent to that $\mathcal{F}(\rho_{\omega^*} - \mu_{per})(0,0) = 0$. As $\mathcal{F}(\rho_{\omega^*} - \mu_{per})(0,k)$ is $C^1(\mathbb{R}^2)$ and bounded, hence $k \rightarrow |k|^{-1}, \mathcal{F}(\rho_{\omega^*} - \mu_{per,sym})(0,k) \in L^2_{per}(\mathbb{R}^2)$. In view of this, there exists a positive constant $C$ such that

$$\sum_{n\in \mathbb{Z}} \int_{\mathbb{R}^2} \left| \frac{\mathcal{F}(\rho_{\omega^*} - \mu_{per,sym})(n,k)}{|k|^2 + 4\pi^2 n^2} \right|^2 dk \leq \int_{|k| \leq 2\pi} \left| \frac{\mathcal{F}(\rho_{\omega^*} - \mu_{per,sym})(0,k)}{|k|^2} \right|^2 dk$$

$$+ \frac{1}{4\pi^2} \left( \int_{|k| > 2\pi} \left| \mathcal{F}(\rho_{\omega^*} - \mu_{per,sym})(0,k) \right|^2 dk + \sum_{n\in \mathbb{Z}, \{0\}} \int_{\mathbb{R}^2} \left| \mathcal{F}(\rho_{\omega^*} - \mu_{per,sym})(n,k) \right|^2 dk \right) \tag{5.7}$$

$$\leq C + \frac{1}{4\pi^2} \int_{|k| \leq 2\pi} \left| \rho_{\omega^*} - \mu_{per,sym} \right|^2 < +\infty.$$ 

In view of the definition of the Coulomb interactions (2.13), we therefore can conclude that

$$D_{\Gamma}(\rho_{\omega^*} - \mu_{per,sym}, \rho_{\omega^*} - \mu_{per,sym}) < +\infty.$$ 

This allows us to conclude that the state $\gamma_{\omega^*} \in \mathcal{F}_{\Gamma,sym} \subseteq \mathcal{F}_{\Gamma}$. Hence $\mathcal{F}_{\Gamma,sym}$ and $\mathcal{F}_{\Gamma}$ are not empty. As any density $\rho_{\gamma}$ associated with $\gamma \in \mathcal{P}_{per,x}$ is integrable, in view of the Remark 2.4 we can conclude that (2.17) holds.

### 5.4 Proof of Theorem 2.6 and Theorem 2.7

First of all we prove the existence of minimizers for the minimization problem (2.18) and (2.19). We also prove that all the minimizers share the same density for each minimization problem. We next define a mean-field Hamiltonian associated with the problem (2.19), and show that the ground state energy is always non-positive. Moreover, the minimizer of (2.19) is uniquely given by the spectral projector of the mean-field Hamiltonian. In the end we show that density of minimizer decays exponentially fast in the $r$-direction, we also show that the mean-field potential belongs to $L^p_{per,x}(\Gamma)$ for $1 < p < +\infty$, which will be useful for further discussions.

For the convenience of the proof let us give an equivalent formulation of the minimization problem (2.18) and (2.19). In view of the rHF energy functional defined in (2.15), remark that the operator $-\frac{1}{2} \Delta_{\xi}$ is not invertible. However, the operator $-\frac{1}{2} \Delta_{\xi} - \kappa$ is positive definite and $\left| -\frac{1}{2} \Delta_{\xi} - \kappa \right|^{-1}$ is bounded for any $\kappa < 0$. Therefore for any $\gamma \in \mathcal{F}_{\Gamma}$, in view of the charge neutrality constant (2.17), we rewrite the periodic rHF energy functional as follows:

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

$$= \tilde{E}_{per,x,\kappa}(\gamma, \mu_{per}) + \kappa \frac{1}{2\pi} \int_{\Gamma^*} \text{Tr} L^2_{per,x}(\Gamma) \left( \gamma_{\xi} \right) d\xi = \tilde{E}_{per,x,\kappa}(\gamma, \mu_{per}) + \kappa \int_{\Gamma} \mu_{per},$$

with

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

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The parameter $\kappa$ can be interpreted as the Lagrangian multiplier associated with the charger neutrality constraint. Therefore by fixing $\kappa < 0$, the minimization problem (2.18) is equivalent to the problem

$$\inf \left\{ \mathcal{E}_{\text{per},x,\kappa}(\gamma, \mu_{\text{per}}); \gamma \in \mathcal{F}_\Gamma \right\}.$$ 

Similarly, the minimization problem (2.19) is equivalent to the problem

$$\inf \left\{ \mathcal{E}_{\text{per},x,\kappa}(\gamma, \mu_{\text{per},\text{sym}}); \gamma \in \mathcal{F}_{\Gamma,\text{sym}} \right\}.$$ 

In the following we consider a fixed $\kappa < 0$ and relate $\kappa$ to the Lagrange multiplier of the charge neutrality constraint when giving the form of the minimizers for the minimization problem (2.19).

**Existence of minimizer.** We prove the existence of minimizers and uniqueness of the density of minimizers for the problem (2.19) by considering a minimizing sequence, and show that there is no loss of compactness. This approach is rather classical [13, 11, 12, 10] for rHF type models. The results for the minimization problem (2.18) are obtained by straightforward adaptations.

**Step 1. Weak convergence of the minimizing sequence.**

First of all it is easy to see that the functional $\mathcal{E}_{\text{per},x,\kappa}(\cdot, \mu_{\text{per},\text{sym}})$ is well defined on the non-empty set $\mathcal{F}_{\Gamma,\text{sym}}$. Consider a minimizing sequence of $\mathcal{E}_{\text{per},x,\kappa}(\cdot, \mu_{\text{per},\text{sym}})$

$$\left\{ \gamma_n := \mathcal{B}^{-1} \left( \int_{\Gamma^*} \gamma_n \frac{d\xi}{2\pi} \mathcal{B} \right) \right\}_{n \geq 1}$$

on $\mathcal{F}_{\Gamma,\text{sym}}$, there exists $C > 0$ such that for all $n \geq 1$:

$$0 \leq \int_{\Gamma^*} \text{Tr}_{L^2_{\text{per},x}(\Gamma)} \left( \left| -\frac{1}{2} \Delta \xi - \kappa \right|^{1/2} \gamma_n \right) \leq C, \quad 0 \leq \text{Tr}_{\Gamma} (\rho_{\gamma_n} - \mu_{\text{per},\text{sym}}, \rho_{\gamma_n} - \mu_{\text{per},\text{sym}}) \leq C.$$ 

The kinetic energy bound (5.8) together with the inequality (2.12) 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 $\forall n \in \mathbb{N}^*$, the density $\rho_{\gamma_n} \in L^p_{\text{per},x}(\Gamma)$ 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 $0 \leq \gamma_n \xi \leq \gamma_n \xi \leq 1$, we obtain that

$$0 \leq \int_{\Gamma^*} \|\gamma_n \xi\|_{L^2_{\text{sym}}(\Gamma)}^2 \leq \int_{\Gamma^*} \text{Tr}_{L^2_{\text{per},x}(\Gamma)} (\gamma_n^2 \xi) \leq \int_{\Gamma^*} \text{Tr}_{L^2_{\text{per},x}(\Gamma)} (\gamma_n \xi) \leq 2\pi Z.$$ 

This implies that the operator-valued function $\xi \mapsto \gamma_n \xi$ is uniformly bounded in $L^2(\Gamma^*; \mathcal{G}_2)$. 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 $L^\infty(\Gamma^*; \mathcal{S}(L^2_{\text{per},x}(\Gamma)))$. Combine these remarks with the uniform energy bound (5.8), we deduce that there exist (up to extraction):

$$\gamma = \mathcal{B}^{-1} \left( \int_{\Gamma^*} \gamma_n \frac{d\xi}{2\pi} \mathcal{B} \right), \quad \mathcal{B} \in L^p_{\text{per},x}(\Gamma), \quad \tilde{\rho}_\gamma - \mu_{\text{per},\text{sym}} \in \mathcal{C}_\Gamma,$$

such that $\gamma_n \xrightarrow{\ast} \gamma$ in the following sense: for any operator-valued function

$$\xi \mapsto U_\xi \in L^2(\Gamma^*; \mathcal{G}_2) + L^1(\Gamma^*; \mathcal{G}_1),$$

we have

$$\int_{\Gamma^*} \text{Tr}_{L^2_{\text{per},x}(\Gamma)} (U_\xi \gamma_n) \frac{d\xi}{n \rightarrow \infty} \int_{\Gamma^*} \text{Tr}_{L^2_{\text{per},x}(\Gamma)} (U_\xi \gamma) \frac{d\xi}{n \rightarrow \infty}.$$ 

(5.10)
The density $\rho_{\gamma_n} \rightharpoonup \bar{\rho}_\gamma$ weakly in $L^p_{\text{per},x}(\Gamma)$ for $1 < p \leq 3$, and the total density $\rho_{\gamma_n} - \mu_{\text{per},\text{sym}} \rightharpoonup \bar{\rho}_\gamma - \mu_{\text{per},\text{sym}}$ weakly in $C_\Gamma$. The convergence (5.10) is due to the fact that the predual of $L^\infty(\Gamma^*; \mathcal{S}(L^2_{\text{per},x}(\Gamma)))$ is $L^1(\Gamma^*; \mathcal{S}_1)$, and that $L^2(\Gamma^*; \mathcal{S}_2)$ is a Hilbert space.

Denote by $\mathcal{D}_{\text{per},x}(\Gamma)$ the functions which are $C^\infty$ on $\mathbb{R}$, 1-periodic in the $x$-direction, and have compact support in the $r$-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 $r$-direction when $|r| \to \infty$.

**Lemma 5.2** (Consistency of densities). Denote by $\rho_\gamma$ the density associated with the density matrix $\gamma$ obtained in the weak limit (5.9). It holds that $\rho_\gamma - \mu_{\text{per},\text{sym}} = \bar{\rho}_\gamma - \mu_{\text{per},\text{sym}}$ in $\mathcal{D}'_{\text{per},x}(\Gamma)$.

We postpone this proof to Section 5.5.

---

Step 2. The state $\gamma$ is a minimizer.

Let us first show that the kinetic energy of $\gamma$ obtained by the weak limit (5.10) is finite. To achieve this, consider an orthonormal basis $\{e_i\}_{i \in \mathbb{N}} \subset \mathcal{H}_{\text{per},x}(\Gamma) \cap L^2_{\text{per},x}(\Gamma)$, and define the following family of operators for $N \in \mathbb{N}^*$:

$$M^N_\xi := \left( \left| \frac{1}{2} \Delta_\xi - \kappa \right|^{1/2} \sum_{i=1}^N |e_i \rangle \langle e_i| \right) - \left( \frac{1}{2} \Delta_\xi - \kappa \right)^{1/2} \left( \sum_{i=1}^N |e_i \rangle \langle e_i| \right) \right).$$

An easy computation shows that for all $\xi \in \Gamma^*$, the operator $M^N_\xi$ belongs to $\mathcal{S}_2$. Moreover, the function $\xi \mapsto M^N_\xi$ can be seen as an operator-valued function belonging to $L^2(\Gamma^*; \mathcal{S}_2)$ as $\Gamma^* = [-\pi, \pi]$ is a finite interval. Recall that $\text{Tr}(AB) = \text{Tr}(BA)$ when $A, B$ are Hilbert-Schmidt operators. On the other hand, it is easy to see that $\left| \frac{1}{2} \Delta_\xi - \kappa \right|^{1/2}$ is a square-integrable function on $\Gamma^*$, and

$$\lim_{N \to \infty} \int_{\Gamma^*} \text{Tr}_{L^2_{\text{per},x}(\Gamma)} \left( M^N_\xi \right) d\xi = 0.$$
In view of (5.11) and (5.12), we conclude that
\[
\mathcal{E}_{\text{per},x}(\gamma, \mu_{\text{per},\text{sym}}) \leq \liminf_{n \to \infty} \mathcal{E}_{\text{per},x}(\gamma_n, \mu_{\text{per},\text{sym}}),
\]
which shows that the state \( \gamma \) obtained in (5.9) is a minimizer of the problem (2.19). Let us prove that all minimizers share the same density: consider two minimizers \( \overline{\gamma}_1 \) and \( \overline{\gamma}_2 \). By the convexity of \( \mathcal{F}_{\Gamma,\text{sym}} \) it holds that \( \frac{1}{2} (\overline{\gamma}_1 + \overline{\gamma}_2) \in \mathcal{F}_{\Gamma,\text{sym}} \). Moreover
\[
\mathcal{E}_{\text{per},x} \left( \frac{\overline{\gamma}_1 + \overline{\gamma}_2}{2}, \mu_{\text{per},\text{sym}} \right) = \frac{1}{2} \mathcal{E}_{\text{per},x} (\overline{\gamma}_1, \mu_{\text{per},\text{sym}}) + \frac{1}{2} \mathcal{E}_{\text{per},x} (\overline{\gamma}_2, \mu_{\text{per},\text{sym}}) - \frac{1}{4} D_1 \left( \rho_{\overline{\gamma}_1} - \rho_{\overline{\gamma}_2}, \rho_{\overline{\gamma}_1} - \rho_{\overline{\gamma}_2} \right),
\]
which shows that \( D_1 \left( \rho_{\overline{\gamma}_1} - \rho_{\overline{\gamma}_2}, \rho_{\overline{\gamma}_1} - \rho_{\overline{\gamma}_2} \right) \equiv 0 \), hence all the minimizers of the problem (2.19) share the same density.

**Non-positivity of the ground state energy.** We begin with the definition of the mean-field potential and the mean-field Hamiltonian, we next study the spectrum of the mean-field Hamiltonian. In the end we prove the non-positivity of the ground state energy by constructing admissible states in \( \mathcal{F}_{\Gamma,\text{sym}} \), escaping to infinity in the \( r \)-direction whenever the ground state energy is positive, decreasing the total energy of the system. Let
\[
V_{\text{per},\text{sym}} := (\rho_{\gamma_{\text{per}}} - \mu_{\text{per},\text{sym}}) \ast_{\Gamma} G,
\]
which is the solution of the Poisson’s equation \(-\Delta V_{\text{per},\text{sym}} = 4\pi (\rho_{\gamma_{\text{per}}} - \mu_{\text{per},\text{sym}})\). Applying the mixed Fourier transform (2.3) to both sides of the above equation
\[
\| \nabla V_{\text{per},\text{sym}} \|_{L^2_{\text{per},x}(\Gamma)} = \left\| \mathcal{F} (V_{\text{per},\text{sym}}) \right\|_{L^2_{\text{per},x}(\Gamma)} = 4\pi \left\| \mathcal{F} \left( \rho_{\gamma_{\text{per}}} - \mu_{\text{per},\text{sym}} \right) \right\|_{L^2_{\text{per},x}(\Gamma)} < +\infty.
\]
Assume that (2.16) holds. Consider a minimizer \( \gamma_{\text{per}} \) of (2.19) with the unique density \( \rho_{\gamma_{\text{per}}} \in L^p_{\text{per},x}(\Gamma) \) where \( 1 \leq p \leq 3 \). It is easy to deduce that \( \int_{\Gamma} r \cdot \rho_{\gamma_{\text{per}}} (x, r) \, dx \, dr \equiv 0 \) by the uniqueness of density. Hence
\[
\int_{\Gamma} r \cdot (\rho_{\gamma_{\text{per}}} - \mu_{\text{per},\text{sym}}) (x, r) \, dx = -i\nu_{\Gamma} \mathcal{F} \left( \rho_{\gamma_{\text{per}}} - \mu_{\text{per},\text{sym}} \right) (0, 0) \equiv 0.
\]
This condition implies that
\[
\int_{\mathbb{R}^2} \left| \mathcal{F} \left( \rho_{\gamma_{\text{per}}} - \mu_{\text{per},\text{sym}} \right) (0, k) \right|^2 |k| \, dk < +\infty.
\]
Hence we obtain that
\[
\| V_{\text{per},\text{sym}} \|_{L^2_{\text{per},x}(\Gamma)} = \left\| \mathcal{F} (V_{\text{per},\text{sym}}) \right\|_{L^2_{\text{per},x}(\Gamma)} = 4\pi \left\| \mathcal{F} \left( \rho_{\gamma_{\text{per}}} - \mu_{\text{per},\text{sym}} \right) \right\|_{L^2_{\text{per},x}(\Gamma)} < +\infty. \tag{5.13}
\]
Therefore \( V_{\text{per},\text{sym}} \) belongs to \( H^2_{\text{per},x}(\Gamma) \) and is continuous. By an interpolation argument we obtain that \( V_{\text{per},\text{sym}} \in L^p_{\text{per},x}(\Gamma) \) for \( 2 \leq p < +\infty \). Approximating \( V_{\text{per},\text{sym}} \) by functions in \( D^0_{\text{per},x}(\Gamma) \) as it belongs to \( L^\infty_{\text{per},x}(\Gamma) \), we deduce that \( V_{\text{per},\text{sym}} \) tends to 0 when \( |r| \) tends to infinity. On the other hand, the mean-field potential \( V_{\text{per},\text{sym}} \) defines a \(-\Delta\)-bounded operator on \( L^2(\mathbb{R}^3) \) with relative bound zero, hence by the Kato–Rellich theorem (see for example [29, Theorem 9.10]) we know that \( H_{\text{per}} = -\frac{1}{2} \Delta + V_{\text{per},\text{sym}} \) 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 \( H_{\text{per}} \) is \( \mathbb{Z} \)-translation invariant in the \( x \)-direction,
\[
H_{\text{per}} = \mathcal{B} \left( -\frac{1}{2} \Delta + V_{\text{per},\text{sym}} \right) \mathcal{B}, \quad H_{\text{per},\xi} := -\frac{1}{2} \Delta \xi + V_{\text{per},\text{sym}}.
\]
1. Spectral properties of $H_{\text{per}}$.
Note that the decomposed Hamiltonian $H_{\text{per},\xi}$ does not have a compact resolvent as $\Gamma$ 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 (2.6) we have
\[
\left\|V_{\text{per},\text{sym}} (1 - \Delta_\xi)^{-1}\right\|_{L^2_{\text{per},\text{sym}}} \leq \frac{1}{2\pi} \left\|V_{\text{per},\text{sym}}\right\|_{L^\infty_{\text{per},\text{sym}}} \left( \frac{1}{(2\pi n + \xi)^2 + |\mathbf{k}|^2 + 1} \right) \frac{dk}{\mathcal{V}} < C'.
\]
In particular $V_{\text{per},\text{sym}}$ is a compact perturbation of $-\Delta_\xi$, introducing at most countably many discrete spectra below 0 bounded from below by $-\|V_{\text{per},\text{sym}}\|_{L^\infty_{\text{per},\text{sym}}}$. Denote by $\{\lambda_n(\xi)\}_{1 \leq n \leq N_H}$ these (negative) discrete spectra for $N_H \in \mathbb{N}^*$ ($N_H$ can be finite or infinite). Therefore 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 (2.20), a result of [48, Theorem XIII.85] gives the following spectral decomposition:
\[
\sigma_{\text{ess}}(H_{\text{per}}) \supseteq \bigcup_{\xi \in \Gamma^*} \sigma_{\text{ess}}(H_{\text{per},\xi}) = [0, +\infty), \quad \sigma_{\text{disc}}(H_{\text{per}}) \subseteq \bigcup_{\xi \in \Gamma^*} \sigma_{\text{disc}}(H_{\text{per},\xi}) = \bigcup_{1 \leq n \leq N_H} \lambda_n(\xi).
\]
We also obtain from [48, 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 (see for example [48, Section XII.2]) and the approach of Thomas [54, Lemma 1], we know that the eigenvalues $\lambda_n(\xi)$ below 0 are analytical functions of $\xi$ and cannot be constant, hence $\{\xi \in \Gamma^* \mid \lambda \in \sigma_{\text{disc}}(H_{\text{per},\xi})\}$ has trivial Lebesgue measure. Hence,
\[
\sigma(H_{\text{per}}) = \sigma_{\text{ess}}(H_{\text{per}}) = \bigcup_{\xi \in \Gamma^*} \sigma(H_{\text{per},\xi}).
\]
2. Ground state energy is always non-positive.
Let us prove that $N_H = F(0) \geq \int_\Gamma \mu_{\text{per},\text{sym}}$ always holds. Physical meaning of this statement is that the ground state energy of the 1D system in the 3D space is always non-positive when mean-field potential tends to 0 in the $r$-direction. We prove this by showing that if $F(0) < \int_\Gamma \mu_{\text{per},\text{sym}}$, we then can always construct (infinitely many) states belonging to $F_{\Gamma,\text{sym}}$ whose total energy are nearly 0 and are smaller than the ground state energy of the problem (2.19).

For any $\xi \in \Gamma^*$ and $H_{\text{per},\xi}$ defined in (2.20), denote by
\[
\gamma^0_{\text{per}} := \mathbb{1}_{(-\infty, 0)}(H_{\text{per}}), \quad \gamma^0_{\text{per},\xi} := \mathbb{1}_{(-\infty, 0)}(H_{\text{per},\xi}).
\]
Therefore,
\[
N_H = F(0) = \frac{1}{|\Gamma^*|} \int_{\Gamma^*} \operatorname{Tr}_{L^2_{\text{per},\text{sym}}(\Gamma)} (\gamma^0_{\text{per},\xi}) \ dx \xi = \int_{\Gamma^*} \rho_{\gamma^0_{\text{per}}}.
\]
(5.14)
The inequality that $F(0) < \int_\Gamma \mu_{\text{per},\text{sym}}$ implies that
\[
Z_{\text{diff}} := \int_{\Gamma} \mu_{\text{per},\text{sym}} - N_H = \int_{\Gamma} \mu_{\text{per},\text{sym}} - \int_{\Gamma} \rho_{\gamma^0_{\text{per}}} \in \mathbb{N}^+.
\]
(5.15)
The condition (5.15) implies that there are at most finitely many states below 0 ($N_H$ is finite). Consider a smooth function $t(r)$ supported in $\{|r| < 1\}$ and equals to one when $|r| < 1/2$ and such that $\|t\|_{L^2(\mathbb{R}^2)} = 1$. For $n \in \mathbb{N}^*$ and $\xi \in \Gamma^*$, let us define
\[
\psi_{n,\xi}(x, r) := n^{-1} \left( \sum_{k \in \mathbb{Z}} e^{-i(x+k)\xi} \right) t \left( \frac{r - (n^2, n^2)}{n} \right).
\]

It is easy to see that $\psi_{n,\xi}$ belongs to $L^2_{\text{per},x} (\Gamma)$, converging weakly to 0 when $n$ tends to infinity and $\|\psi_{n,\xi}\|_{L^2_{\text{per},x} (\Gamma)} = 1$. Moreover, as $V_{\text{per,sym}}$ tends to 0 in the $r$-direction, hence for any $\epsilon > 0$ there exists an integer $N_\epsilon$ such that $|V_{\text{per,sym}}(\cdot, (n^2, n^2))| \leq \epsilon$ when $n \geq N_\epsilon$. Therefore for $n \geq N_\epsilon$,

$$\left\| H_{\text{per},x} \psi_{n,\xi} \right\|_{L^2_{\text{per},x} (\Gamma)} = \left\| -n^{-1} \Delta_r \left( \frac{(n^2, n^2)}{n} \right) + V_{\text{per,sym}} \psi_{n,\xi} \right\|_{L^2_{\text{per},x} (\Gamma)} \leq \frac{1}{n^2} + \epsilon. \quad (5.16)$$

Remark that $\gamma_{\text{per},\xi} \psi_{n,\xi}$ for any $\xi \neq 0$ is a compact operator, where $P_1(H_{\text{per},x})$ the spectral projector of $H_{\text{per},x}$. There exists an orthonormal basis $\{e_{n,\xi}\}_{n \geq 1}$ of $L^2_{\text{per},x} (\Gamma)$ belonging to $H^1_{\text{per},x} (\Gamma)$ such that $\gamma_{\text{per},\xi} \psi_{n,\xi} e_{\xi,n} = \lambda_n(\xi)e_{\xi,n}$ for $n \leq N_H$, and $\gamma_{\text{per},\xi} \psi_{n,\xi} e_{\xi,n} = 0$ for $n > N_H$. For $N_0 \in \mathbb{N}^+$ to be precised 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

$$\gamma_{N_0,\xi} := \sum_{n=1}^{N_0} \gamma_{\text{per},\xi} e_{\xi,n} \cdot e_{\xi,n} + \sum_{n=N_0+1}^{N_0+Z_{\text{diff}}} \left( 1 - \gamma_{\text{per},\xi} \right) |\psi_{n,\xi} \rangle \langle \psi_{n,\xi}| .$$

**Lemma 5.3.** For any $N_0 \in \mathbb{N}^+$, the state $\gamma_{N_0}$ belongs to the admissible set $\mathcal{F}_{\Gamma,\text{sym}}$.

**Proof.** It is easy to see that $0 \leq \gamma_{N_0} \leq 1$. The density of $\gamma_{N_0}$ can be written as

$$\rho_{\gamma_{N_0}} = \frac{1}{2\pi} \int_{\Gamma^*} \int_{\Gamma} |e_{\xi,n}|^2 d\xi + \frac{1}{2\pi} \sum_{n=N_0+1}^{N_0+Z_{\text{diff}}} \int_{\Gamma^*} |e_{\xi,n}|^2 d\xi .$$

The density $\rho_{\gamma_{N_0}}$ belongs to $L^p_{\text{per}} (\Gamma)$ for $1 \leq p \leq 3$ as $\{e_{\xi,n}\}_{n \geq 1}$ and $\{\psi_{n,\xi}\}_{n \geq 1}$ belong to $H^1_{\text{per},x} (\Gamma)$. Besides, in view of (5.14)

$$\int_{\Gamma} \rho_{\gamma_{N_0}} = \frac{1}{2\pi} \int_{\Gamma^*} \int_{\Gamma} Tr L^2_{\text{per},x} (\Gamma) \left( \gamma_{\text{per},\xi} \right) d\xi + \frac{1}{2\pi} \sum_{n=N_0+1}^{N_0+Z_{\text{diff}}} \int_{\Gamma^*} |e_{\xi,n}|^2 L^2_{\text{per},x} (\Gamma) d\xi$$

$$= N_H + Z_{\text{diff}} = \int_{\Gamma} \mu_{\text{per,sym}} .$$

A simple calculation shows that $|\nabla |\gamma_{N_0}| | \nabla |$ is trace-class on $L^2_{\text{per},x} (\Gamma)$. Hence $\gamma_{N_0}$ belongs to $\mathcal{F}_{\text{per},x}$. Let us show that $\rho_{\gamma_{N_0}} - \mu_{\text{per,sym}}$ belongs to $C^1$. Following similar calculations as (5.7), we only need to prove that $k \mapsto |k|^{-1} \mathcal{F}(\rho_{\gamma_{N_0}} - \mu_{\text{per,sym}})(0, k)$ is square-integrable near $k = 0$ since $\rho_{\gamma_{N_0}} - \mu_{\text{per,sym}}$ belongs to $L^2_{\text{per},x} (\Gamma)$. Remark that $\mathcal{F}(\rho_{\gamma_{N_0}} - \mu_{\text{per,sym}})(0, 0) = \int_{\Gamma} \rho_{\gamma_{N_0}} - \mu_{\text{per,sym}} = 0$ and

$$\left| \partial_k \mathcal{F}(\rho_{\gamma_{N_0}} - \mu_{\text{per,sym}})(0, k) \right| = \left| \int_{\Gamma} \partial_k \left( \rho_{\gamma_{N_0}} - \mu_{\text{per,sym}} \right) (x, r) d\xi d\rho \right|$$

$$\leq \frac{1}{2\pi} \sum_{n=1}^{N_H} \int_{\Gamma^*} \int_{\Gamma} |e_{\xi,n}|^2 (x, r) d\xi d\rho + \frac{1}{2\pi} \sum_{n=N_0+1}^{N_0+Z_{\text{diff}}} \int_{\Gamma^*} \int_{\Gamma} |e_{\xi,n}|^2 (x, r) d\xi d\rho$$

$$+ \int_{\Gamma} |\mu_{\text{per,sym}}(x, r) d\xi < +\infty ,$$

where we have used the fact that the eigenfunctions of $H_{\text{per},x}$ decays exponentially [32, Theorem 3.4] [14, Theorem 1] so that $\int_{\Gamma} |e_{\xi,n}|^2 (x, r) d\xi d\rho < +\infty$ for $1 \leq n \leq N_H$, and the fact that $\{\psi_{n,\xi}\}_{N_0+1 \leq n \leq N_0+Z_{\text{diff}}}$ has compact support in the $r$-direction. Therefore $\mathcal{F}(\rho_{\gamma_{N_0}} - \mu_{\text{per,sym}})(0, k)$ is $C^1$ near $k = 0$. The rest follows similar arguments as in (5.7). The terminates the proof of Lemma 5.3. \qed
Lemma 5.3 implies that we can construct many admissible states in \( \mathcal{F}_{\Gamma, \text{sym}} \) by varying \( N_0 \). Let us show that we can always find \( N_0 \) such that \( \gamma_{N_0} \) has smaller total energy than the ground state energy of (2.19) if \( N_H < \int_{\Gamma^*} \mu_{\text{per, sym}} \).

Given \( \gamma^* \) a minimizer of (2.19), simple expansion around minimal shows that [11] that \( \gamma^* \) also minimizes the functional

\[
\gamma \mapsto \int_{\Gamma^*} \text{Tr}_{L^2_{\text{per, x}}(\Gamma)} \left( H_{\text{per, x}} \gamma \xi \right) d\xi
\]
on \( \mathcal{F}_{\Gamma, \text{sym}} \). Therefore given \( N_0 \in \mathbb{N}^+ \) we have

\[
0 \leq \int_{\Gamma^*} \text{Tr}_{L^2_{\text{per, x}}(\Gamma)} \left( H_{\text{per, x}} \left( \gamma_{N_0} \xi - \overline{\gamma\xi} \right) \right) d\xi = \int_{\Gamma^*} \text{Tr}_{L^2_{\text{per, x}}(\Gamma)} \left( \gamma_{0, \text{per, x}} \left( H_{\text{per, x}} \gamma_{N_0} \xi - \overline{\gamma\xi} \right) \right) d\xi
\]
\[
+ \int_{\Gamma^*} \text{Tr}_{L^2_{\text{per, x}}(\Gamma)} \left( (1 - \gamma_{0, \text{per, x}}) H_{\text{per, x}} \gamma_{N_0} \xi - \overline{\gamma\xi} \right) d\xi
\]
\[
= M + \int_{\Gamma^*} \text{Tr}_{L^2_{\text{per, x}}(\Gamma)} \left( (1 - \gamma_{0, \text{per, x}}) H_{\text{per, x}} \gamma_{N_0} \xi - \overline{\gamma\xi} \right) d\xi - \int_{\Gamma^*} \text{Tr}_{L^2_{\text{per, x}}(\Gamma)} \left( (1 - \gamma_{0, \text{per, x}}) H_{\text{per, x}} \overline{\gamma\xi} \right) d\xi,
\]
where by the fact that \( 0 \leq \overline{\gamma\xi} \leq 1 \) and \( \{ \lambda_n(\cdot) \}_{1 \leq n \leq N_H} < 0 \)

\[
M := \int_{\Gamma^*} \sum_{n=1}^{N_H} \lambda_n(\xi) \left| e_n, \xi \right| \frac{1 - \gamma_{0, \text{per, x}} \overline{\gamma\xi}}{e_n, \xi} \right) d\xi \leq 0. \tag{5.19}
\]

In view of (5.16) and by the Cauchy-Schwarz inequality we deduce that, for \( N_0 \geq N_\epsilon \),

\[
\int_{\Gamma^*} \text{Tr}_{L^2_{\text{per, x}}(\Gamma)} \left( (1 - \gamma_{0, \text{per, x}}) H_{\text{per, x}} \gamma_{N_0} \xi \right) d\xi
\]
\[
= \int_{\Gamma^*} \sum_{n=0}^{N_0+\text{diff}} \sum_{m=1}^{\infty} \left| e_{m, \xi} \right| \left| (1 - \gamma_{0, \text{per, x}}) H_{\text{per, x}} \psi_n, \xi \right| \left| \psi_{m, \xi} \right| d\xi
\]
\[
\leq \int_{\Gamma^*} \sum_{n=0}^{N_0+\text{diff}} \left( \sum_{m=1}^{\infty} \left| e_{m, \xi} \right| \left| (1 - \gamma_{0, \text{per, x}}) H_{\text{per, x}} \psi_{n, \xi} \right| \right)^{1/2} \left( \sum_{m=1}^{\infty} \left| e_{m, \xi} \right| (1 - \gamma_{0, \text{per, x}}) H_{\text{per, x}} \psi_{n, \xi} \right)^{1/2} d\xi
\]
\[
= \int_{\Gamma^*} \sum_{n=0}^{N_0+\text{diff}} \left\| \psi_{n, \xi} \right\|_{L^2_{\text{per, x}}(\Gamma)} \left\| (1 - \gamma_{0, \text{per, x}}) H_{\text{per, x}} \psi_{n, \xi} \right\|_{L^2_{\text{per, x}}(\Gamma)} d\xi
\]
\[
\leq \int_{\Gamma^*} \sum_{n=0}^{N_0+\text{diff}} \left( \frac{1}{\eta^2 + \epsilon} \right) d\xi \leq 2\pi \text{diff} \left( \frac{1}{N_0^2} + \epsilon \right).
\]

On the other hand,

\[
\int_{\Gamma^*} \text{Tr}_{L^2_{\text{per, x}}(\Gamma)} \left( (1 - \gamma_{0, \text{per, x}}) H_{\text{per, x}} \overline{\gamma\xi} \right) = \int_{\Gamma^*} \text{Tr}_{L^2_{\text{per, x}}(\Gamma)} \left( H_{\text{per, x}} \left( 1 - \gamma_{0, \text{per, x}} \overline{\gamma\xi} \right) \right) \geq 0. \tag{5.21}
\]

In view of the inequality (5.19), let us separate the case when \( M \equiv 0 \) and \( M < 0 \). When \( M \equiv 0 \), the inequality (5.19) implies that \( \overline{\gamma\xi} = \gamma_{0, \text{per, x}} \) for almost all \( \xi \in \Gamma^* \). In view of the the inequalities (5.20) and (5.21). The inequality (5.18) imply that,

\[
\forall N_0 \geq N_\epsilon, \quad 0 \leq \int_{\Gamma^*} \text{Tr}_{L^2_{\text{per, x}}(\Gamma)} \left( (1 - \gamma_{0, \text{per, x}}) H_{\text{per, x}} \overline{\gamma\xi} \right) d\xi \leq 2\pi \text{diff} \left( \frac{1}{N_0^2} + \epsilon \right). \tag{5.22}
\]

When \( N_0 \) tends to infinity, it is easy to deduce that \( (1 - \gamma_{0, \text{per, x}}) \overline{\gamma\xi} = 0 \) for almost all \( \xi \in \Gamma^* \). Together with the fact that \( \overline{\gamma\xi} = \gamma_{0, \text{per, x}} \) we deduce that \( \overline{\gamma\xi} = \gamma_{0, \text{per, x}} \) for almost all \( \xi \in \Gamma^* \). In view of (5.14) and (5.15), by the charge neutrality we obtain that

\[
Z_{\text{diff}} = \int_{\Gamma^*} \mu_{\text{per, sym}} - N_H = \int_{\Gamma^*} \rho - N_H = \frac{1}{\Gamma^*} \int_{\Gamma^*} \text{Tr}_{L^2_{\text{per, x}}(\Gamma)} \left( 0 \right) d\xi - N_H \equiv 0.
\]
Hence $\int_{\Gamma} \mu_{\text{per,sym}} = N_H = F(0)$. This also shows that the minimizer of the problem (2.19) equals to $\gamma_{\text{per}}^0$ when $N_H = F(0) = \int_{\Gamma} \mu_{\text{per,sym}}$. When $M < 0$ strictly and $Z_{\text{diff}} \neq 0$, we can always find $\epsilon > 0$ and $N_0 \geq N_e$ such that $2\pi Z_{\text{diff}} \left( \frac{1}{N_0^2} + \epsilon \right) \leq -M/2$. In view of the the inequalities (5.20) and (5.21). The inequality (5.18) imply that,

$$\forall N_0 \geq N_e, \quad 0 \leq \int_{\Gamma^*} \text{Tr} \gamma_{\text{per,}\xi}(\Gamma) \left( (1 - \gamma_{\text{per,}\xi}){H_{\text{per,}\xi}} \right) d\xi \leq M/2 < 0,$$

which is a contradiction. This leads to the conclusion that $F(0) \geq \int_{\Gamma} \mu_{\text{per,sym}}$ and the ground state energy of the 1D system in the 3D space is always non-positive.

**Form of the minimizer.** 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 equals to $\gamma_{\text{per}}^0$ and the Fermi level $\epsilon_F \equiv 0$. 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 $F(\epsilon)$ 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 [11, Theorem 1] by using similar spectral projector decomposition as in (A.2) of [11, Theorem 1], that is, the unique minimizer can be written as

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

where $\gamma_{\text{per,}\xi} := 1_{(-\infty, \epsilon_F]}(H_{\text{per,}\xi})$. The Fermi level $\epsilon_F$ can be considered as the Lagrange multiplier associated with the charge neutrality condition

$$F(\epsilon_F) = \int_{\Gamma} \rho_{\gamma_{\text{per}}} = \int_{\Gamma} \mu_{\text{per,sym}}.$$

**Integrability of the mean-field potential.** Once the unique minimizer is shown to be a spectral projector, we can obtain more information on $V_{\text{per,sym}}$ by using the exponentially decaying property of the eigenfunctions of $H_{\text{per,}\xi}$ in the $r$-direction via the Combe–Thomas estimate [14, Theorem 1]: for almost all $\xi \in \Gamma^*$, there exist positive constant $C(\xi)$ and $\alpha(\xi)$ such that

$$\forall 1 \leq n \leq N_H, \quad |e_{n,\xi}(x, r)| \leq C(\xi) e^{-\alpha(\xi)|r|}.$$

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 $\epsilon_F$ for all $\xi \in \Gamma^*$. Therefore there exist positive constants $C_{\epsilon_F}$ and $\alpha_{\epsilon_F}$ such that

$$0 \leq \rho_{\gamma_{\text{per}}}(x, r) \leq \frac{1}{2\pi} \int_{\Gamma^*} \sum_{n=1}^{N_H} \mathcal{I}(\lambda_n(\xi) \leq \epsilon_F) C^2(\xi) e^{-2\alpha(\xi)|r|} d\xi \leq C_{\epsilon_F} e^{-\alpha_{\epsilon_F}|r|}.$$

Denote by $\rho = \rho_{\gamma_{\text{per}}} - \mu_{\text{per,sym}}$, hence $\int_{\Gamma} \rho = 0$ by the charge neutrality condition and $\int_{\Gamma} r \rho(x, r) dx dr = 0$ by the symmetry condition. Moreover, as $\mu_{\text{per,sym}}$ has compact support in the $r$-direction, it is easy to see that there exist positive constants $C_\rho$, $\alpha_\rho$, such that

$$|\rho(x, r)| \leq C_\rho e^{-\alpha_\rho|r|}.$$  

(5.24)

As $V_{\text{per,sym}}$ belongs to $L^p_{\text{per,}\xi}(\Gamma)$ for $2 \leq p \leq +\infty$ by results following (5.13), let us prove that $V_{\text{per,sym}} \in L^p_{\text{per,}\xi}(\Gamma)$ for $1 < p < 2$ so we can conclude that $V_{\text{per,sym}}$ belongs to $L^p_{\text{per,}\xi}(\Gamma)$ for $1 < p \leq +\infty$. Let us rewrite $V_{\text{per,sym}}$ as

$$V_{\text{per,sym}}(x, r) = (\rho \star_{\Gamma} G)(x, r) = \rho \star_{\Gamma} \tilde{G}(x, r) + T(r),$$

where

$$T(r) = -2 \int_{\mathbb{R}^2} \rho_x(r') \log(|r - r'|) dr'.$$

(5.25)
and $0 \leq \rho_z(r) := \int_{|r| \leq 2} \rho(x, r) \, dx$ such that $|\rho_z(r)| \leq C e^{-\alpha |r|}$ by (5.24). As $\tilde{G}$ belongs to $L^p_{\text{per}, r}(\Gamma)$ for $1 \leq p < 2$, by Young’s convolution inequality we deduce that $\rho \ast \tilde{G}$ belongs to $L^q_{\text{per}, r}(\Gamma)$ for $1 \leq q \leq +\infty$. It remains to prove that $T(r)$ belongs to $L^p(\mathbb{R}^2)$ for $1 < p < 2$. Let us use the partition $\mathbb{R}^2 = \{|r| \leq 2R\} \cup \{|r| > 2R\}$ for the integration domain of $T(r)$. First of all remark that $\log(|r|)$ is $L^p_{\text{loc}}(\mathbb{R}^2)$ for $1 \leq q < +\infty$. Therefore by the Minkowski inequality, there exists a positive constant $C_R$, such that for $p' = p/(p-1) \in (2, +\infty)$:

$$
\left(\int_{|r| \leq 2R} |T(r)|^p \, dr \right)^{1/p} \leq 2 \left(\int_{|r| \leq 2R} \left| \int_{|r'| \leq 3R} \rho_x(r') \log \left(|r - r'| \right) \, dr' \right|^p \, dr \right)^{1/p} + 2C_p \left(\int_{|r| \leq 2R} \left| \int_{|r'| > 3R} e^{-\alpha |r'|} \log \left(|r - r'| \right) \, dr' \right|^p \, dr \right)^{1/p} \leq C_R,
$$

(5.26)

Let us look at the integration domain $\{|r| > 2R\}$. Remark that by the charge neutrality condition and the symmetry condition on $\rho_x$, $\int_{\mathbb{R}^2} \rho_x(r') \log (|r|) \, dr' = 0$, $\int_{\mathbb{R}^2} \rho_x(r') \frac{r'r}{|r|^2} \, dr' = 0$.

Denote by $Q(r, r') := \log(|r - r'|) - \log(|r|) - \frac{r'r}{|r|^2} = \frac{1}{2} \log \left(1 - \frac{2rr'}{|r|^2} + \frac{|r'|^2}{|r|^2} \right) - \frac{r'r}{|r|^2}$, hence $T(r) = -2 \int_{\mathbb{R}^2} \rho_x(r')Q(r, r') \, dr'$. Remark that when $|r| > 2R$ and $|r'| < \varepsilon_R$ for some fixed $\varepsilon_R > 0$ small enough, by the Taylor’s expansion we know that there exists a positive constant $C$ such that $|Q(r, r')| \leq C \frac{|r'|^2}{|r|^2}$. This motivates the partition of $\mathbb{R}^2$ given $|r| > 2R$:

$$
\mathbb{R}^2 = \mathbb{B}_{\varepsilon_R} \cup \mathbb{B}_{\varepsilon_R}^c, \quad \mathbb{B}_{\varepsilon_R} := \left\{ r' \mid \frac{|r'|}{|r|} \leq \varepsilon_R \right\}, \quad \mathbb{B}_{\varepsilon_R}^c := \left\{ r' \mid \frac{|r'|}{|r|} > \varepsilon_R \right\}.
$$

Hence

$$
T(r) = T_1(r) + T_0(r), \quad T_1(r) := \int_{\mathbb{B}_{\varepsilon_R}} \rho_x(r')Q(r, r') \, dr', \quad T_0(r) := \int_{\mathbb{B}_{\varepsilon_R}^c} \rho_x(r')Q(r, r') \, dr'.
$$

Therefore for $1 < p < 2$

$$
\int_{|r| > 2R} |T_1(r)|^p \, dr \leq 2C^p \int_{|r| > 2R} \left| \int_{\mathbb{B}_{\varepsilon_R}} \rho_x(r') \frac{|r'|^2}{|r|^2} \, dr' \right|^p \, dr \leq 2C^p \int_{|r| > 2R} \left| \int_{|r'| \leq \varepsilon_R} e^{-\alpha |r'|} \frac{|r'|^2}{|r|^2} \, dr' \right|^p |r|^{-2p} \, dr < +\infty.
$$

(5.27)
Similarly,
\[ \int_{|r| > 2R} |T_0(r)|^p \, dr \leq C_1 \int_{|r| > 2R} \left( \int_{|r'| > \varepsilon R/|r|} e^{-\alpha_{r'}|r'|} |Q(r, r')| \, dr' \right)^p \, dr \]
\[ \leq C_1 \int_{|r| > 2R} \left( \frac{e^{-\alpha_{r'} \varepsilon R/2} e^{-\alpha_{r'}|r'|/2} |Q(r, r')| \, dr'}{e^{-\alpha_{r'}|r'|}} \right)^p \, dr < +\infty. \]  
(5.28)

In view of the results obtained by (5.26), (5.27) and (5.28) we conclude that \( T(r) \) belongs to \( L^p(\mathbb{R}^2) \) for \( 1 < p < 2 \). This leads to the conclusion that \( V_{per, sym} \) belongs to \( L^p_{per, x}(\Gamma) \) for \( 1 < p \leq +\infty \).

5.5 Proof of Lemma 5.2

Equality of \( \tilde{\rho}_\gamma \) and \( \overline{\rho}_\gamma \). The proof follows similar ideas as in [10, Lemma 3.5] by considering a test function in \( D_{per, x}(\Gamma) \) and replacing the Fourier transform by the mixed Fourier transform defined in (2.3). Consider a test function \( w \in D_{per, x}(\Gamma) \). The weak convergence of \( \rho_\gamma \rightarrow \overline{\rho}_\gamma \) in \( L^p_{per, x}(\Gamma) \) with \( 1 < p \leq 3 \) implies that
\[ \langle \rho_\gamma - \mu_{per, sym}, w \rangle \rightarrow_{n \rightarrow \infty} \langle \overline{\rho}_\gamma - \mu_{per, sym}, w \rangle. \]

On the other hand,
\[ \langle \rho_\gamma - \mu_{per, sym}, w \rangle = \int_\Gamma (\rho_\gamma - \mu_{per, sym}) \, w = \sum_{n \in \mathbb{Z}^2} \int_\mathbb{R}^2 \mathcal{F} (\rho_\gamma - \mu_{per, sym}) (n, k) \mathcal{F} w(n, k) \, dk \]
\[ = 4\pi \sum_{n \in \mathbb{Z}^2} \frac{\mathcal{F} (\rho_\gamma - \mu_{per, sym}) (n, k) \mathcal{F} f(n, k)}{4\pi^2 n^2 + |k|^2} \, dk, \]
(5.29)

where \( f = -\frac{1}{4\pi} \Delta w \). Note that \( f \) belongs to the Coulomb space \( C_1 \) defined in (2.14) since for all \( n \in \mathbb{Z} \), \( \mathcal{F} f(n, \cdot) \in L^1_{loc}(\mathbb{R}^2) \), and
\[ D_\Gamma(f, f) = 4\pi \sum_{n \in \mathbb{Z}^2} \int_\mathbb{R}^2 \frac{|\mathcal{F} f(n, k)|^2}{|k|^2 + 4\pi^2 n^2} \, dk = \frac{1}{4\pi} \sum_{n \in \mathbb{Z}^2} \int_\mathbb{R}^2 (|k|^2 + 4\pi^2 n^2) \frac{|\mathcal{F} w(n, k)|^2}{|k|^2} \, dk \]
\[ = \frac{1}{4\pi} \sum_{n \in \mathbb{Z}^2} \int_\mathbb{R}^2 \frac{|\mathcal{F} (\nabla w)(n, k)|^2}{|k|^2} \, dk = \frac{1}{4\pi} \int_\Gamma |\nabla w|^2 < +\infty. \]

Therefore in view of (5.29), the convergence of \( D_\Gamma(\rho_\gamma - \mu_{per, sym}, f) \rightarrow_{n \rightarrow \infty} D_\Gamma(\tilde{\rho}_\gamma - \mu_{per, sym}, f) \) implies that
\[ \langle \rho_\gamma - \mu_{per, sym}, w \rangle \rightarrow_{n \rightarrow \infty} \langle \tilde{\rho}_\gamma - \mu_{per, sym}, w \rangle. \]

The uniqueness of limit in the sense of distribution allows us to conclude.

Equality of \( \rho_\gamma \) and \( \overline{\rho}_\gamma \). Let us prove that \( \rho_\gamma = \overline{\rho}_\gamma \) in \( D'_{per, x}(\Gamma) \). The fact that \( \rho_\gamma \rightarrow \overline{\rho}_\gamma \) weakly in \( L^p_{per, x}(\Gamma) \) implies that
\[ \langle \rho_\gamma, w \rangle \rightarrow_{n \rightarrow \infty} \langle \overline{\rho}_\gamma, w \rangle. \]

Therefore it suffices to prove that the operator-valued function \( \xi \mapsto w_{\gamma, \xi} \in L^1(\Gamma^*; \mathcal{S}_1) \) converges in the following sense:
\[ \frac{1}{2\pi} \int_{\Gamma^*} \text{Tr}_{L^2_{per, x}(\Gamma)}(w_{\gamma, \xi}) \, d\xi = \langle \rho_\gamma, w \rangle \rightarrow_{n \rightarrow \infty} \langle \rho_\gamma, w \rangle = \frac{1}{2\pi} \int_{\Gamma^*} \text{Tr}_{L^2_{per, x}(\Gamma)}(w_{\gamma, \xi}) \, d\xi. \]
(5.30)

The weak convergence (5.10) does not guarantee the above convergence since the function \( w \) does not belong to any Schatten class. We prove (5.30) by using the kinetic energy bound (5.8), which implies that the operator-valued function
\[ \xi \mapsto \left| -\frac{1}{2} \Delta_\xi - \kappa \right|^{1/2} \gamma_{n, \xi} = \left( \left| -\frac{1}{2} \Delta_\xi - \kappa \right|^{1/2} \gamma_{n, \xi} \right)^{1/2} \left| -\frac{1}{2} \Delta_\xi - \kappa \right|^{-1/2} \]
is uniformly bounded in $L^1(\Gamma^*; S_1)$ as $\left| -\frac{1}{2} \Delta_\xi - \kappa \right|^{1/2}$ is uniformly bounded with respect to $\xi \in \Gamma^*$. Moreover, the energy bounded (5.8) also implies that $\xi \mapsto \left| -\frac{1}{2} \Delta_\xi - \kappa \right|^{1/2} \sqrt{\gamma_{n, \xi}}$ is uniformly bounded in $L^2(\Gamma^*; S_2)$. 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 $L^2(\Gamma^*; S_2)$ as $0 \leq \gamma_{n, \xi} \leq 1$. Therefore

$$\xi \mapsto \left| -\frac{1}{2} \Delta_\xi - \kappa \right|^{1/2} \gamma_{n, \xi}$$

is uniformly bounded in $L^1(\Gamma^*; S_1) \cap L^2(\Gamma^*; S_2)$, hence in $L^q(\Gamma^*; S_q)$ for $1 \leq q \leq 2$ by interpolation. Therefore up to extraction the following weak convergence holds: for any operator-valued function $\xi \mapsto W_\xi \in L^{q'}(\Gamma^*; S_{q'})$ where $q' = \frac{q}{q-1}$ for $1 < q < 2$,

$$\int_{\Gamma^*} \text{Tr}_{L^2_{per, x}(\Gamma)} \left( W_\xi \left| -\frac{1}{2} \Delta_\xi - \kappa \right|^{1/2} \gamma_{n, \xi} \right) d\xi \xrightarrow{n \to \infty} \int_{\Gamma^*} \text{Tr}_{L^2_{per, x}(\Gamma)} \left( W_\xi \left| -\frac{1}{2} \Delta_\xi - \kappa \right|^{1/2} \gamma_{n, \xi} \right) d\xi. \quad (5.31)$$

On the other hand by the inequality (2.6) we obtain that for any $\xi \in \Gamma^*$,

$$\left\| \left| -\frac{1}{2} \Delta_\xi - \kappa \right|^{1/2} \right\|_{S_{q'}} \leq \frac{1}{(2\pi)^{2/3}} \left( \sum_{n \in \mathbb{Z}} \left( \frac{2}{(2\pi n + \xi)^2 + |r|^2 - 2\kappa r''/r''} \right)^{q'/2} \right)^{1/q'} \left\| u \right\|_{L^{q'}_{per, x}(\Gamma)}.$$ 

Upon choosing for example $q' = 4$, the right hand side of the above quantity is finite. Therefore upon taking $W_\xi = u \left| -\frac{1}{2} \Delta_\xi - \kappa \right|^{-1/2}$ in (5.31) we obtain that

$$\frac{1}{2\pi} \int_{\Gamma^*} \text{Tr}_{L^2_{per, x}(\Gamma)} (u \gamma_{n, \xi}) d\xi \xrightarrow{n \to \infty} \frac{1}{2\pi} \int_{\Gamma^*} \text{Tr}_{L^2_{per, x}(\Gamma)} \left( u \left| -\frac{1}{2} \Delta_\xi - \kappa \right|^{-1/2} \gamma_{n, \xi} \right) d\xi.$$

Hence (5.30) holds. Therefore $\rho_\gamma = \nabla \gamma$ in $D'_{per, x}(\Gamma)$. This terminates the proof of the lemma.

### 5.6 Proof of Lemma 3.1

From the last item of Theorem 2.7 we know that $V_{per, L} \in L^p_{per, x}(\Gamma_L)$ (resp. $V_{per, R} \in L^p_{per, x}(\Gamma_R)$) for $1 < p \leq +\infty$. Remark also that $\partial_\xi (\bar{\chi}^2), \bar{\chi}^2$ are continuous and have support in $[-a_L/2, a_L/2] \times \mathbb{R}^2$. The proof therefore relies on the $L^p$-estimates of $\partial_\xi V_{per, L}$ and $\partial_\xi V_{per, R}$. We treat $\partial_\xi V_{per, L}$, the $L^p$-estimates of $\partial_\xi V_{per, R}$ following similar arguments. First of all in view of the form of the minimizer (5.23), by the Cauchy–Schwarz inequality

$$\partial_\xi \mu_{per, L} = \partial_\xi \left( \frac{1}{2\pi} \int_{\Gamma^*} \sum_{n \geq 1} \mathbb{1}(\Lambda_n(\xi) \leq \epsilon_L) |e_n(\xi, \cdot)|^2 d\xi \right)$$

$$\leq \frac{1}{\pi} \int_{\Gamma^*} \left( \sum_{n \geq 1} \mathbb{1}(\Lambda_n(\xi) \leq \epsilon_L) |\partial_\xi e_n(\xi, \cdot)|^2 \right)^{1/2} \left( \sum_{n \geq 1} \mathbb{1}(\Lambda_n(\xi) \leq \epsilon_L) |e_n(\xi, \cdot)|^2 \right)^{1/2} d\xi$$

$$\leq \frac{1}{\pi} \sqrt{K_{\xi, L} \sqrt{\rho_{per, L}},$$

where $K_{\xi, L}(x) := \int_{\Gamma^*} \sum_{n \geq 1} \mathbb{1}(\Lambda_n(\xi) \leq \epsilon_L) |\partial_\xi e_n(\xi, x)|^2 d\xi$. We also have used the fact that $|\nabla f| \leq |\nabla f|$ for any complex-valued function $f$. In view of the potential decomposition (5.25), the term $T(r)$ does not contribute to the $x$-directional derivative, hence

$$|\partial_\xi V_{per, L}| = |\partial_\xi (\mu_{per, L} - \mu_{per, L})| \leq \left( \frac{1}{2\pi} \sqrt{K_{\xi, L} \sqrt{\rho_{per, L}} + |\partial_\xi \mu_{per, L}|} \right) \left| \nabla \tilde{G}_{a_L} \right|.$$
On the other hand, finite kinetic energy condition (2.10) implies that $K_{\xi,L} \in L^1_{\text{per},x}(\Gamma_L)$. Moreover, we have $\sqrt{\rho_{\text{per},L}}$ belongs to $H^{1}_{\text{per},x}(\Gamma_L)$ hence in $L^s_{\text{per},x}(\Gamma_L)$ for $2 \leq s \leq 6$. Therefore, by the Hölder’s inequality, for $p, m \geq 1$:

$$\int_{\Gamma_L} (K_{\xi,L} \rho_{\text{per},L})^{p/2} \leq \left( \int_{\Gamma_L} K_{\xi,L}^{pm/2} \right)^{1/m} \left( \int_{\Gamma_L} \rho_{\text{per},L}^{pm/(m-1)} \right)^{(m-1)/m},$$

with the condition that $pm = 2$ and $2 \leq pm/(m-1) \leq 6$. This implies that $4/3 \leq m \leq 2$ and $1 \leq p \leq 3/2$. As $\delta_{\rho_{\text{per},L}}$ is in $L^p_{\text{per},x}(\Gamma_L)$ for any $1 \leq p \leq +\infty$ and $G_{\rho_{\text{per},L}} \in L^q_{\text{per},x}(\Gamma_L)$ for $1 \leq q < 2$ by Lemma 2.3, we obtain by the Young’s convolution inequality that $\delta_{\rho_{\text{per},L}}$ behaves like $H^{s}_{\text{per},x}(\Gamma_L)$ for $1 \leq s < 6$. This allows us to conclude the lemma.

### 5.7 Proof of Proposition 3.2

Let us emphasis the fact that the function $\chi$ being translation-invariant in the $r$-direction makes it difficult to control the compactness in the $r$-direction across the junction surface. Our geometry is very different from the cylindrical geometry considered in [31] which automatically provides compactness in the $r$-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 $n\alpha_L$-translation (resp. $n\alpha_R$-translation) are still Weyl sequences of $H_{\text{per},L}$ (resp. $H_{\text{per},R}$) for any $n \in \mathbb{Z}$. This implies that one can construct Weyl sequences of $H_{\chi}$ by properly translating Weyl sequences of $H_{\text{per},L}$ or $H_{\text{per},R}$, as $H_{\chi}$ 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 $H_{\chi}$ is much more difficult, as the supports of Weyl sequences are essentially away from any compact, making it difficult to control their behaviors. One naive approach is to cut-off Weyl sequences of $H_{\chi}$ by the function $\chi$ in order to construct Weyl sequences of $H_{\text{per},L}$ or $H_{\text{per},R}$. However, one quickly remarks that the commutator $[-\Delta, \chi]$ being not compact, it is hard to ensure that the cut-off sequence to be Weyl sequence of $H_{\text{per},L}$. Another naive approach is to use a cut-off function $\chi_c$ which has compact support in the $r$-direction. However as mentioned before, it is also difficult to ensure that the Weyl sequences leave any mass in the support of $\chi_c$ as Weyl sequences essentially have supports away from any compact.

The proof is organized as follows: we first prove that $[0, +\infty) \subset \sigma_{\text{ess}}(H_{\chi})$, as $[0, +\infty)$ belongs to the essential spectrum of $H_{\text{per},L}$ and $H_{\text{per},R}$. The proof relies on an explicit construction of Weyl sequences for any $\lambda > 0$, and the fact that the accumulation points of $\sigma_{\text{ess}}(H_{\chi})$ also belong to $\sigma_{\text{ess}}(H_{\chi})$. We next prove for any $\lambda < 0$ such that $\lambda \in \sigma_{\text{ess}}(H_{\text{per},L}) \cup \sigma_{\text{ess}}(H_{\text{per},R})$, then $\lambda \in \sigma_{\text{ess}}(H_{\chi})$. 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 $[0, +\infty)$. Consider a $C^\infty_c(\mathbb{R})$ function $f(z)$ supported on $[0, 1]$ with $\int_{\mathbb{R}} |f|^2 = 1$, and $g \in C^\infty_c(\mathbb{R}^2)$ 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 $\{\psi_n\}_{n \in \mathbb{N}^\ast}$ defined as follows:

$$\psi_n(x, y, z) := n^{-3/2}e^{\sqrt{\lambda}z} f((z - 2n)/n)g(x/n, y/n).$$

It is easy to see that $\int_{\mathbb{R}^3} |\psi_n|^2 = 1$ for all $n \in \mathbb{N}^\ast$, and $\psi_n$ tends weakly to 0 in $L^2(\mathbb{R}^3)$. On the other hand

$$(H_{\chi} - \lambda) \psi_n(x, y, z) = \left( -n^{-2}f''((z - 2n)/n) - 2i\sqrt{\lambda}n^{-1}f'((z - 2n)/n) \right) n^{-3/2}e^{\sqrt{\lambda}z}g(x/n, y/n)$$

$$- n^{-7/2}e^{\sqrt{\lambda}z} f((z - 2n)/n) (\Delta g) (x/n, y/n) + V_{\chi} \psi_n(x, y, z).$$

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Recall also that by the results of Theorem 2.7, there exists for any \( \epsilon > 0 \) an integer \( N_\epsilon \) such that \( |V(x, y, 2n)| \leq \epsilon \) when \( n \geq N_\epsilon \). Therefore, for \( n \geq N_\epsilon \), there exists a positive constant \( C \) such that

\[
\left\| (H_\lambda - \lambda) \psi_n \right\|_{L^2(\mathbb{R}^2)} \leq \frac{1}{n^2} \left\| f' \right\|_{L^2(\mathbb{R}^2)} \left\| g \right\|_{L^2(\mathbb{R}^2)} + \frac{2\sqrt{\lambda}}{n} \left\| f' \right\|_{L^2(\mathbb{R}^2)} \left\| g \right\|_{L^2(\mathbb{R}^2)} + \frac{1}{n^2} \left\| f \right\|_{L^2(\mathbb{R}^2)} \left\| \Delta g \right\|_{L^2(\mathbb{R}^2)} \\
+ \left( \frac{1}{n} \int_{\mathbb{R}^2} \left( \int_{2n}^{3n} |V_\lambda(x, y, z)f((z - 2n)/n)|^2 \, dz \right) |g(x/n, y/n)|^2 \, dx \, dy \right)^{1/2} \\
\leq C + \left( \frac{1}{n} \int_{\mathbb{R}^2} \left( \int_{2n}^{3n} |V_\lambda(nx, ny, 2n + nz)f(z)|^2 \, dz \right) |g(x, y)|^2 \, dx \, dy \right)^{1/2} \\
\leq C + \epsilon \left\| f \right\|_{L^2(\mathbb{R}^2)} \left\| g \right\|_{L^2(\mathbb{R}^2)} = \frac{C}{n} + \epsilon.
\]

This shows that \( \{ \psi_n \}_{n \in \mathbb{N}^*} \) is a Weyl sequence of \( H_\lambda \) associated with \( \lambda > 0 \). It is easy to see that \( 0 \) is an accumulation point of \( \sigma_{\text{ess}}(H_\lambda) \), therefore \( \{ 0, +\infty \} \subset \sigma_{\text{ess}}(H_\lambda) \).

The union of \( \sigma_{\text{ess}}(H_{\text{per}, L}) \cup \sigma_{\text{ess}}(H_{\text{per}, R}) \) is included in \( \sigma_{\text{ess}}(H_\lambda) \). Without loss of generality we prove that when \( \lambda_L < 0 \) belongs to \( \sigma_{\text{ess}}(H_{\text{per}, L}) \) then \( \lambda_L \in \sigma_{\text{ess}}(H_\lambda) \). Consider a Weyl sequence \( \{ w_n \}_{n \in \mathbb{N}^*} \) of \( H_{\text{per}, L} \) associated with \( \lambda_L \), let us construct a Weyl sequence of \( H_\lambda \) from \( \{ w_n \}_{n \in \mathbb{N}^*} \). Given \( n \in \mathbb{N}^* \) and for \( \epsilon > 0 \) small enough, there exists a sequence \( \{ v_k \}_{k \in \mathbb{N}^*} \) belonging to \( C^\infty_c(\mathbb{R}^3) \) and a \( K_\lambda \in \mathbb{N}^* \) such that for any \( k(n) \geq K_\lambda \),

\[
\left\| v_k(n),n - w_n \right\|_{H^2(\mathbb{R}^3)} \leq \epsilon.
\]

It is easy to see that \( v_k(n),n \) tends weakly to 0 in \( L^2(\mathbb{R}^3) \) as \( n \to \infty \). Since \( v_k(n),n \) has compact support, for any fixed \( n \in \mathbb{N}^* \), when \( m \in \mathbb{N}^* \) tends to \( +\infty \),

\[
\text{supp} \left( \tau_{a_L, m} v_k(n),n \right) \cap \left( [-a_L/2, +\infty) \times \mathbb{R}^2 \right) \cup \mathcal{B}_n = \emptyset,
\]

where \( \mathcal{B}_n \) denotes the ball of radius \( n \) centered at 0 in \( \mathbb{R}^3 \). Remark that the above equation also ensures that \( \tau_{a_L, m} v_k(n),n \) tends weakly to 0 in \( L^2(\mathbb{R}^3) \) when \( m \to +\infty \) for \( n \) fixed. In view of (5.32) and (5.33), let \( \tilde{w}_\ell := \tau_{a_L, m} v_k(n,\ell) \) for \( \ell \in \mathbb{N}^* \) such that when \( \ell \) tends to \( +\infty \), \( m(\ell) \to +\infty \) and \( n(\ell) \to +\infty \). Remark that by (5.33) for \( \ell \) large enough

\[
\text{supp} \left( \tilde{w}_\ell \right) \cap \left( [-a_L/2, +\infty) \times \mathbb{R}^2 \right) \cup \mathcal{B}_n = \emptyset.
\]

This implies that \( \tilde{w}_\ell \) tends weakly to 0 in \( L^2(\mathbb{R}^3) \) when \( \ell \to +\infty \). Moreover, in view of (5.32) and by the definition of the Weyl sequence

\[
\left\| (H_\lambda - \lambda) \tilde{w}_\ell \right\|_{L^2} = \left\| (H_\lambda - \lambda) \tau_{a_L, m} v_k(n,\ell) \right\|_{L^2} = \left\| (H_{\text{per}, L} - \lambda) \tau_{a_L, m} v_k(n,\ell) \right\|_{L^2} \\
\leq \left\| \tau_{a_L, m} (H_{\text{per}, L} - \lambda) (v_k(n,\ell) - w_n) \right\|_{L^2} + \left\| \tau_{a_L, m} (H_{\text{per}, L} - \lambda) w_n \right\|_{L^2} \\
\leq (1 + \left\| V_{\text{per}} \right\|_{L^\infty} - \lambda) \left\| v_k(n,\ell) - w_n \right\|_{H^2} + \left\| (H_{\text{per}, L} - \lambda) w_n \right\|_{L^2} \quad \ell \to +\infty \to 0.
\]

Therefore the sequence \( \tilde{w}_\ell / \| \tilde{w}_\ell \|_{L^2} \) is a Weyl sequence of \( H_\lambda \) associated with \( \lambda_L \). This leads to the conclusion that

\[
\sigma_{\text{ess}}(H_{\text{per}, L}) \cup \sigma_{\text{ess}}(H_{\text{per}, R}) \subseteq \sigma_{\text{ess}}(H_\lambda).
\]

The essential spectrum \( \sigma_{\text{ess}}(H_\lambda) \) is included in \( \sigma_{\text{ess}}(H_{\text{per}, L}) \cup \sigma_{\text{ess}}(H_{\text{per}, R}) \). We prove that for \( \lambda < 0 \) and \( \lambda \in \sigma_{\text{ess}}(H_\lambda) \) then \( \lambda \in \sigma_{\text{ess}}(H_{\text{per}, L}) \cup \sigma_{\text{ess}}(H_{\text{per}, R}) \). The main technique is to use spreading sequences (Zhislin sequences) [22, Definition 5.12], which is a Weyl sequence 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 \( \hat{O} \) on \( L^2(\mathbb{R}^3) \) associated with \( \lambda \) if the following properties are satisfied:
• for all $n$, $\psi_n$ is in the domain of the operator $O$ and $\|\psi_n\|_{L^2(\mathbb{R}^3)} = 1$;
• for any bounded set $G \subset \mathbb{R}^3$, $\text{supp}(\psi_n) \cap G = \emptyset$ for $n$ sufficiently large. As a consequence, $\psi_n \to 0$ weakly in $L^2(\mathbb{R}^3)$;
• $\lim_{n \to +\infty} \|(O-\lambda) \psi_n\|_{L^2(\mathbb{R}^3)} = 0$.

As $V_{\text{per},L}$ and $V_{\text{per},R}$ are continuous and in $L^\infty(\mathbb{R}^3)$ by Theorem 2.7, it holds by [22, Theorem 5.14] that

$$\sigma_{\text{ess}}(H_\theta) = \{ \lambda \in \mathbb{C} | \text{there is a spreading sequence for } H_\theta \text{ and } \lambda \}$$

for $H_\theta$ being $H_\chi$, $H_{\text{per},L}$ or $H_{\text{per},R}$. Given $\varepsilon > 0$, results of Theorem 2.7 also imply that there exists a constant $R_\varepsilon$ such that

$$\max \left( \|V_{\text{per},L} \mathbb{1}_{|r| > R_\varepsilon} \|_{L^\infty(\mathbb{R}^3)}, \|V_{\text{per},R} \mathbb{1}_{|r| > R_\varepsilon} \|_{L^\infty(\mathbb{R}^3)} \right) < \varepsilon. \quad (5.35)$$

Consider a spreading sequence $\{\phi_n\}_{n \in \mathbb{N}^*}$ of $H_\chi$ associated with $\lambda \leq 0$. For all $n \in \mathbb{N}^*$, it is easy to see that either $\|\phi_n\|_{L^2((0, +\infty) \times \mathbb{R}^2)} \geq 1/2$ or $\|\phi_n\|_{L^2((-\infty, 0) \times \mathbb{R}^2)} \geq 1/2$. Without loss of generality, in the following we assume 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 cut-off function $\rho$ which has non-trivial mass on $(0, +\infty) \times \mathbb{R}^2$ and the derivatives of which decay rapidly:

$$\rho(x) := \frac{\int_{-\infty}^{x} \eta(y) dy}{\|\eta\|_{L^1(\mathbb{R})}},$$

where $\eta$ satisfies the following one-dimensional Yukawa equation

$$-\eta'' - \lambda \eta = e^{-2\sqrt{-\lambda}|x|}. \quad (5.36)$$

The following lemma summarizes some properties of the cut-off function $\rho$, which will be useful in the construction of Weyl sequence.

**Lemma 5.4.** It holds that $0 \leq \rho \leq 1$ and $\lim_{n \to +\infty} \|\rho\phi_n\|_{L^2} \neq 0$. Moreover,

$$\|\rho'' \phi_n + 2\rho' \partial_x \phi_n\|_{L^2} \to 0, \quad \|\rho \chi^2 (V_{\text{per},L} - V_{\text{per},R})\|_{L^2(\mathbb{R}^3)}. \quad (5.37)$$

We postpone the proof of this lemma to Section 5.8. 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 $\lambda$. First of all the sequence $\{w_n\}_{n \in \mathbb{N}^*}$ is well defined at least for large $n$ as $\lim_{n \to +\infty} \|\rho \phi_n\|_{L^2} \neq 0$. It is also easy to see that $\|w_n\|_{L^2} = 1$ for all $n \in \mathbb{N}^*$. For any bounded set $G \subset \mathbb{R}^3$, it holds $\text{supp}(w_n) \cap G = \emptyset$ for $n$ sufficiently large as $\{\phi_n\}_{n \in \mathbb{N}^*}$ is a spreading sequence. Note that

$$\left( H_{\text{per},R} - \lambda \right) w_n = \frac{1}{\|\rho \phi_n\|_{L^2}} (\rho (H_\chi - \lambda) \phi_n + A \phi_n), \quad (5.38)$$

where $A := -\frac{1}{2} \rho'' - \rho' \partial_x + \rho \chi^2 (V_{\text{per},L} - V_{\text{per},R})$. As $\lim_{n \to +\infty} \|\rho (H_\chi - \lambda) \phi_n\|_{L^2} = 0$ by the definition of the spreading sequence, hence $\lim_{n \to +\infty} \| \left( H_\chi - \lambda \right) \phi_n \|_{L^2} = 0$. It therefore suffices to prove that (possibly up to extraction) $\lim_{n \to +\infty} \| A \phi_n \|_{L^2} = 0$. By the Kato–Seiler–Simon inequality (5.1) we obtain that

$$\left\| (1 - \Delta)^{-1} \rho \chi^2 (V_{\text{per},L} - V_{\text{per},R}) \right\|_{L^2(\mathbb{R}^3)} \leq \frac{1}{2 \sqrt{\pi}} \left\| \rho \chi^2 (V_{\text{per},L} - V_{\text{per},R}) \right\|_{L^2(\mathbb{R}^3)},$$

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, 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 $f \in L^2(\mathbb{R}^3)$,

$$(v, f)_{L^2} = \lim_{n \to +\infty} \left( \rho \chi^2 (V_{\text{per},L} - V_{\text{per},R}) w_n, f \right)_{L^2} = \lim_{n \to +\infty} \left( w_n, \rho \chi^2 (V_{\text{per},L} - V_{\text{per},R}) f \right)_{L^2} = 0,$$
where we have used the fact that \( w_n \to 0 \) and \( \rho \chi^2 (V_{\text{per},L} - V_{\text{per},R}) \in L^2(\mathbb{R}^3) \) so \( \rho \chi^2 (V_{\text{per},L} - V_{\text{per},R}) f \in L^2(\mathbb{R}^3) \). Therefore by uniqueness of weakly convergence, \( \rho \chi^2 (V_{\text{per},L} - V_{\text{per},R}) w_n \) converges strongly to \( v \equiv 0 \). Together with (5.37) we conclude that \( \lim_{n \to \infty} ||A\phi_n||_{L^2} = 0 \). Therefore in view of (5.38), it holds

\[
\lim_{n \to \infty} \| (H_{\text{per},R} - \lambda) w_n \|_{L^2} = 0.
\]

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 \( H_\chi \) 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 \( H_\chi \) has non-trivial mass on \(( -\infty, 0 ] \times \mathbb{R}^2 \) or \(( 0, +\infty ) \times \mathbb{R}^2 \). This allows us to conclude that

\[
\sigma_{\text{ess}}(H_\chi) \subseteq \sigma_{\text{ess}}(H_{\text{per},L}) \cup \sigma_{\text{ess}}(H_{\text{per},R}).
\]

By gathering the result of (5.34) and (5.39) 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, this is independent of the function \( \chi \in \mathcal{X} \).

### 5.8 Proof of Lemma 5.4

The solution of the one-dimensional Yukawa equation (5.36) is

\[
0 < \eta(x) = \int_{\mathbb{R}} \frac{e^{-\sqrt{-\lambda} |x-y|}}{\sqrt{-\lambda}} e^{-2\sqrt{-\lambda} |y|} dy \leq \int_{\mathbb{R}} \frac{e^{-\sqrt{-\lambda} |x+y|}}{\sqrt{-\lambda}} dy \leq \frac{2}{-\lambda} e^{-\sqrt{-\lambda} |x|}.
\]

This implies that \( \eta \) belongs to \( L^p(\mathbb{R}) \) for \( 1 \leq p \leq +\infty \). As \( \eta > 0 \) is integrable, the cut-off function \( \rho(x) = \frac{\int_{\mathbb{R}} \eta(y) dy}{\| \eta \|_{L^1(\mathbb{R})}} \) 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 \( \rho(x) \geq 1/2 \) for \( x \geq 0 \), it is easy to see that \( \lim_{n \to \infty} \| \rho \phi_n \|_{L^2(\mathbb{R}^3)} \neq 0 \). Let us prove that \( \| \rho'' \phi_n + 2\rho' \partial_x \phi_n \|_{L^2} \to 0 \) as \( n \to \infty \). In view of (5.40),

\[
|\eta'(x)| = \left| \int_{-\infty}^{+\infty} e^{-\sqrt{-\lambda} |x-y| - 2\sqrt{-\lambda} |y|} (1_{x<y} - 1_{x>y}) dy \right| \leq 2 \int_{-\infty}^{+\infty} e^{-\sqrt{-\lambda} |x-y| - 2\sqrt{-\lambda} |y|} dy = 2\sqrt{-\lambda} \eta(x) \leq \frac{4}{\sqrt{-\lambda}} e^{-\sqrt{-\lambda} |x|}.
\]

Combining the above inequality with (5.40) we obtain that

\[
\| \rho'' \phi_n + 2\rho' \partial_x \phi_n \|_{L^2(\mathbb{R}^3)}^2 = \| \eta'' \phi_n + 2\eta' \partial_x \phi_n \|_{L^2(\mathbb{R}^3)}^2 \leq \frac{2}{\| \eta \|_{L^1(\mathbb{R})}^2} \int_{\mathbb{R}^3} \left( (\eta')^2 |\phi_n|^2 + 4\eta^2 |\partial_x \phi_n|^2 \right) \leq \frac{32}{\lambda |\eta|^2} \int_{\mathbb{R}^3} e^{-2\sqrt{-\lambda} |y|} |\phi_n|^2 + \frac{8|\eta\|_{L^\infty}^2}{\| \eta \|_{L^2}^2} \int_{\mathbb{R}^3} \eta |\partial_x \phi_n|^2.
\]

It suffices to prove that each integral of the last term of (5.41) tends to 0 when \( n \to \infty \). Remark that the integrands of these terms appear when one does an explicit calculation of \( (\eta (-\Delta - \lambda) \phi_n, (-\Delta - \lambda) \phi_n)_{L^2(\mathbb{R}^3)} \). Let us therefore first prove that

\[
(\eta (-\Delta - \lambda) \phi_n, (-\Delta - \lambda) \phi_n)_{L^2(\mathbb{R}^3)} \to 0 \text{ as } n \to \infty.
\]

For this purpose, we prove that \( \| \eta (-\Delta - \lambda) \phi_n \|_{L^2(\mathbb{R}^3)} \to 0 \) strongly and \( (-\Delta - \lambda) \phi_n \to 0 \) weakly in \( L^2(\mathbb{R}^3) \). In view of (5.40), for any \( \varepsilon > 0 \) there exists \( x_\varepsilon > 0 \) such that when \( |x| > x_\varepsilon \), \( 0 \leq \eta(x) \leq \varepsilon \). Together with (5.35) and the fact that \( \{\phi_n\}_{n \in \mathbb{N}} \) is a spreading sequence, it holds

\[
\| \eta_{\chi} \phi_n \|_{L^2(\mathbb{R}^3)}^2 = \int_{\mathbb{R} \times \{|x| > R_n\}} |\eta_{\chi} \phi_n|^2 + \int_{\mathbb{R} \times \{|x| \leq R_n\}} |\eta_{\chi} \phi_n|^2 + \int_{\mathbb{R} \times \{|x| \leq R_n\}} |\eta_{\chi} \phi_n|^2 \leq \varepsilon \| \eta \|_{L^\infty(\mathbb{R})}^2 + \| \eta_{\chi} \|_{L^\infty(\mathbb{R})}^2 \| \phi_n \|_{L^2(\mathbb{R}^3)}^2 + \varepsilon \| \eta_{\chi} \|_{L^\infty(\mathbb{R})}^2 \| \phi_n \|_{L^2(\mathbb{R}^3)}^2 \to 0 \text{ as } n \to \infty.
\]
The above convergence allows us to conclude that
\[
\|\eta (\Delta - \lambda) \phi_n\|_{L^2(\mathbb{R}^3)} \leq \|\eta (H_\chi - \lambda) \phi_n\|_{L^2(\mathbb{R}^3)} + \|\eta V_\chi \phi_n\|_{L^2(\mathbb{R}^3)} \to 0. \tag{5.42}
\]
Moreover, \(\phi_n \in H^2(\mathbb{R}^3) \hookrightarrow L^\infty(\mathbb{R}^3)\) with continuous embedding for all \(n \in \mathbb{N}^+\). Approximating \(\phi_n\) by \(C_c^\infty(\mathbb{R}^3)\) functions we deduce that \(\lim_{|x| \to \infty} |\phi_n(x)| = 0\). Furthermore, remark that for any \(\psi \in C_c^\infty(\mathbb{R}^3)\) it holds
\[
((-\Delta - \lambda)\phi_n, \psi)_{L^2(\mathbb{R}^3)} = (\phi_n, (\Delta - \lambda)\psi)_{L^2(\mathbb{R}^3)} \to 0, \quad n \to \infty,
\]
which implies the weak convergence \((-\Delta - \lambda)\phi_n \to 0\) by the density of \(C_c^\infty(\mathbb{R}^3)\) in \(L^2(\mathbb{R}^3)\). This leads to, together with the strong convergence (5.42) and the integration by parts,
\[
(\eta (-\Delta - \lambda) \phi_n, (-\Delta - \lambda) \phi_n)_{L^2(\mathbb{R}^3)} = \int_{\mathbb{R}^3} \eta |\Delta \phi_n|^2 + \eta \lambda \Delta \phi_n \phi_n + \lambda \eta \Delta \phi_n \phi_n + \eta \lambda^2 |\phi_n|^2
\]
\[
= \int_{\mathbb{R}^3} \eta |\Delta \phi_n|^2 - 2 \eta \lambda |\nabla \phi_n|^2 + \lambda^2 \eta |\phi_n|^2
\]
\[
= \int_{\mathbb{R}^3} \eta |\Delta \phi_n|^2 + (\lambda \eta \lambda + \lambda^2 \eta) |\phi_n|^2 - 2 \eta \lambda |\nabla \phi_n|^2 \to 0, \quad n \to \infty.
\]
In view of (5.36) we have \((\lambda \eta \lambda + \lambda^2 \eta) = -\lambda e^{-2\sqrt{-\lambda}|x|} > 0\), hence the integrand of the above integral is positive. This implies that
\[
\int_{\mathbb{R}^3} e^{-2\sqrt{-\lambda}|x|} |\phi_n|^2 \to 0, \quad \int_{\mathbb{R}^3} \eta |\nabla \phi_n|^2 \to 0. \tag{5.43}
\]
In view of (5.41) and (5.43), we deduce that
\[
0 \leq \|\rho' \phi_n + 2 \rho' \hat{\nabla} x \phi_n\|_{L^2(\mathbb{R}^3)}^2 \leq -\frac{32}{\lambda |\eta|^2} \int_{\mathbb{R}^3} e^{-2\sqrt{-\lambda}|x|} |\phi_n|^2 + \frac{8 |\eta|^2}{|\eta|^2} \int_{\mathbb{R}^3} \eta |\hat{\nabla} x \phi_n|^2 \to 0, \quad n \to \infty.
\]
Finally let us prove that \(\rho \chi^2 (V_{\text{per},L} - V_{\text{per},R}) \in L^2(\mathbb{R}^3)\). By definition of \(\chi\), the function \(\rho \chi^2\) has support in \((-\infty, a_R/2]\) and is equal to \(\rho(x)\) when \(x \in (-\infty, -aL/2)\). Remark also that (5.40) implies that
\[
\forall x < 0, \quad \rho(x) \leq \frac{1}{|\eta|^2} \int_{-\infty}^{x} \frac{2}{\lambda} e^{-\sqrt{-\lambda}|y|} dy \leq \frac{2}{(-\lambda)^{1/2} |\eta|^2} e^{\sqrt{-\lambda} x}.
\]
Hence, as \(V_{\text{per},L} \in L^s_{\text{per,x}} (\Gamma_L)\) for \(1 < s \leq \infty\) by Theorem 2.7,
\[
\int_{\mathbb{R}^3} (\rho \chi^2 V_{\text{per},L})^2 = \int_{(-\infty, -aL/2) \times \mathbb{R}^2} (\rho V_{\text{per},L})^2 + \int_{[-aL/2, aR/2] \times \mathbb{R}^2} (\rho \chi^2 V_{\text{per},L})^2
\]
\[
\leq 4 |\rho V_{\text{per},L}|^2 \chi L^2(\mathbb{R}^2) \int_{-\infty}^{x} e^{-2\sqrt{-\lambda}a_L n} + \int_{[-aL/2, aR/2] \times \mathbb{R}^2} V_{\text{per},L}^2 \leq +\infty.
\]
This implies that \(\rho \chi^2 V_{\text{per},L} \in L^2(\mathbb{R}^3)\). Similar arguments show that \(\rho \chi^2 V_{\text{per},R} \in L^2(\mathbb{R}^3)\). This concludes the proof of the lemma.

### 5.9 Proof of Proposition 3.3

In view of Proposition 3.2, consider a contour \(\mathcal{C}\) in the complex plan enclosing the spectra of \(H_\chi\) below the Fermi level \(\epsilon_F\) without intersecting them, crossing the real axis at \(c < \inf \{ -\| V_{\text{per},L} \|_{L^\infty}, -\| V_{\text{per},R} \|_{L^\infty} \}\) (See Fig. 7). This is possible even if \(\epsilon_F\) is an eigenvalue: by the definition of discrete spectra one can always slightly move the curve \(\mathcal{C}\) below \(\epsilon_F\) in order not to intersect at \(\epsilon_F\) but still contain all the spectra of \(H_\chi\) below \(\epsilon_F\). Let us first introduce the following estimates, which are useful to characterizer the decay property of the densities of operators.
Lemma 5.5 (Combes-Thomas estimate [35, 14, 21, 35]). Consider $H := -\frac{1}{2} \Delta + V$ with $V \in L^\infty(\mathbb{R}^3)$. Then, for any $(\alpha, \beta) \in \mathbb{Z}^3 \times \mathbb{Z}^3$, 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 $\zeta \notin \sigma(H)$,

$$
\left\| w_\alpha(\zeta - H)^{-p} w_\beta \right\|_{\mathcal{E}_\varepsilon} \leq C(p, q) \left(1 + \frac{1}{\theta(\zeta, V)}\right)^{4p} e^{-\varepsilon \theta(\zeta, V)|\alpha - \beta|},
$$

(5.44)

where $\theta(\zeta, V) = \frac{\text{dist}(\zeta, \sigma(H))}{|\zeta| + \|V\|_{L^\infty} + 1}$.

With $V_\chi$ belonging to $L^\infty(\mathbb{R}^3)$, the following lemma is a direct adaption of [11, Lemma 1]:

Lemma 5.6. Under Assumption 1, for all $\zeta \in \mathcal{C}$ there exist two positive constants $c_1, c_2$ such that

$$
c_1 (1 - \Delta) \leq |H_\chi - \zeta| \leq c_2 (1 - \Delta)
$$

as operators on $L^2(\mathbb{R}^3)$. In particular

$$
\left\| H_\chi - \zeta \right\|^{1/2} (1 - \Delta)^{-1/2} \leq \sqrt{c_2}, \quad \left\| H_\chi - \zeta \right\|^{-1/2} (1 - \Delta)^{1/2} \leq \frac{1}{\sqrt{c_1}}.
$$

Moreover, $(H_\chi - \zeta)(1 - \Delta)^{-1}$ and its inverse are bounded operators.

Let us turn to the proof of Proposition 3.3. First of all let us show that $\gamma_\chi$ is locally trace class. Let $\varrho \in C_{c,0}(\mathbb{R}^3)$. Remark that $\gamma_\chi$ is a spectral projector. In view of Lemma 5.6, by Cauchy’s resolvent formula and the Kato–Seiler–Simon inequality (5.1), there exists a positive constant $C_\chi$ such that

$$
\| \varrho \gamma_\chi \|_{\mathcal{E}_1} = \left\| \varrho \gamma_\chi \gamma_\chi \varrho \right\|_{\mathcal{E}_1} \leq \left\| \varrho \gamma_\chi \right\|_{\mathcal{E}_2}^2 = \left\| \varrho \int \frac{1}{2\pi} \frac{1}{\zeta - H_\chi} d\zeta \right\|_{\mathcal{E}_2} \leq C_\chi \left\| \varrho \frac{1}{1 - \Delta} \right\|_{\mathcal{E}_2}^2 \leq \frac{C_\chi}{4\pi} \| \varrho \|_{L^2(\mathbb{R}^3)}^2.
$$

(5.44)

This implies that $\gamma_\chi$ is locally trace class so that its density $\rho_\chi$ 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 $\rho_\chi$. We construct a density operator $\gamma_d$ whose density $\rho_d$ is equal to $\chi^2 \rho_{\text{per}, L} + (1 - \chi^2) \rho_{\text{per}, R} - \rho_\chi$:

$$
\gamma_d := \gamma_{d,1} + \gamma_{d,2}, \quad \gamma_{d,1} := \chi (\gamma_{\text{per}, L} - \gamma_\chi) \chi, \quad \gamma_{d,2} := \sqrt{1 - \chi^2} (\gamma_{\text{per}, R} - \gamma_\chi) \sqrt{1 - \chi^2}.
$$

(5.45)

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 $\rho_d$ is in $L^p(\mathbb{R}^3)$ for $1 < p \leq 2$. The proof of $\rho_d \in L^p(\mathbb{R}^3)$ relies on duality arguments: denote 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 $|\text{Tr}_{L^2(\mathbb{R}^3)}(\gamma_d W)| \leq \frac{K_q}{q}$.
By symmetry of the problem, let us prove 

\[ K_q \| W \|_{L^q}. \]

By Cauchy’s formula we have

\[
\begin{align*}
\gamma_{d,1} &= \frac{1}{2\pi i} \oint_{\mathcal{E}} \chi \left( \frac{1}{z - H_{\text{per},L}} - \frac{1}{z - H_{\chi}} \right) \chi \, dz, \\
\gamma_{d,2} &= \frac{1}{2\pi i} \oint_{\mathcal{E}} \sqrt{1 - \chi^2} \left( \frac{1}{z - H_{\text{per},R}} - \frac{1}{z - H_{\chi}} \right) \sqrt{1 - \chi^2} \, dz.
\end{align*}
\]

(5.46)

By symmetry of the problem, let us prove \( \exists K_q^1 > 0 \) such that

\[ \| \text{Tr}_{L^2(\mathbb{R}^3)}(\gamma_{d,1} W) \| \leq K_q^1 \| W \|_{L^q}. \]

Similar arguments can be used 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 \( V_d \chi \) belongs to \( L^r(\mathbb{R}^3) \) for \( 1 < r \leq +\infty \) by Theorem 2.7.

For any \( \zeta \in \mathcal{E} \), 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 \( \chi \) being translation-invariant in the \( r \)-direction, hence is not in any \( L^p \) space in \( \mathbb{R}^3 \), which prevents us using the standard techniques such as calculating the commutator \( [-\Delta, \chi] \). By writing \( 1 = \gamma_{\text{per},L} + \gamma_{\text{per},L}^1 \) and \( 1 = \gamma_{\chi} + \gamma_{\chi}^1 \), the following decomposition holds

\[
D(\zeta) = \chi \frac{\gamma_{\text{per},L}}{\zeta - H_{\text{per},L}} V_d \frac{1}{\zeta - H_{\chi}} \chi + \chi \frac{\gamma_{\text{per},L}^1}{\zeta - H_{\text{per},L}} V_d \frac{\gamma_{\chi}^1}{\zeta - H_{\chi}} \chi + \chi \frac{\gamma_{\text{per},L}}{\zeta - H_{\text{per},L}} V_d \frac{\gamma_{\chi}^1}{\zeta - H_{\chi}} \chi.
\]

(5.47)

By the residue theorem we know that

\[
\int_{\mathcal{E}} \chi \frac{\gamma_{\text{per},L}}{\zeta - H_{\text{per},L}} V_d \frac{\gamma_{\chi}^1}{\zeta - H_{\chi}} \chi \, d\zeta = 0.
\]

(5.48)

**Lemma 5.7.** Consider a self-adjoint operator \( H = -\Delta + V \) defined on \( L^2(\mathbb{R}^3) \) with domain \( H^2(\mathbb{R}^3) \) and \( V \in L^\infty(\mathbb{R}^3) \). For \( E \in \mathbb{R} \setminus \sigma(H) \) denote by \( \gamma = 1_{(-\infty, E]}(H) \). Then for any \( a, b \in \mathbb{R} \), the operator \( (1 - \Delta)^a \gamma (1 - \Delta)^b \) is bounded. Moreover, if \( \gamma \in \mathcal{S}_k \) for some \( k \geq 1 \), then \( (1 - \Delta)^a \gamma (1 - \Delta)^b \in \mathcal{S}_k \).

**Proof.** Similar as in Lemma 5.6 we can deduce 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 \( \lambda_0 := -\| V \|_{L^\infty} - \delta \). We have \( \lambda_0 \notin \sigma(H) \). By writing \( \gamma = \gamma^2 \), there exists a positive constant \( C \) such that

\[
\left\| (1 - \Delta)^a \gamma (1 - \Delta)^b \right\|_{\mathcal{S}_k} \leq C \left\| (\lambda_0 - H)^a \gamma (\lambda_0 - H)^b \right\|_{\mathcal{S}_k} = C \left\| \gamma^2 (\lambda_0 - H)^{a+b} \right\|_{\mathcal{S}_k} < +\infty,
\]

as \( \gamma \in \mathcal{S}_k \) and \( (\lambda_0 - H)^{a+b} \) is a bounded operator. The proof of the boundedness in operator norm follows the same lines.

**Lemma 5.8.** For any \( 1 < p \leq 2 \), there exist positive constants \( d_{p,1} \) and \( d_{p,2} \), such that for all \( \zeta \in \mathcal{E} \),

\[
\left\| \chi \frac{\gamma_{\text{per},L}}{\zeta - H_{\text{per},L}} V_d \right\|_{\mathcal{S}_p} \leq d_{p,1} \| V_d \chi \|_{L^p(\mathbb{R}^3)}, \quad \left\| V_d \frac{\gamma_{\chi}^1}{\zeta - H_{\chi}} \chi \right\|_{\mathcal{S}_p} \leq d_{p,2} \| V_d \chi \|_{L^p(\mathbb{R}^3)}.
\]

(5.49)
Proof. Let us prove the statement for $\chi \gamma\per.L(\zeta - H\per.L)^{-1} V_d$, the proof of the bound of $V_d\gamma\per.L(\zeta - H\per.L)^{-1}$ follows similar arguments. Fix $R > 0$. Recall that $\mathcal{B}_R$ is the ball in $\mathbb{R}^3$ centered at 0 with radius $R$. Denote by $\varphi_R$ the characteristic function of $\mathcal{B}_R$. For any $R > 0$, by the Kato–Seiler–Simon inequality (5.1) and the boundedness of $(1 - \Delta)(\zeta - H\per.L)^{-1}$ it is easy to see that $\varphi_R(\zeta - H\per.L)^{-1}$ and $(\zeta - H\per.L)^{-1} V_d \varphi_R$ belong to $\mathcal{S}_2$. The operator $\gamma\per.L(\zeta - H\per.L)^m$ is a bounded for any $m \in \mathbb{R}$ in view of Lemma 5.8. Therefore

$$\varphi_R \left( \chi \gamma\per.L(\zeta - H\per.L)^{-1} V_d \right) \varphi_R = \left( \varphi_R \chi \gamma\per.L(\zeta - H\per.L)^{-1} V_d \right) \in \mathcal{S}_1.$$ 

For $1 < p \leq 2$, by the cyclicity of the trace the following estimate holds

$$\left\| \varphi_R \chi \gamma\per.L(\zeta - H\per.L)^{-1} V_d \right\|_{\mathcal{S}_1} = \left\| \varphi_R \chi \gamma\per.L(\zeta - H\per.L)^{-1} V_d \right\|_{\mathcal{S}_1} \leq \left\| \varphi_R \chi \gamma\per.L(\zeta - H\per.L)^{-1} V_d \right\|_{\mathcal{S}_1}$$

By taking the limit $R \to +\infty$ we obtain the desired results.

Consider $W \in L^p(\mathbb{R}^3)$ for $q = \frac{p}{1+\frac{1}{2}} \in [2, +\infty)$. In view of (5.47), (5.48) and (5.49), by similar manipulation as in the proof of Lemma 5.8 we obtain that

$$\left\| \gamma_d W \right\|_{\mathcal{S}_1} = \frac{1}{2\pi} \left\| \int_\mathbb{S} D(\zeta) \, d\zeta W \right\|_{\mathcal{S}_1} \leq C \left\| \gamma_d W \right\|_{\mathcal{S}_1} \leq \left\| K_1^1 \right\|_{L^p(\mathbb{R}^3)}$$

where we have used the Kato–Seiler–Simon inequality (5.1) as well as the fact that $\left\| \gamma \right\|_{L^\infty} = 1$. Similar estimates hold for $\gamma_d$. Therefore we can conclude that $\rho_d = \chi^2 \rho\per.L + (1 - \chi^2) \rho\per.R - \rho_\gamma$ 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 $\chi^2 \rho\per.L + (1 - \chi^2) \rho\per.R - \rho_\gamma$ decays exponentially fast in the $x$-direction. Note that there exists $N_L \in \mathbb{N}$ such that $N_L \leq -a_L/2 < N_L + 1$. Denote by $\mathbb{H}_{a_L} := [-a_L/2, +\infty) \times \mathbb{R}^2$, we prove the exponential decay when $\supp (w_\alpha) \subset \mathbb{R}^3 \setminus \mathbb{H}_{a_L}$. 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

$$I_{\mathbb{H}_{a_L}} \left( \sum_{\beta_x > N_L} \sum_{\beta_y, \beta_z \in \mathbb{Z}} w_\beta \right) = I_{\mathbb{H}_{a_L}} V_d, \quad I_{\mathbb{H}_{a_L}} V_d = V_d, \quad \alpha_x < -\frac{a_L}{2} < N_L + 1 \leq \beta_x + 1.$$
The above relations imply, together with (5.49) and the Combes–Thomas estimate (5.44), that there exist a positive constants $C_1$ and $t_1$ such that for $1 < p \leq 2$ and $q = \frac{p}{p+1} \geq 2$:

\[
\|w_\alpha \gamma_d w_\alpha\|_{\mathcal{E}_1} = \left\| w_\alpha \gamma_{d,1} w_\alpha \right\|_{\mathcal{E}_1} \leq \left\| \frac{1}{2\pi} \int_c \left( w_\alpha \chi \frac{\gamma_{\text{per},L}}{\zeta - \bar{H}_{\text{per},L}} V_d \chi w_\alpha + w_\alpha \chi \frac{\gamma_{\text{per},L}}{\zeta - \bar{H}_{\text{per},L}} V_d \chi w_\alpha \right) d\zeta \right\|_{\mathcal{E}_1}
\]

\[
\leq \frac{1}{2\pi} \int_c \left( \| w_\alpha \chi \frac{\gamma_{\text{per},L}}{\zeta - \bar{H}_{\text{per},L}} V_d \chi w_\alpha \|_{\mathcal{E}_p} + \| w_\alpha \chi \frac{\gamma_{\text{per},L}}{\zeta - \bar{H}_{\text{per},L}} V_d \chi w_\alpha \|_{\mathcal{E}_q} \right) d\zeta
\]

\[
\leq \frac{\| V_d \chi \|_{L^p(\mathbb{R}^3)}}{2\pi} \int_c \left( \sum_{\beta, \gamma} + \sum_{\beta, \gamma} \right) \left( \| w_{\beta} \chi \frac{\gamma_{\text{per},L}}{\zeta - \bar{H}_{\text{per},L}} w_{\alpha} \|_{\mathcal{E}_q} + \| w_{\alpha} \chi \frac{\gamma_{\text{per},L}}{\zeta - \bar{H}_{\text{per},L}} w_{\beta} \|_{\mathcal{E}_q} \right) d\zeta
\]

\[
\leq K \sum_{\beta, \gamma} \sum_{\beta, \gamma} \| w_{\beta} \chi \|_{\mathcal{E}_p} \| w_{\alpha} \chi \|_{\mathcal{E}_p} \| w_{\beta} \chi \|_{\mathcal{E}_p} \| w_{\alpha} \chi \|_{\mathcal{E}_p} \leq C e^{-t_1|z|}.
\]

The last step relies on the uniform distance of $\zeta \in \mathcal{E}$ to $\sigma(H_\lambda)$ and $\sigma(H_{\text{per},L})$. Similar estimates hold when the support of $w_\alpha$ is in $[a R^2, +\infty) \times \mathbb{R}^2$. There exist therefore positive constants $C$ and $t$ such that $\|w_\alpha \gamma_d w_\alpha\|_{\mathcal{E}_1} = \int_{\mathbb{R}^3} |w_\alpha \rho_d w_\alpha| \leq C e^{-t|z|}$, which concludes the proof.

5.10 Proof of Proposition 3.4

The following statements assert that the problem (3.13) is well-defined: a duality argument shows that densities of operators in $Q_\chi$ are well defined. The energy functional (3.14) is well defined and is bounded from below. The proofs are direct adaptations of [11, Proposition 1, Lemma 2, Corollary 1 and Corollary 2].

1. For any $Q \in Q_\chi$, it holds that $QW \in \mathcal{E}_1^{1,5}$ for $W = W_1 + W_2 \in \mathcal{C} + L^2(\mathbb{R}^3)$. Moreover, there exists a positive constant $C_\chi$ such that:

\[
|\text{Tr}_{\gamma_\chi}(QW)| \leq C_\chi \|Q\|_{\mathcal{Q}_\chi}(\|W_1\|_{\mathcal{C}} + \|W_2\|_{L^2(\mathbb{R}^3)}).
\]

Moreover, there exists a uniquely defined function $\rho_Q \in \mathcal{C} \cap L^2(\mathbb{R}^3)$ such that:

\[
\forall W = W_1 + W_2 \in \mathcal{C} + L^2(\mathbb{R}^3), \quad \text{Tr}_{\gamma_\chi}(QW) = \langle \rho_Q, W_1 \rangle_{C',C} + \int_{\mathbb{R}^3} \rho_Q W_2.
\]

The linear map $Q \in Q_\chi \mapsto \rho_Q \in \mathcal{C} \cap L^2(\mathbb{R}^3)$ is continuous:

\[
\|\rho_Q\|_{C} + \|\rho_Q\|_{L^2(\mathbb{R}^3)} \leq C_\chi \|Q\|_{\mathcal{Q}_\chi}.
\]

Moreover, if $Q \in \mathcal{E}_1 \subset \mathcal{E}_1^{1,5}$, then $\rho_Q(x) = Q(x, x)$ where $Q(x, x)$ the integral kernel of $Q$.

2. For any $\kappa \in (\Sigma_{N,\chi}, \epsilon_F)$ and any state $Q \in K_\chi$, the following inequality holds:

\[
0 \leq c_1 \text{Tr}((1 - \Delta)^{1/2}(Q^+ - Q^-))(1 - \Delta)^{1/2} \leq \text{Tr}_{\gamma_\chi}(H_\lambda Q) - \kappa \text{Tr}_{\gamma_\chi}(Q) \leq c_2 \text{Tr}((1 - \Delta)^{1/2}(Q^+ - Q^-))(1 - \Delta)^{1/2},
\]

where $c_1$ and $c_2$ are the same constants as in Lemma 5.6.
3. Assume that Assumption 1 holds. There are positive constants \( \tilde{d}_1, \tilde{d}_2 \), such that
\[
E_\chi(Q) - \kappa \text{Tr}_{\gamma_\chi}(Q) \geq \tilde{d}_1 \left( \|Q^+\|_{\mathfrak{L}_1} + \|Q^-\|_{\mathfrak{L}_1} + \|\nabla Q^+\|_{\mathfrak{L}_1} + \|\nabla Q^-\|_{\mathfrak{L}_1} \right) \\
+ \tilde{d}_2 \left( \|\nabla Q\|^2_{\mathfrak{L}_2} + \|Q\|^2_{\mathfrak{L}_2} \right) - \frac{1}{2} D(\nu_\chi, \nu_\chi).
\]

Hence \( E_\chi(\cdot) - \kappa \text{Tr}_{\gamma_\chi}(\cdot) \) is bounded from below and coercive on \( K_\chi \).

The existence and the form of the minimizers are direct adaptations of [11, Theorem 2].

### 5.11 Proof of Theorem 3.5

We prove this theorem by taking two arbitrary cut-off functions \( \chi_1, \chi_2 \) belonging to \( \mathcal{X} \), and prove that \( \rho_{\chi_1} + \rho_{\chi_2} = \rho_{\chi_2} + \rho_{\chi_1} \). For \( i = 1, 2 \), consider reference states with Hamiltonian \( H_{\chi_i} \) associated with cut-off functions \( \chi_i \). Denote by \( \gamma_{\chi_i} \), the spectral projector of \( H_{\chi_i} \), below \( \epsilon_F \) and by \( Q_{\chi_i} \), the solutions of (3.15) associated with \( \chi_i \). Consider a test state
\[
\tilde{Q} := \gamma_{\chi_1} - Q_{\chi_1} - \gamma_{\chi_2}.
\]

We show that \( \tilde{Q} \) is a minimizer of the problem (3.13) associated with the cut-off function \( \chi_2 \), so that \( \rho_{\tilde{Q}} = \rho_{Q_{\chi_2}} \) by the uniqueness of density. Note that Assumption 1 and Proposition 3.2 guarantee that there is a common spectral gap for \( H_{\chi_1} \) 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
\[
K_{\chi_2} := \{ Q \in Q_{\chi_2} \mid -\gamma_{\chi_2} \leq Q \leq 1 - \gamma_{\chi_2} \},
\]

hence is an admissible state for the minimization problem (3.13) associated with \( \chi_2 \). We next show that \( \tilde{Q} \) is a minimizer.

The test state \( \tilde{Q} \in K_{\chi_2} \). We begin by proving that \( \tilde{Q} \) is in \( Q_{\chi_2} \). Let us prove that \( \tilde{Q} \) is \( \gamma_{\chi_2} \)-trace class. The following lemma will be useful.

**Lemma 5.9.** The difference of the spectral projectors \( \gamma_{\chi_1} - \gamma_{\chi_2} \) belongs to \( \mathfrak{S}_1^{\gamma_{\chi_2}} \). Moreover,
\[
|\nabla| (\gamma_{\chi_1} - \gamma_{\chi_2}) \in \mathfrak{S}_2, \quad (\gamma_{\chi_1} - \gamma_{\chi_2}) |\nabla| \in \mathfrak{S}_2.
\]

**Proof.** By Cauchy’s resolvent formula and the Kato–Seiler–Simon inequality (5.1)
\[
\|\gamma_{\chi_1} - \gamma_{\chi_2}\|_{\mathfrak{L}_2} = \left\| \frac{1}{2\pi i} \int (\zeta - H_{\chi_1})^{-1} (\chi_1^2 - \chi_2^2) (V_{\text{per},L} - V_{\text{per},R}) (\zeta - H_{\chi_2})^{-1} d\zeta \right\|_{\mathfrak{L}_2} \\
\leq C \left\| (1 - \Delta)^{-1} (\chi_1^2 - \chi_2^2) (V_{\text{per},L} - V_{\text{per},R}) \right\|_{\mathfrak{L}_2} < +\infty.
\]

As \( |\nabla| (\zeta - H_{\chi_1})^{-1} \) is uniformly bounded with respect to \( \zeta \in \mathcal{C} \) following the results of Lemma 5.6. By similar calculations as in (5.53),
\[
\left\| |\nabla| (\gamma_{\chi_1} - \gamma_{\chi_2}) \right\|_{\mathfrak{L}_2} \leq c_1 \left\| (\chi_1^2 - \chi_2^2) (V_{\text{per},L} - V_{\text{per},R}) (1 - \Delta)^{-1} \right\|_{\mathfrak{L}_2} < +\infty,
\]
\[
\left\| (\gamma_{\chi_1} - \gamma_{\chi_2}) |\nabla| \right\|_{\mathfrak{L}_2} \leq c_2 \left\| (1 - \Delta)^{-1} (\chi_1^2 - \chi_2^2) (V_{\text{per},L} - V_{\text{per},R}) \right\|_{\mathfrak{L}_2} < +\infty.
\]

As \( \gamma_{\chi_1} \) is a bounded operator, in view of (5.53) and by writing \( \gamma_{\chi_1} = \gamma_{\chi_2} - \gamma_{\chi_2} \) and using the fact that \( \gamma_{\chi_1} + \gamma_{\chi_2} = 1 \),
\[
\gamma_{\chi_2}^\perp (\gamma_{\chi_1} - \gamma_{\chi_2}) \gamma_{\chi_2} = \gamma_{\chi_2}^\perp \gamma_{\chi_2} (\gamma_{\chi_1} - \gamma_{\chi_2}) \gamma_{\chi_2} (\gamma_{\chi_1} - \gamma_{\chi_2}) \gamma_{\chi_2} = \gamma_{\chi_2}^\perp \gamma_{\chi_2}^\perp \gamma_{\chi_2} = \gamma_{\chi_2}^\perp (\gamma_{\chi_1} - \gamma_{\chi_2})^2 \in \mathfrak{S}_1.
\]

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Together with (5.53) we conclude that $\gamma_{x_1} - \gamma_{x_2}$ belongs to $\mathcal{S}^{\gamma_{x_2}}$ by definition.

The following lemma is a consequence of [23, Lemma 1] and the fact that $\gamma_{x_1} - \gamma_{x_2} \in \mathcal{S}_2$:

**Lemma 5.10.** Any self-adjoint operator $A$ is in $\mathcal{S}^{\gamma_{x_1}}$ if and only if $A$ is in $\mathcal{S}^{\gamma_{x_2}}$. Moreover $\text{Tr}(\gamma_{x_1} A) = \text{Tr}(\gamma_{x_2} A)$.

The fact that $Q_{x_1} \in \mathcal{S}^{\gamma_{x_1}}$ implies that $|\nabla|Q_{x_1} \in \mathcal{S}_2$, and $Q_{x_1} \in \mathcal{S}^{\gamma_{x_2}}$ by Lemma 5.10. In view of this and Lemma 5.9 we know that $\hat{Q} = \gamma_{x_1} - \gamma_{x_2} + Q_{x_1}$ belongs to $\mathcal{S}^{\gamma_{x_2}}$. The inequality (5.54) implies that $\|\nabla|\hat{Q} = |\nabla|Q_{x_1} + |\nabla|(\gamma_{x_1} - \gamma_{x_2}) \in \mathcal{S}_2$. It remains to prove that $|\nabla|\gamma_{x_2} \hat{Q} \gamma_{x_2} |\nabla| \in \mathcal{S}_1$ and $|\nabla|\gamma_{x_2} \gamma_{x_2} \gamma_{x_2} |\nabla| \in \mathcal{S}_1$. In view of (5.51) we have

$$
|\nabla|\gamma_{x_2} \hat{Q} \gamma_{x_2} |\nabla| = |\nabla|\gamma_{x_2} Q_{x_1} \gamma_{x_2} |\nabla| + |\nabla|\gamma_{x_2} (\gamma_{x_1} - \gamma_{x_2}) \gamma_{x_2} |\nabla|,
$$

$$
|\nabla|\gamma_{x_2} \hat{Q} \gamma_{x_2} |\nabla| = |\nabla|\gamma_{x_2} Q_{x_1} \gamma_{x_2} |\nabla| + |\nabla|\gamma_{x_2} (\gamma_{x_1} - \gamma_{x_2}) \gamma_{x_2} |\nabla|.
$$

We estimate (5.56) term by term. By Lemma 5.7 we know that $\|\nabla|\gamma_{x_1} \| \leq \|\nabla|((1 - \Delta)^{-1})(1 - \Delta)\gamma_{x_1} \| < \infty$. Moreover, by writing $\gamma_{x_2} = 1 - \gamma_{x_1} + \gamma_{x_1} - \gamma_{x_2}$ and $\gamma_{x_2} = \gamma_{x_1} + \gamma_{x_2} - \gamma_{x_1}$, in view of (5.54),

$$
\left\| \nabla|\gamma_{x_2} Q_{x_1} \gamma_{x_2} \nabla| \right\|_{\mathcal{S}_1} \leq \left\| \nabla|\gamma_{x_1} Q_{x_1} \gamma_{x_1} \nabla| \right\|_{\mathcal{S}_1} + \left\| \nabla|Q_{x_1} (\gamma_{x_1} - \gamma_{x_2}) \nabla| \right\|_{\mathcal{S}_1} + \left\| \nabla|\gamma_{x_1} Q_{x_1} (\gamma_{x_1} - \gamma_{x_2}) \nabla| \right\|_{\mathcal{S}_1}
$$

$$
+ \left\| \nabla|(\gamma_{x_1} - \gamma_{x_2}) Q_{x_1} \gamma_{x_2} \nabla| \right\|_{\mathcal{S}_1} + \left\| \nabla|(\gamma_{x_1} - \gamma_{x_2}) Q_{x_1} \gamma_{x_2} \nabla| \right\|_{\mathcal{S}_1}
$$

and similarly

$$
\left\| \nabla|\gamma_{x_2} Q_{x_1} \gamma_{x_2} \nabla| \right\|_{\mathcal{S}_1} = \left\| \nabla|\gamma_{x_1} Q_{x_1} \gamma_{x_1} \nabla| \right\|_{\mathcal{S}_1} + \left\| \nabla|Q_{x_1} (\gamma_{x_1} - \gamma_{x_2}) \nabla| \right\|_{\mathcal{S}_1} + \left\| \nabla|\gamma_{x_1} Q_{x_1} (\gamma_{x_1} - \gamma_{x_2}) \nabla| \right\|_{\mathcal{S}_1}
$$

$$
+ \left\| \nabla|(\gamma_{x_1} - \gamma_{x_2}) Q_{x_1} \gamma_{x_2} \nabla| \right\|_{\mathcal{S}_1} + \left\| \nabla|(\gamma_{x_1} - \gamma_{x_2}) Q_{x_1} \gamma_{x_2} \nabla| \right\|_{\mathcal{S}_1}
$$

From (5.55) we know that

$$
\left\| \nabla|\gamma_{x_2} (\gamma_{x_1} - \gamma_{x_2}) \gamma_{x_2} \nabla| \right\|_{\mathcal{S}_1} = \left\| \nabla|\gamma_{x_1} Q_{x_1} (\gamma_{x_1} - \gamma_{x_2}) \nabla| \right\|_{\mathcal{S}_1} \leq \left\| \nabla|(\gamma_{x_1} - \gamma_{x_2}) \nabla| \right\|_{\mathcal{S}_1} \leq \left\| \nabla|(\gamma_{x_1} - \gamma_{x_2}) \nabla| \right\|_{\mathcal{S}_1} \leq \left\| \nabla|(\gamma_{x_1} - \gamma_{x_2}) \nabla| \right\|_{\mathcal{S}_1} < \infty,
$$

$$
\left\| \nabla|\gamma_{x_2} (\gamma_{x_1} - \gamma_{x_2}) \gamma_{x_2} \nabla| \right\|_{\mathcal{S}_1} = \left\| \nabla|\gamma_{x_1} Q_{x_1} (\gamma_{x_1} - \gamma_{x_2}) \nabla| \right\|_{\mathcal{S}_1} \leq \left\| \nabla|(\gamma_{x_1} - \gamma_{x_2}) \nabla| \right\|_{\mathcal{S}_1} \leq \left\| \nabla|(\gamma_{x_1} - \gamma_{x_2}) \nabla| \right\|_{\mathcal{S}_1} < \infty.
$$

This shows that $|\nabla|\gamma_{x_2} \hat{Q} |\nabla| \in \mathcal{S}_1$ and $|\nabla|\gamma_{x_2} \gamma_{x_2} |\nabla| \in \mathcal{S}_1$. This allows us to conclude that $\hat{Q} \in Q_{x_2}$. On the other hand, it is easy to see that $-\gamma_{x_2} \leq \hat{Q} = \gamma_{x_1} + Q_{x_1} - \gamma_{x_2} \leq 1 - \gamma_{x_2}$, which shows that $\hat{Q}$ belongs to the convex set $K_{x_2}$. 

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The state $\tilde{Q}$ is a minimizer. We now prove that $\tilde{Q}$ is a minimizer of the problem (3.13) associated with the cut-off function $\chi_2$. As $Q \in K_{\chi_2}$, the fact that $Q_{\chi_2}$ is a minimizer implies that

$$\mathcal{E}_{\chi_2} (\tilde{Q}) - \kappa \text{Tr}_{\gamma_{\chi_2}} (\tilde{Q}) \geq \mathcal{E}_{\chi_2} (Q_{\chi_2}) - \kappa \text{Tr}_{\gamma_{\chi_2}} (Q_{\chi_2}).$$

(5.57)

Define $\Theta := \tilde{Q} - Q_{\chi_2} = Q_{\chi_1} - Q_{\chi_2} + \gamma_{\chi_1} - \gamma_{\chi_2}$. The inequality (5.57) can therefore also be written as

$$\mathcal{E}_{\chi_2} (\Theta) - \kappa \text{Tr}_{\gamma_{\chi_2}} (\Theta) + D (\rho_\Theta, \rho_{Q_{\chi_2}}) \geq 0.$$  

(5.58)

It is easy to see that $-1 \leq \Theta \leq 1$ and $\Theta$ belongs to $Q_{\chi_2}$ (not necessarily in the convex $K_{\chi_2}$), which also implies that the density $\rho_\Theta$ of $\Theta$ is well defined and belongs to the Coulomb space $C$ by proofs of Proposition 3.4. Therefore (5.58) is well defined. Introduce another state by exchanging the indices $1 \leftrightarrow 2$ of $\tilde{Q}$:

$$\tilde{Q}_1 := \gamma_{\chi_2} + Q_{\chi_2} - \gamma_{\chi_1}.$$  

We can also deduce that $\tilde{Q}_1 \in K_{\chi_1}$ by similar arguments that we have used to prove $\tilde{Q} \in K_{\chi_2}$. By definition we get $Q_{\chi_1} = \Theta + \tilde{Q}_1$. Since $Q_{\chi_1}$ minimizes the problem (3.13) associated with $\chi_1$ and $\tilde{Q}_1 \in K_{\chi_1}$,

$$\mathcal{E}_{\chi_1} (\tilde{Q}_1) - \kappa \text{Tr}_{\gamma_{\chi_1}} (\tilde{Q}_1) \geq \mathcal{E}_{\chi_1} (\Theta + \tilde{Q}_1) - \kappa \text{Tr}_{\gamma_{\chi_1}} (\Theta + \tilde{Q}_1).$$

The above equation can be simplified as

$$\mathcal{E}_{\chi_1} (\Theta) - \kappa \text{Tr}_{\gamma_{\chi_1}} (\Theta) + D (\rho_\Theta, \rho_{\tilde{Q}_1}) \leq 0.$$  

(5.59)

Let us show that the left hand sides of (5.58) and (5.59) are equal. First of all as $\Theta$ belongs to $Q_{\chi_2}$, we know that $\text{Tr}_{\gamma_{\chi_2}} (\Theta) = \text{Tr}_{\gamma_{\chi_1}} (\Theta)$ by Lemma 5.10. Remark also that $\rho_{\tilde{Q}_1} = \rho_{\chi_2} - \rho_{\chi_1} + \rho_{Q_{\chi_2}}$, by Lemma 5.10

$$\mathcal{E}_{\chi_2} (\Theta) - \kappa \text{Tr}_{\gamma_{\chi_2}} (\Theta) + D (\rho_\Theta, \rho_{Q_{\chi_2}}) - \mathcal{E}_{\chi_1} (\Theta) \geq \mathcal{E}_{\chi_1} (\Theta) - \kappa \text{Tr}_{\gamma_{\chi_1}} (\Theta) + D (\rho_\Theta, \rho_{\tilde{Q}_1}).$$

(5.60)

We show that (5.60) is equal to zero by first showing that $(V_{\chi_2} - V_{\chi_1}) \Theta \in \mathcal{S}_1 \subset \mathcal{S}_1^{\chi_2}$. We start by showing that $(1 - \Delta)Q_{\chi_1} \in \mathcal{S}_2$. By Cauchy’s resolvent formula,

$$Q_{\chi_1} = \frac{1}{2\pi i} \int \left( \frac{1}{z-H_{\gamma_{\chi_1}}} - \frac{1}{z-H_{\chi_1}} \right) d\zeta = Q_{1,i} + Q_{2,i} + Q_{3,i},$$

where

$$Q_{1,i} = \frac{1}{2\pi i} \int \frac{1}{z-H_{\chi_1}} \left( (\rho_{\chi_1} - \nu_{\chi_1}) \ast \frac{1}{|\cdot|} \right) \frac{1}{z-H_{\chi_1}} d\zeta,$$

$$Q_{2,i} = \frac{1}{2\pi i} \int \frac{1}{z-H_{\chi_1}} \left( (\rho_{\chi_1} - \nu_{\chi_1}) \ast \frac{1}{|\cdot|} \right) \frac{1}{z-H_{\chi_1}} \left( (\rho_{\chi_1} - \nu_{\chi_1}) \ast \frac{1}{|\cdot|} \right) \frac{1}{z-H_{\chi_1}} d\zeta,$$

$$Q_{3,i} = \frac{1}{2\pi i} \int \frac{1}{z-H_{\gamma_{\chi_1}}} \left( (\rho_{\chi_1} - \nu_{\chi_1}) \ast \frac{1}{|\cdot|} \right) \frac{1}{z-H_{\chi_1}} \left( (\rho_{\chi_1} - \nu_{\chi_1}) \ast \frac{1}{|\cdot|} \right) \frac{1}{z-H_{\chi_1}} d\zeta.$$
Following arguments similar to the ones used in the proof of [11, Proposition 2], we can conclude that \((1 - \Delta)Q_x, \in \mathcal{S}_2\). Remark that \(V_{x_1} - V_{x_2} = (\chi_1^2 - \chi_2^2)(V_{\text{per},L} - V_{\text{per},R}) \in L^\infty(\mathbb{R}^3) \cap L^2(\mathbb{R}^3)\). By definition of \(\Theta\), by the Kato–Seiler–Simon inequality and use similar calculations as in (5.53)

\[
\left\| (V_{x_1} - V_{x_2}) \Theta \right\|_{\mathcal{S}_1} \leq \left\| (V_{x_1} - V_{x_2}) (1 - \Delta)^{-1} \right\|_{\mathcal{S}_2} \left( \left\| (1 - \Delta)(Q_{x_1} - Q_{x_2}) \right\|_{\mathcal{S}_2} + \left\| (1 - \Delta)(\gamma_{x_1} - \gamma_{x_2}) \right\|_{\mathcal{S}_2} \right) 
\]

\[
\leq \frac{1}{2\sqrt{\pi}} \left\| V_{x_1} - V_{x_2} \right\|_{L^2} \left( \left\| (1 - \Delta)(Q_{x_1} - Q_{x_2}) \right\|_{\mathcal{S}_2} + \left\| (\chi_1^2 - \chi_2^2)(V_{\text{per},L} - V_{\text{per},R})(1 - \Delta)^{-1} \right\|_{\mathcal{S}_2} \right) < \infty ,
\]

which proves that \((V_{x_1} - V_{x_2}) \Theta \) belongs to \(\mathcal{S}_1\) hence

\[
\text{Tr}_{\gamma_{x_2}} ((V_{x_2} - V_{x_1}) \Theta) = \text{Tr} ((V_{x_2} - V_{x_1}) \Theta).
\]

On the other hand, by the definition of \(V_{x_i}\) in (3.10) and \(\nu_i\) in (3.11) for \(i = 1, 2\), we deduce that

\[
\text{Tr} ((V_{x_2} - V_{x_1}) \Theta) = D (\rho_{\Theta}, (\rho_{x_2} - \mu_{x_2}) - (\rho_{x_1} - \mu_{x_1})) = D (\rho_{\Theta}, \rho_{x_2} - \rho_{x_1} + \nu_{x_2} - \nu_{x_1}).
\]

The above equation implies that (5.60) equals to 0. Hence in view of (5.58) and (5.59)

\[
\mathcal{E}_{x_2} (\Theta) - \kappa \text{Tr}_{\gamma_{x_2}} (\Theta) + D (\rho_{\Theta}, \rho_{Q_{x_2}}) = \mathcal{E}_{x_1} (\Theta) - \kappa \text{Tr}_{\gamma_{x_1}} (\Theta) + D (\rho_{\Theta}, \rho_{Q_1}) \equiv 0.
\]

In view of (5.57) we conclude that

\[
\mathcal{E}_{x_2} (\tilde{Q}) - \kappa \text{Tr}_{\gamma_{x_2}} (\tilde{Q}) \equiv \mathcal{E}_{x_2} (Q_{x_2}) - \kappa \text{Tr}_{\gamma_{x_2}} (Q_{x_2}).
\]

Therefore \(\tilde{Q}\) is a minimizer of the problem (3.13) associated with the cut-off function \(\chi_2\). From Theorem 3.4 we know that \(\rho_{\tilde{Q}} \equiv \rho_{Q_{x_2}}\), which is equivalent to that \(\rho_{Q_{x_2}} + \rho_{x_2} = \rho_{x_1} + \rho_{Q_{x_1}}\). By the arbitrariness when choosing \(\chi_1, \chi_2\) we deduce that \(\rho_{\chi} + \rho_{Q_\chi}\) is independent of the cut-off function \(\chi \in \mathcal{X}\).

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