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MEAN-FIELD MODEL FOR THE JUNCTION OF TWO QUASI-1-DIMENSIONAL QUANTUM COULOMB SYSTEMS

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Junctions appear naturally when one studies surface states or transport properties of quasi-1-dimensional materials such as carbon nanotubes, polymers and quantum wires. These materials can be seen as 1-dimensional systems embedded in the 3-dimensional space. We first establish a mean-field description of reduced Hartree–Fock-type for a 1-dimensional periodic system in the 3-dimensional space (a quasi-1-dimensional system), the unit cell of which is unbounded. With mild summability condition, we next show that a quasi-1-dimensional quantum system in its ground state can be described by a mean-field Hamiltonian. We also prove that the Fermi level of this system is always negative. A junction system is described by two different infinitely extended quasi-1-dimensional systems occupying separate half-spaces in three dimensions, where coulombic electron-electron interactions are taken into account and without any assumption on the commensurability of the periods. We prove the existence of the ground state for a junction system, the ground state is a spectral projector of a mean-field Hamiltonian, and the ground state density is unique.

1. Introduction

1A. ***Physical background and mathematical models.*** Atomic junctions of quasi-1-dimensional systems appear for instance when studying the surface states of 1-dimensional crystals [Aerts 1960; Shockley 1939], quantum thermal transport in nanostructures [Wang et al. 2008], and p-n junctions [Baugher et al. 2014; Pospischil et al. 2014], which are the foundation of the modern semiconductor electronic devices. Besides, electronic transport in carbon nanotubes [Laird et al. 2015] and in molecular wires [Nitzan and Ratner 2003], which recently attracted a lot of interest, is often modeled by the junction of two semi-infinite systems with different chemical potentials. In recent years, studies of various quantum Hall effects and topological insulators focused attention on 2-dimensional materials; see [Hasan and Kane 2010]. These 2-dimensional materials often possess periodicity in one dimension and can therefore be

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reduced to quasi-1-dimensional materials by momentum representation in the periodic direction [Hatsugai 1993]. Furthermore, when studying edge states properties (see [Hatsugai 1993; Avila et al. 2013]) of 2-dimensional materials, they can be seen as a junction with the vacuum.

Real world materials are often described by periodic [Catto et al. 2001; Cancès et al. 2008] or ergodically periodic [Cancès et al. 2013] systems in mathematical modeling. In this article we consider a junction of two different quasi-1-dimensional periodic systems without any assumption on the commensurability of the periods. Generally speaking, there are two regimes for the junction of two different periodic systems: when the chemical potentials of the underlying periodic systems are separated by some occupied bands (nonequilibrium regime, see Figure 3), and when the chemical potentials are in a common spectral gap (equilibrium regime, see Figure 4). The nonequilibrium regime models a persistent (nonperturbative) current in the junction system [Bruneau et al. 2015; 2016a; 2016b; Cornean et al. 2012], 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 [Cornean et al. 2008]. In this article we consider the equilibrium regime, and only briefly comment on the nonequilibrium regime in Section 3B, as the study of this situation requires different techniques.

The most prominent feature of quasi-1-dimensional materials is the presence of strong electron-electron interactions due to low screening effect [Brus 2010; 2014] as electrons interact through the 3-dimensional space. For finite systems, one can use a N-body Schrödinger model to describe the electron-electron interactions. Nevertheless, this is impossible for infinite systems. Mean-field theory is a good candidate for infinite systems: it consists of replacing the N-body interactions by a 1-body interaction with an effective average field, leading to a quasiparticle description of the system. However, mean-field models are rarely available for quasi-1-dimensional periodic systems, as periodic systems are often considered either in the 3-dimensional space (see [Lieb and Simon 1977; Catto et al. 1998] for Thomas–Fermi-type models and [Catto et al. 2001] for Hartree–Fock-type models), or strictly in a 1-dimensional geometry (see [Blanc and Le Bris 2002] for Thomas–Fermi type models). To our knowledge, the work on Thomas–Fermi-type models [Blanc and Le Bris 2000] for polymers is the only literature available for a 1-dimensional periodic system with interactions through the 3-dimensional space. Furthermore, nonperiodic infinite systems are difficult to handle mathematically, as they do not possess any symmetry; hence the usual Bloch decomposition of periodic systems [Reed and Simon 1978; Catto et al. 2001] is not applicable, and the definition of the ground state energy needs to be examined [Blanc et al. 2003].

In this article, we establish a mean-field model to describe the junction of two different quasi-1-dimensional periodic systems (see Figure 2) in the 3-dimensional space with Coulomb interactions, under the framework of the reduced Hartree–Fock (rHF) description [Solovej 1991]. Note that the rHF model is strictly convex in the density, and can be seen as a good approximation of Kohn–Sham LDA model [Kohn and Sham 1965; Anantharaman and Cancès 2009; Lewin et al. 2020], which is widely used in condensed matter physics. This nonlinear model can be employed to describe the junction of two nanotubes, or a more realistic model of the junction of two quasi-1-dimensional crystals for electronic structure calculations. It can be further explored to study the linear response with respect to different Fermi levels between two semi-infinite chains: recall that the famous Landauer–Büttiker formalism [Landauer 1970; Büttiker

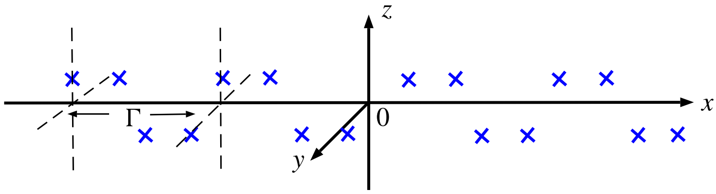

Figure 1. An example of nuclei configuration of a quasi-1-dimensional periodic system.

et al. 1985] for electronic (thermal) transport, which is based on the lead-device-lead description, can be seen as the junction of two different quasi-1-dimensional systems (leads) with different chemical (thermal) potentials, and the device as a perturbation of this junction. Note also that p-n junctions of carbon nanotubes without external battery [Léonard and Tersoff 1999; Lee et al. 2004] correspond to the equilibrium regime, and can thus be described by the model we consider. Furthermore, our model can also be easily adapted to describe 1-dimensional dislocation problems in the 3-dimensional space, while the linear 1-dimensional dislocation problems have been studied in [Korotyaev 2000; 2005] and some generalizations have been provided for higher-dimensional systems [Dohnal et al. 2011; Hempel and Kohlmann 2011; Hempel et al. 2015].

1B. ***Summary of main results.*** The organization of this article and the main results are as follows: in Section 2 we consider a quasi-1-dimensional periodic system, which is described by nuclei arranged periodically alongside the x-axis (see Figure 1) with electrons occupying the 3-dimensional space, as it is a building block for the junction system. We define a periodic rHF energy functional (2-15) by taking into account the real Coulomb interactions in the 3-dimensional space. In Theorem 2.6 we show that this rHF functional admits minimizers, and that the ground state electronic density is unique. Note that this is different from [Catto et al. 2001; Cancès et al. 2008] as the system is periodic only in the x-direction, the unit cell Γ being unbounded so that additional compactness proofs are needed when dealing with the ground state problem. With a mild summability condition (2-18) on the unique density of minimizers, we are able to obtain a mean-field Hamiltonian $H_{\text{per}} = -\frac{1}{2}\Delta + V_{\text{per}}$ to describe a quasi-1-dimensional periodic system, where V_{per} is the mean-field potential that tends to 0 in the $\boldsymbol{r} := (y, z)$-direction. In Theorem 2.7 we prove that the Fermi level ϵ_F of the quasi-1-dimensional system, which represents the highest energy occupied by electrons under this quasiparticle description, is always negative. We also prove that the unique minimizer is a spectral projector of the mean-field Hamiltonian $\gamma_{\text{per}} = \mathbb{1}_{(-\infty,\epsilon_F]}(H_{\text{per}})$.

In Section 3, under certain symmetry assumptions on the nuclear densities $\mu_{\text{per},L}$ and $\mu_{\text{per},R}$ of two different quasi-1-dimensional periodic systems, the junction system is described by considering the following nuclear configuration (see Figure 2):

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

where ν describes how the junction is initiated. We aim at establishing a quasiparticle description of this infinitely extended junction system with Coulomb interactions and show the existence of ground state. As we do not assume any commensurability of periods of the two quasi-1-dimensional systems, the junction

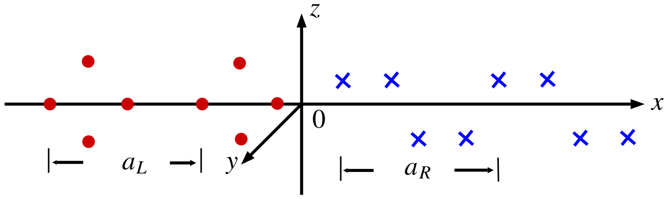

Figure 2. Nuclei configuration of the junction system with period a_L on $(-\infty, 0] \times \mathbb{R}^2$ and a_R on $(0, +\infty) \times \mathbb{R}^2$.

system does not possess any translation-invariant symmetry. The main idea is to establish a well-suited reference system based on the linear combination of periodic systems, and use perturbative techniques which have been widely used for mean-field type models [Hainzl et al. 2005a; 2007; 2009; Cancès et al. 2008; Frank et al. 2013] to justify the construction. More precisely, we define a reference Hamiltonian

$$H_\chi = \chi H_{\mathrm{per},L}\chi + \sqrt{1-\chi^2} H_{\mathrm{per},R}\sqrt{1-\chi^2}$$

with χ a smooth cut-off function approximating $\mathbb{1}_{x\le 0}$, where $H_{\mathrm{per},L}$ and $H_{\mathrm{per},R}$ are the mean-field Hamiltonians of the quasi-1-dimensional periodic systems. Denote by $\sigma(A) = \sigma_{\mathrm{disc}}(A) \cup \sigma_{\mathrm{ess}}(A)$ the spectrum of A, where $\sigma_{\mathrm{disc}}(A)$ and $\sigma_{\mathrm{ess}}(A)$ denote the discrete and essential spectra of an operator A respectively. Denote also by $\sigma_{\mathrm{ac}}(A)$ the purely absolutely continuous spectrum of A. We first show in Proposition 3.1 that

$$\sigma_{\mathrm{ess}}(H_\chi) = \sigma_{\mathrm{ess}}(H_{\mathrm{per},L}) \cup \sigma_{\mathrm{ess}}(H_{\mathrm{per},R}), \quad \sigma_{\mathrm{ess}}(H_\chi) \cap (-\infty, 0] \subseteq \sigma_{\mathrm{ac}}(H_\chi).$$

This implies that the essential spectrum of the reference Hamiltonian is independent of the cut-off function χ, and the linear junction preserves the scattering channels of the underlying systems, since the purely absolutely continuous spectrum of the Hamiltonian has not been modified; hence the linear junction can be used to study the electronic conductance with the Landauer–Büttiker formalism (see for example [Bruneau et al. 2015; 2016a; 2016b] as well as the discussion following Proposition 3.1).

After introducing a reference state $\gamma_\chi := \mathbb{1}_{(-\infty,\epsilon_F)}(H_\chi)$, we show in Proposition 3.2 that the electronic density ρ_χ is close to the linear combination of the underlying periodic electronic densities, and that the difference with these reference densities decays exponentially fast. The quasiparticle description of the nonlinear junction state can be constructed by considering

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

where Q_χ is a trial density matrix which encodes the nonlinear effects of the junction system. Following the idea developed in [Cancès et al. 2008], we associate Q_χ with some minimization problem in Proposition 3.5, and denote by $\bar{Q}_\chi$ a minimizer. We prove in Theorem 3.6 that

$$\rho_{\gamma_J} = \rho_\chi + \rho_{\bar{Q}_\chi} \quad \text{is independent of } \chi.$$

This implies that the ground state of the junction system with Coulomb interactions exists and its density is independent of the choice of the reference state; see Corollary 3.6.1.

2. A reduced Hartree–Fock description of quasi-1-dimensional periodic systems

In this section we give a mathematical description of a quasi-1-dimensional periodic system in the framework of the reduced Hartree–Fock (rHF) approach. In Section 2A, we introduce some mathematical preliminaries. In Section 2B we construct a periodic rHF energy functional for a quasi-1-dimensional system.

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 $\boldsymbol{x} = (x, \boldsymbol{r})$, where $x \in \mathbb{R}$. For a given separable Hilbert space $\mathfrak{H}$, we denote by $\mathcal{L}(\mathfrak{H})$ the space of bounded linear operators acting on $\mathfrak{H}$, by $\mathcal{S}(\mathfrak{H})$ the space of bounded self-adjoint operators acting on $\mathfrak{H}$, and by $\mathfrak{S}_p(\mathfrak{H})$ the Schatten class of operators acting on $\mathfrak{H}$. For $1 \le p < \infty$, a compact operator A belongs to $\mathfrak{S}_p(\mathfrak{H})$ if and only if $\|A\|_{\mathfrak{S}_p} := (\mathrm{Tr}(|A|^p))^{1/p} < \infty$. Operators in $\mathfrak{S}_1(\mathfrak{H})$ and $\mathfrak{S}_2(\mathfrak{H})$ are respectively called trace-class and Hilbert–Schmidt. If $A \in \mathfrak{S}_1(L^2(\mathbb{R}^d))$, there exists a unique function $\rho_A \in L^1(\mathbb{R}^d)$ such that,

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

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

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

$$\text{for all } \phi \in C_c^\infty(\mathbb{R}^d), \quad \mathrm{Tr}(A\phi) = \int_{\mathbb{R}^d} \rho_A \phi.$$

Let $\mathscr{S}(\mathbb{R}^d)$ be the Schwartz space of rapidly decreasing functions on $\mathbb{R}^d$, and $\mathscr{S}'(\mathbb{R}^d)$ the space of tempered distributions on $\mathbb{R}^d$. We denote by $\hat{\phi}$ and $\check{\phi}$ the Fourier and inverse Fourier transforms on $\mathscr{S}'(\mathbb{R}^d)$, with the normalization,

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

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

2A. ***Mathematical preliminaries.*** We first introduce a decomposition of the operator which is $\mathbb{Z}$-translation-invariant in the x-direction based on the partial Bloch transform. In order to describe the 1-dimensional periodic system in the 3-dimensional space, we next introduce a mixed Fourier transform. We also introduce a Green's function which is periodic only in the x-direction. Finally we introduce the kinetic energy space of density matrices and Coulomb interactions for quasi-1-dimensional systems.

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

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

An operator A on $L^2(\mathbb{R}^3)$ is called $\mathbb{Z}$-translation-invariant in the x-direction if it commutes with τ_k^x for all $k \in \mathbb{Z}$. In order to decompose operators which are $\mathbb{Z}$-translation-invariant in the x-direction, let us without loss of generality choose a unit cell

$$\Gamma := \left[-\tfrac{1}{2}, \tfrac{1}{2}\right) \times \mathbb{R}^2,$$

and introduce the L^p spaces and H^1 spaces of functions which are 1-periodic in the x-direction: for $1 \le p \le +\infty$,

$$L^p_{\mathrm{per},x}(\Gamma) := \{u \in L^p_{\mathrm{loc}}(\mathbb{R}^3) \mid \|u\|_{L^p(\Gamma)} < +\infty,\ \tau_k^x u = u \text{ for all } k \in \mathbb{Z}\},$$
$$H^1_{\mathrm{per},x}(\Gamma) := \{u \in L^2_{\mathrm{per},x}(\Gamma) \mid \nabla u \in (L^2_{\mathrm{per},x}(\Gamma))^3\}.$$

Let us also introduce the constant fiber direct integral of Hilbert spaces [Reed and Simon 1978]

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

with the base $\Gamma^* := [-\pi, \pi) \times \{0\}^2 \equiv [-\pi, \pi)$. The partial Bloch transform $\mathscr{B}$ is a unitary operator from $L^2(\mathbb{R}^3)$ to $L^2(\Gamma^*; L^2_{\mathrm{per},x}(\Gamma))$, defined on the dense subspace of $C_c^\infty(\mathbb{R}^3)$ of $L^2(\mathbb{R}^3)$:

$$\text{for all } (x, \boldsymbol{r}) \in \Gamma, \text{ for all } \xi \in \Gamma^*, \quad (\mathscr{B}\phi)_\xi(x, \boldsymbol{r}) := \sum_{k\in\mathbb{Z}} \mathrm{e}^{-\mathrm{i}(x+k)\xi}\phi(x+k, \boldsymbol{r}).$$

Its inverse is given, for $f_\bullet = (f_\xi)_{\xi\in\Gamma^*}$, by

$$\text{for all } k \in \mathbb{Z}, \text{ for a.a. } (x, \boldsymbol{r}) \in \Gamma, \quad (\mathscr{B}^{-1} f_\bullet)(x+k, \boldsymbol{r}) := \int_{\Gamma^*} \mathrm{e}^{\mathrm{i}(k+x)\xi} f_\xi(x, \boldsymbol{r})\,\frac{d\xi}{2\pi}.$$

The partial Bloch transform has the property that any operator A on $L^2(\mathbb{R}^3)$ which commutes with τ_k^x for $k \in \mathbb{Z}$ is decomposed by $\mathscr{B}$: for any $A \in \mathcal{L}(L^2(\mathbb{R}^3))$ such that $\tau_k^x A = A\tau_k^x$, there exists $A_\bullet \in L^\infty(\Gamma^*; \mathcal{L}(L^2_{\mathrm{per},x}(\Gamma)))$ such that, for all $u \in L^2(\mathbb{R}^3)$,

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

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

$$A = \mathscr{B}^{-1}\left(\int_{\Gamma^*}^{\oplus} A_\xi\,\frac{d\xi}{2\pi}\right)\mathscr{B}.$$

In addition, $\|A\|_{\mathcal{L}(L^2(\mathbb{R}^3))} = \|\|A_\bullet\|_{\mathcal{L}(L^2_{\mathrm{per},x}(\Gamma))}\|_{L^\infty(\Gamma^*)}$. In particular, if A is positive and locally trace-class, then, for almost all $\xi \in \Gamma^*$, A_ξ is locally trace-class. The densities of these operators are related by the formula

$$\rho_A(\boldsymbol{x}) = \frac{1}{2\pi}\int_{\Gamma^*} \rho_{A_\xi}(\boldsymbol{x})\,d\xi. \tag{2-1}$$

If A is a (not necessarily bounded) self-adjoint operator such that $\tau_k^x(A+\mathrm{i})^{-1} = (A+\mathrm{i})^{-1}\tau_k^x$ for all $k \in \mathbb{Z}$, then A is decomposed by $\mathcal{U}$; see [Reed and Simon 1978, Theorems XIII.84 and XIII.85]. In particular, denoting by Δ the Laplace operator acting on $L^2(\mathbb{R}^3)$, the kinetic energy operator $-\frac{1}{2}\Delta$ on $L^2(\mathbb{R}^3)$ is decomposed by $\mathscr{B}$ as follows:

$$-\frac{1}{2}\Delta = \mathscr{B}^{-1}\biggl(\int_{\Gamma^*} -\frac{1}{2}\Delta_\xi \,\frac{d\xi}{2\pi}\biggr)\mathscr{B}, \quad -\Delta_\xi = (-\mathrm{i}\nabla_\xi)^2 = (\mathrm{i}\partial_x - \xi)^2 - \Delta_{\boldsymbol{r}}, \tag{2-2}$$

where $\Delta_{\boldsymbol{r}}$ is the Laplace operator acting on $L^2(\mathbb{R}^2)$.

Mixed Fourier transform. The mixed Fourier transform consists of a Fourier series transform in the x-direction and an integral Fourier transform in the $\boldsymbol{r}$-direction. Denote by $\mathscr{S}_{\mathrm{per},x}(\Gamma)$ the space of functions that are C^∞ on $\mathbb{R}^3$ and Γ-periodic, decaying faster than any power of $|\boldsymbol{r}|$ when $|\boldsymbol{r}|$ tends to infinity, as well as their derivatives. Denote by $\mathscr{S}'_{\mathrm{per},x}(\Gamma)$ the dual space of $\mathscr{S}_{\mathrm{per},x}(\Gamma)$. The mixed Fourier transform is the unitary transform $\mathscr{F} : L^2_{\mathrm{per},x}(\Gamma) \to \ell^2(\mathbb{Z}, L^2(\mathbb{R}^2))$ defined on the dense subspace $\mathscr{S}_{\mathrm{per},x}(\Gamma)$ of $L^2_{\mathrm{per},x}(\Gamma)$ by

$$\text{for all } \phi \in \mathscr{S}_{\mathrm{per},x}(\Gamma), \text{ for all } (n, \boldsymbol{k}) \in \mathbb{Z}\times\mathbb{R}^2, \quad \mathscr{F}\phi(n,\boldsymbol{k}) := \frac{1}{2\pi}\int_\Gamma \phi(x,\boldsymbol{r})\,\mathrm{e}^{-\mathrm{i}(2\pi n x + \boldsymbol{k}\cdot\boldsymbol{r})}\,dx\,d\boldsymbol{r}. \tag{2-3}$$

Its inverse is given by,

$$\text{for all } (\psi_n(\boldsymbol{k}))_{n\in\mathbb{Z},\boldsymbol{k}\in\mathbb{R}^2} \in \ell^2(\mathbb{Z}; L^2(\mathbb{R}^2)), \quad \mathscr{F}^{-1}\psi(x,\boldsymbol{r}) := \frac{1}{2\pi}\sum_{n\in\mathbb{Z}}\int_{\mathbb{R}^2}\psi_n(\boldsymbol{k})\,\mathrm{e}^{\mathrm{i}(2\pi n x + \boldsymbol{k}\cdot\boldsymbol{r})}\,d\boldsymbol{k}.$$

Note that $\mathscr{F}$ can be extended from $\mathscr{S}'_{\mathrm{per},x}(\Gamma)$ to $\mathscr{S}'(\mathbb{R}^3)$. One can easily see that $\mathscr{F}$ is an isometry from $L^2_{\mathrm{per},x}(\Gamma)$ to $\ell^2(\mathbb{Z}, L^2(\mathbb{R}^2))$ in the following sense:

$$\text{for all } f, g \in L^2_{\mathrm{per},x}(\Gamma), \quad \int_\Gamma \overline{f(x,\boldsymbol{r})}g(x,\boldsymbol{r})\,dx\,d\boldsymbol{r} = \sum_{n\in\mathbb{Z}}\int_{\mathbb{R}^2}\overline{\mathscr{F}f(n,\boldsymbol{k})}\mathscr{F}g(n,\boldsymbol{k})\,d\boldsymbol{k}. \tag{2-4}$$

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

$$\mathscr{F}(f \star_\Gamma g) = 2\pi(\mathscr{F}f)(\mathscr{F}g), \tag{2-5}$$

where $(f \star_\Gamma g)(\boldsymbol{x}) := \int_\Gamma f(\boldsymbol{x}-\boldsymbol{x}')g(\boldsymbol{x}')\,d\boldsymbol{x}'$. As an application of the mixed Fourier transform, let us introduce a Kato–Seiler–Simon-type inequality [Seiler and Simon 1975] for the operator $-\mathrm{i}\nabla_\xi = (-\mathrm{i}\partial_x + \xi, -\mathrm{i}\partial_{\boldsymbol{r}})$ for all $\xi \in \Gamma^*$, which will be repeatedly used in the proofs.

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

$$\|f(-\mathrm{i}\nabla_\xi)g\|_{\mathfrak{S}_p(L^2_{\mathrm{per},x}(\Gamma))} \le (2\pi)^{-2/p}\|g\|_{L^p_{\mathrm{per},x}(\Gamma)}\biggl(\sum_{n\in\mathbb{Z}}\|f(2\pi n+\xi,\cdot)\|^p_{L^p(\mathbb{R}^2)}\biggr)^{1/p} \tag{2-6}$$

for any $2 \le p < \infty$ and

$$\|f(-\mathrm{i}\nabla_\xi)g\| \le \|g\|_{L^\infty_{\mathrm{per},x}(\Gamma)}\sup_{n\in\mathbb{Z}}\|f(2\pi n+\xi,\cdot)\|_{L^\infty(\mathbb{R}^2)},$$

when $p = +\infty$.

The proof is an easy adaptation of the proof of the classical Kato–Seiler–Simon inequality (4-1) by replacing the Fourier transform with the mixed Fourier transform $\mathscr{F}$. The detailed proof of this lemma can be read in [Cao 2019b, Lemma 2.1].

Periodic Green's function. We introduce a 3-dimensional Green's function which is 1-periodic in the x-direction in the same spirit as in [Blanc and Le Bris 2000; Lieb and Simon 1977].

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

$$G(x,\boldsymbol{r}) = -2\log(|\boldsymbol{r}|) + \widetilde{G}(x,\boldsymbol{r}), \quad \widetilde{G}(x,\boldsymbol{r}) := 4\sum_{n\geq 1} K_0(2\pi n|\boldsymbol{r}|)\cos(2\pi n x), \tag{2-7}$$

where $K_0(\alpha) := \int_0^{+\infty} \mathrm{e}^{-\alpha\cosh(t)}\, dt$ is the modified Bessel function of the second kind.

Note that $-2\log(|\boldsymbol{r}|)$ is the solution of the equation

$$-\Delta u = 4\pi\delta_{\boldsymbol{r}=0} \quad \text{in } \mathscr{S}'(\mathbb{R}^2),$$

where $\delta_a \in \mathscr{S}'(\mathbb{R}^d)$ is the Dirac distribution at $a \in \mathbb{R}^d$. It is also known as the 2-dimensional Coulomb kernel of the whole space Poisson equation. It appears here since we consider the Green's function which is periodic only in the x-direction and has a free boundary condition in the $\boldsymbol{r}$-direction. The following lemma summarizes the properties of the periodic Green's function defined in (2-7).

Lemma 2.3. (1) *The Green's function $G(x, \boldsymbol{r})$ defined in (2-7) satisfies the following Poisson equation*:

$$-\Delta G(x,\boldsymbol{r}) = 4\pi\sum_{n\in\mathbb{Z}} \delta_{(x,\boldsymbol{r})=(n,0)} \in \mathscr{S}'(\mathbb{R}^3).$$

Moreover $G \in \mathscr{S}'_{\mathrm{per},x}(\Gamma)$ and

$$\mathscr{F}(G)(n,\boldsymbol{k}) = \frac{2}{4\pi^2 n^2 + |\boldsymbol{k}|^2} \in \mathscr{S}'(\mathbb{R}^3). \tag{2-8}$$

(2) *The function $\widetilde{G}$ defined in (2-7) belongs to $L^p_{\mathrm{per},x}(\Gamma)$ for $1 \leq p < 2$ and satisfies $\int_\Gamma \widetilde{G} \equiv 0$. Moreover, there exist positive constants d_1 and d_2 such that*

$$|\widetilde{G}(\cdot,\boldsymbol{r})| \leq d_1 \frac{\mathrm{e}^{-2\pi|\boldsymbol{r}|}}{\sqrt{|\boldsymbol{r}|}}$$

when $|\boldsymbol{r}| \to +\infty$, and $|\widetilde{G}(\cdot,\boldsymbol{r})| \leq d_2/|\boldsymbol{r}|$ when $|\boldsymbol{r}| \to 0$, uniformly with respect to x. Finally, the function $\widetilde{G}(x,\boldsymbol{r})$ can also be written as

$$\widetilde{G}(x,\boldsymbol{r}) = \sum_{n\in\mathbb{Z}}\left(\frac{1}{\sqrt{(x-n)^2+|\boldsymbol{r}|^2}} - \int_{-1/2}^{1/2} \frac{1}{\sqrt{(x-y-n)^2+|\boldsymbol{r}|^2}}\, dy\right). \tag{2-9}$$

The proof of this lemma is an easy and direct computation and can be read in Section A1 of the Appendix.

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., [Cancès et al. 2008; Frank et al. 2013]. Recall that for a finite system with N electrons, a density matrix is a trace-class self-adjoint operator $\gamma \in \mathcal{S}(L^2(\mathbb{R}^3)) \cap \mathfrak{S}_1(L^2(\mathbb{R}^3))$ satisfying the Pauli principle $0 \leq \gamma \leq 1$ and the normalization condition $\mathrm{Tr}(\gamma) = \int_{\mathbb{R}^3} \rho_\gamma = N$. The kinetic energy of γ is given by $\mathrm{Tr}(-\frac{1}{2}\Delta\gamma) := \frac{1}{2}\mathrm{Tr}(|\nabla|\gamma|\nabla|)$; see [Catto et al. 2001; Cancès et al. 2008; Cancès and Stoltz 2012].

Consider a 1-dimensional periodic system in the 3-dimensional space, where atoms are arranged periodically in the x-direction with unit cell Γ and first Brillouin zone Γ^*. Since the rHF model is strictly convex in the density [Solovej 1991], we do not expect any spontaneous symmetry breaking. Therefore the electronic state of this quasi-1-dimensional system will be described by a one-body density matrix which commutes with the translations $\{\tau_k^x\}_{k\in\mathbb{Z}}$, and hence is decomposed by the partial Bloch transform $\mathscr{B}$. In view of the decomposition (2-2), we define the following admissible set of one-body density matrices, which guarantees that the number of electrons per unit cell and the kinetic energy per unit cell are finite:

$$\mathcal{P}_{\text{per},x} := \left\{ \gamma \in \mathcal{S}(L^2(\mathbb{R}^3)) \;\middle|\; 0 \le \gamma \le 1 \text{ for all } k \in \mathbb{Z},\; \tau_k^x \gamma = \gamma \tau_k^x,\; \int_{\Gamma^*} \mathrm{Tr}_{L^2_{\text{per},x}}\big(\sqrt{1-\Delta_\xi}\,\gamma_\xi \sqrt{1-\Delta_\xi}\big)\, d\xi < \infty \right\}, \tag{2-10}$$

where

$$\gamma = \mathscr{B}^{-1}\left(\int_{\Gamma^*} \gamma_\xi \frac{d\xi}{2\pi}\right)\mathscr{B}. \tag{2-11}$$

For any $\gamma \in \mathcal{P}_{\text{per},x}$, it is easy to see that $\rho_\gamma \in L^1_{\text{per},x}(\Gamma)$. Moreover, a Hoffmann-Ostenhof-type inequality [Hoffmann-Ostenhof and Hoffmann-Ostenhof 1977] can also be deduced from [Catto et al. 2001, equation (4.42)]:

$$\int_\Gamma |\nabla \sqrt{\rho_\gamma}|^2 \le \int_{\Gamma^*} \mathrm{Tr}_{L^2_{\text{per},x}}(-\Delta_\xi \gamma_\xi)\frac{d\xi}{2\pi}. \tag{2-12}$$

Therefore $\sqrt{\rho_\gamma}$ is in $H^1_{\text{per},x}(\Gamma)$, and hence is in $L^6_{\text{per},x}(\Gamma)$ by Sobolev embeddings, so that $\rho_\gamma \in L^p_{\text{per},x}(\Gamma)$ for $1 \le p \le 3$ 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

$$D(f,g) := \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \frac{f(\boldsymbol{x})g(\boldsymbol{x}')}{|\boldsymbol{x}-\boldsymbol{x}'|}\,d\boldsymbol{x}\,d\boldsymbol{x}' = 4\pi \int_{\mathbb{R}^3} \frac{\overline{\hat{f}(\boldsymbol{k})}\hat{g}(\boldsymbol{k})}{|\boldsymbol{k}|^2}.$$

In order to describe Coulomb interactions in the reciprocal space for a quasi-1-dimensional periodic system, 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 $\mathscr{S}_{\text{per},x}(\Gamma)$ as

$$D_\Gamma(f,g) := 4\pi \sum_{n\in\mathbb{Z}} \int_{\mathbb{R}^2} \frac{\overline{\mathscr{F}(f)}(n,\boldsymbol{k})\mathscr{F}(g)(n,\boldsymbol{k})}{|\boldsymbol{k}|^2 + 4\pi^2 n^2}\,d\boldsymbol{k}. \tag{2-13}$$

It is easy to see that $D_\Gamma(\cdot\,,\cdot)$ is a positive definite bilinear form on $\mathscr{S}_{\text{per},x}(\Gamma)$. Let us introduce the Coulomb space for the 1-dimensional periodic system in the 3-dimensional space as

$$\mathcal{C}_\Gamma := \{f \in \mathscr{S}'_{\text{per},x}(\Gamma) \mid \text{for all } n \in \mathbb{Z},\ \mathscr{F}(f)(n,\cdot) \in L^1_{\text{loc}}(\mathbb{R}^2),\ D_\Gamma(f,f) < +\infty\}, \tag{2-14}$$

which is a Hilbert space endowed with the inner product $D_\Gamma(\cdot\,,\cdot)$.

Remark 2.4. Charge densities in $\mathcal{C}_\Gamma$ are neutral in some weak sense. Indeed, for $f \in \mathcal{C}_\Gamma \bigcap L^1_{\text{per},x}(\Gamma)$, the condition

$$\int_{\mathbb{R}^2} \frac{|\mathscr{F}(f)(0,\boldsymbol{k})|^2}{|\boldsymbol{k}|^2}\,d\boldsymbol{k} < +\infty$$

implies that $\mathscr{F}(f)(0,\boldsymbol{0}) = \int_\Gamma f(x,\boldsymbol{r})\,dx\,d\boldsymbol{r} = 0$.

2B. ***Reduced Hartree–Fock description for a quasi-1-dimensional periodic system.*** Based on the kinetic energy space and Coulomb interactions defined in the previous section, we construct here an rHF energy functional for a quasi-1-dimensional periodic system which is 1-periodic only in the x-direction. We show that its ground state is given by the solution of some minimization problem. Denote by $Z \in \mathbb{N}^*$ the total nuclear charge in each unit cell. For the sake of technical reasons we model the nuclear density of a quasi-1-dimensional system by a smooth function (smeared nuclei) which is 1-periodic in the x-direction

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

where $m(x, \boldsymbol{r})$ is a nonnegative $C_c^\infty(\Gamma)$ function such that $\int_{\mathbb{R}^3} m = 1$. In particular $\int_\Gamma \mu_{\text{per}} = Z$.

For any trial density matrix γ which commutes with the translations τ_k^x in the x-direction, the periodic rHF energy functional for a quasi-1-dimensional system associated with the nuclear density μ_{per} is defined as

$$\mathcal{E}_{\text{per},x}(\gamma) := \frac{1}{2\pi} \int_{\Gamma^*} \text{Tr}_{L^2_{\text{per},x}(\Gamma)}\Big(-\frac{1}{2}\Delta_\xi \gamma_\xi\Big) d\xi + \frac{1}{2} D_\Gamma(\rho_\gamma - \mu_{\text{per}}, \rho_\gamma - \mu_{\text{per}}). \tag{2-15}$$

Let us introduce the following set of admissible density matrices for this rHF energy functional, which guarantees that the kinetic energy and Coulomb interaction energy per unit cell are finite:

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

where $\mathcal{P}_{\text{per},x}$ is the kinetic energy space defined in (2-10) and $\mathcal{C}_\Gamma$ is the Coulomb space defined in (2-14).

Lemma 2.5. *The set $\mathcal{F}_\Gamma$ is not empty. Moreover, for any $\gamma \in \mathcal{F}_\Gamma$,*

$$\int_\Gamma \rho_\gamma = \int_\Gamma \mu_{\text{per}}. \tag{2-16}$$

The proof of Lemma 2.5 relies on an explicit construct of an element in $\mathcal{F}_\Gamma$ and can be read in Section 4A.

The periodic rHF ground state energy (per unit cell) of a quasi-1-dimensional system can then be written as the minimization problem

$$I_{\text{per}} = \inf\{\mathcal{E}_{\text{per},x}(\gamma) \mid \gamma \in \mathcal{F}_\Gamma\}. \tag{2-17}$$

The minimization problem similar to (2-17) under the Thomas–Fermi-type models has been studied in [Blanc and Le Bris 2000], where the authors proved the uniqueness of the minimizers, and justified the model by a thermodynamic limit argument. For a 3-dimensional periodic crystal, the minimization problem (2-17) has been examined in [Catto et al. 2001], where the authors showed the existence of minimizers and the uniqueness of the density of the minimizers. The characterization of the minimizers is given in [Cancès et al. 2008, Theorem 1]: the minimizer is unique and is a spectral projector satisfying a self-consistent equation. The following theorem provides similar results for a quasi-1-dimensional system: we show that the minimizer of (2-17) exists, and that the density of the minimizers is unique. Let us emphasize that the unit cell of a quasi-1-dimensional system is an unbounded domain Γ; hence we need to deal with the possible escaping of electrons in the $\boldsymbol{r}$-direction, a situation which need not be considered for bounded unit cells as in [Catto et al. 2001; Cancès et al. 2008].

Theorem 2.6 (existence of rHF ground state). *The minimization problem (2-17) admits a minimizer γ_{per} with density $\rho_{\gamma_{\text{per}}}$ belonging to $L^p_{\text{per},x}(\Gamma)$ for $1 \le p \le 3$. Additionally, all the minimizers share the same density.*

The proof of Theorem 2.6 relies on a classical variational argument and can be read in Section 4B.

In order to treat the junction of quasi-1-dimensional systems in Section 3, it is useful to define and study the mean-field potential $V_{\text{per}} = (\rho_{\gamma_{\text{per}}} - \mu_{\text{per}}) \star_\Gamma G$, where $\star_\Gamma$ denotes the convolution operator in the unit cell Γ and G is the x-periodic Green's function defined in (2-7). It is also critical to obtain some decay estimates of V_{per} in the $\boldsymbol{r}$-direction. However, since the Green's function G has a log-growth in the $\boldsymbol{r}$-direction, the L^p integrability of $\rho_{\gamma_{\text{per}}}$ obtained in Theorem 2.6 does not imply the decay of the mean-field potential V_{per} in the $\boldsymbol{r}$-direction. Moreover, the uniform bound given by the energy functional (2-15) does not provide any L^p bounds or a decay property of V_{per}. In view of this, we introduce the following assumption on $\rho_{\gamma_{\text{per}}}$. Note that this assumption, which called "summability condition", is common when treating the 2-dimensional Poisson equation [Lieb and Loss 2001, Theorem 6.21].

Assumption 1. *The unique ground state density $\rho_{\gamma_{\text{per}}}$ of the problem (2-17) satisfies*

$$\int_\Gamma |\boldsymbol{r}| \rho_{\gamma_{\text{per}}}(x, \boldsymbol{r})\, dx\, d\boldsymbol{r} < +\infty. \tag{2-18}$$

With this mild summability condition (2-18) on $\rho_{\gamma_{\text{per}}}$, we prove in Theorem 2.7 that $\rho_{\gamma_{\text{per}}}$ actually decays exponentially fast in the $|\boldsymbol{r}|$-direction (equation (2-22)), and the highest occupied energy (Fermi level) of electrons for a quasi-1-dimensional system in its ground state is always negative. This coincides with the physical reality: the additional summability condition on the density is sufficient to guarantee that the mean-field potential tends to 0 in the $\boldsymbol{r}$-direction. If the Fermi level is nonnegative, electrons can escape to infinity in the $\boldsymbol{r}$-direction, decreasing the energy of the system, and hence the system is not at ground state. Furthermore, we are able to characterize the unique minimizer as a spectral projector of the mean-field Hamiltonian. We comment on Assumption 1 in Remark 2.9, and we give an explicit example in which Assumption 1 is satisfied.

Example. If the mean-field potential V_{per} tends to 0 when $|\boldsymbol{r}|$ tends to $+\infty$, the density $\rho_{\gamma_{\text{per}}}$ decays exponentially fast in the $|\boldsymbol{r}|$-direction (see the proof of (2-22) in Section 4C); hence a posteriori Assumption 1 is satisfied.

Theorem 2.7 (properties of the rHF ground state with summability condition on the density). *Assume that Assumption 1 holds for the unique ground state density $\rho_{\gamma_{\text{per}}}$ of the minimization problem (2-17):*

(1) (the integrability of mean-field potential) *The mean-field potential*

$$V_{\text{per}} := (\rho_{\gamma_{\text{per}}} - \mu_{\text{per}}) \star_\Gamma G$$

belongs to $L^p_{\text{per},x}(\Gamma)$ for $2 < p \le +\infty$. Moreover, V_{per} is continuous and tends to zero in the $\boldsymbol{r}$-direction when $|\boldsymbol{r}| \to \infty$.

(2) (spectral properties of the mean-field Hamiltonian) *The mean-field Hamiltonian*

$$H_{\mathrm{per}} = \mathscr{B}^{-1}\left(\int_{\Gamma^*} H_{\mathrm{per},\xi}\,\frac{d\xi}{2\pi}\right)\mathscr{B} = -\frac{1}{2}\Delta + V_{\mathrm{per}}, \qquad H_{\mathrm{per},\xi} := -\frac{1}{2}\Delta_\xi + V_{\mathrm{per}}, \tag{2-19}$$

is a self-adjoint operator acting on $L^2(\mathbb{R}^3)$ *with domain* $H^2(\mathbb{R}^3)$ *and form domain* $H^1(\mathbb{R}^3)$. *There exists* $N_H \in \mathbb{N}^*$ *which can be finite or infinite and a sequence* $\{\lambda_n(\xi)\}_{\xi\in\Gamma^*,\,1\le n\le N_H}$ *such that*

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

Moreover, *the following spectral decomposition holds*:

$$\sigma(H_{\mathrm{per}}) = \sigma_{\mathrm{ess}}(H_{\mathrm{per}}) = \bigcup_{\xi\in\Gamma^*} \sigma(H_{\mathrm{per},\xi}), \qquad \bigcup_{\xi\in\Gamma^*} \sigma_{\mathrm{disc}}(H_{\mathrm{per},\xi}) \subseteq \sigma_{\mathrm{ac}}(H_{\mathrm{per}}). \tag{2-20}$$

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

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

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

is continuous and nondecreasing on $(-\infty, 0]$. *The inequality*

$$N_H = F(0) \ge \int_\Gamma \mu_{\mathrm{per}}$$

holds, *which means that there are always enough negative energy levels for the electrons. Moreover*, *there exists* $\epsilon_F < 0$ *called the Fermi level* (*chemical potential*) *such that* $F(\epsilon_F) = \int_\Gamma \mu_{\mathrm{per}} = Z$, *which represents the highest occupied energy level by electrons*, *and can be interpreted as the Lagrange multiplier associated with the charge neutrality condition* (2-16).

(4) (the unique minimizer is a spectral projector) *The minimizer of the problem* (2-17) *is unique and satisfies the following self-consistent equation*:

$$\gamma_{\mathrm{per}} = \mathbb{1}_{(-\infty,\epsilon_F]}(H_{\mathrm{per}}) = \mathscr{B}^{-1}\left(\int_{\Gamma^*} \gamma_{\mathrm{per},\xi}\,\frac{d\xi}{2\pi}\right)\mathscr{B}, \qquad \gamma_{\mathrm{per},\xi} := \mathbb{1}_{(-\infty,\epsilon_F]}(H_{\mathrm{per},\xi}). \tag{2-21}$$

Furthermore, *there exist positive constants* C_{ϵ_F} *and* α_{ϵ_F} *which depend on the Fermi level* ϵ_F, *such that*

$$0 \le \rho_{\gamma_{\mathrm{per}}}(x, \boldsymbol{r}) \le C_{\epsilon_F}\mathrm{e}^{-\alpha_{\epsilon_F}|\boldsymbol{r}|}. \tag{2-22}$$

The proof of Theorem 2.7 can be read in Section 4C.

Remark 2.8. As the unit cell of the 1-dimensional system in the 3-dimensional space is an unbounded domain Γ, the decomposed mean-field Hamiltonian $H_{\mathrm{per},\xi}$ does not have a compact resolvent, which is a significant difference compared to the situation considered in [Catto et al. 2001; Cancès et al. 2008].

Remark 2.9. Let us comment on Assumption 1. The exponential decay of the density (2-22) implies the summability condition (2-18). However, we were not able to directly prove (2-18). This failure is mainly due to the lack of a priori summability bounds for the density matrices in $\mathcal{F}_\Gamma$. One might argue that we can add the condition (2-18) to the definition of $\mathcal{F}_\Gamma$. However, the set $\mathcal{F}_\Gamma$ with the condition (2-18) is not closed for the usual weak-$*$ topology when considering a minimizing sequence of (2-15). Another attempt is to use a Schauder fixed-point algorithm as in [Lions 1987; Cancès et al. 2009] to prove that (2-21) admits a solution. The most crucial step is to guarantee that there are enough negative bound states to meet the charge neutrality constraint (2-16). The number of bound states is controlled by the decay rate of potentials. With exponentially decaying densities we can show that [Blanc and Le Bris 2000, Lemma 2.5] there exists $C \in \mathbb{R}^+$ such that $|V_{\text{per}}(\cdot, \boldsymbol{r})| \le C|\boldsymbol{r}|^{-1}$. Nevertheless this condition is not sufficient to guarantee that there are enough bound states with negative energies, as the critical decay rate for numbers of bound states to be finite or infinite is $-|\boldsymbol{r}|^{-2}$ [Reed and Simon 1978, Theorem XIII.6]. In other words, we do not have a uniform bound over the Fermi level ϵ_F at each fixed-point iteration. On the other hand, the summability condition (2-18) is a sufficient but probably not a necessary condition for the negativity of the Fermi level and the characterization of the minimizers. The main difficult is to control the decay of the mean-field potential V_{per} in the $\boldsymbol{r}$-direction by just controlling the nuclear density μ_{per}, given that the Green's function defined in (2-7) has log-growth in the $\boldsymbol{r}$-direction. Furthermore, different decay scenarios of V_{per} in the $\boldsymbol{r}$-direction lead to different characterizations of the spectrum of the Hamiltonian H_{per}: if V_{per} is bounded from below, and positive with log-growth when $|\boldsymbol{r}| \to \infty$, one can show that the spectrum of $H_{\text{per},\xi}$ is purely discrete and the spectrum of H_{per} has a band structure. The Fermi level of the system could be positive in this case. We are not able to prove the above statements without Assumption 1. But we managed to show that the weak decay of Assumption 1 implies an exponential decay (2-22).

In order to describe the junction of quasi-1-dimensional systems, more specifically to guarantee that the Coulomb energy generated by the perturbative state is finite, the integrability of the mean-field potential provided in Theorem 2.7 is not sufficient in view of Lemma 3.3 below. In order to make use of this result, let us introduce a class of nuclear densities such that the x-averaged density is rotationally invariant in the $\boldsymbol{r}$-direction:

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

where $m_{\text{s}}(x, \boldsymbol{r})$ is a nonnegative $C_c^\infty(\Gamma)$ function such that $\int_{\mathbb{R}^3} m_{\text{s}} = 1$. Moreover, there exists $m_{\text{sym}}(|\boldsymbol{r}|) \in C_c^\infty(\mathbb{R}^2)$ such that

$$\text{for all } \boldsymbol{r} \in \mathbb{R}^2, \quad \int_{-1/2}^{1/2} m_{\text{s}}(x, \boldsymbol{r})\, dx \equiv m_{\text{sym}}(|\boldsymbol{r}|). \tag{2-23}$$

Lemma 2.10. *Suppose that Assumption 1 holds. Under the symmetry condition (2-23) on the nuclear density μ_{per}, all the results of Theorem 2.7 hold for the minimization problem (2-17). Additionally, the mean-field potential V_{per} belongs to $L^p_{\text{per},x}(\Gamma)$ for $1 < p \le +\infty$.*

The proof of this lemma can be read in Section A2. The nuclei of many actual materials can be modeled with a smear nuclear density satisfying the condition (2-23): for instance nanotubes and polymers with rotational symmetry in the $\boldsymbol{r}$-direction.

3. Mean-field stability for the junction of quasi-1-dimensional systems

In this section, we construct an rHF model for the junction of two different quasi-1-dimensional periodic systems. The junction system is described by periodic nuclei satisfying the symmetry condition (2-23) with different periodicities and possibly different charges per unit cell, occupying separately the left and right half-spaces (i.e., $(-\infty, 0] \times \mathbb{R}^2$ and $(0, +\infty) \times \mathbb{R}^2$); see Figure 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 perturbative approaches when treating infinitely extended systems [Hainzl et al. 2005a; 2005b; 2007; 2009; Cancès et al. 2008], the idea is to find an appropriate reference state which is close enough to the actual one. Section 3A gives a mathematical description of the junction system. Section 3B is devoted to a rigorous construction of a reference Hamiltonian H_χ and a reference one-particle density matrix defined as a spectral projector of H_χ. In Section 3C we construct a perturbative state, which encodes the nonlinear effects due to the electron-electron interaction in the rHF approximation, and associate the ground state energy of this perturbative state to some minimization problem in Section 3D.

3A. ***Mathematical description of the junction system.*** Consider two quasi-1-dimensional periodic systems with periods $a_L > 0$ and $a_R > 0$. The unit cells are respectively denoted by $\Gamma_L := [-a_L/2, a_L/2) \times \mathbb{R}^2$ and $\Gamma_R := [-a_R/2, a_R/2) \times \mathbb{R}^2$ with their duals $\Gamma_L^* := [-\pi/a_L, \pi/a_L)$ and $\Gamma_R^* := [-\pi/a_R, \pi/a_R)$. We consider nuclear densities fulfilling the symmetry condition (2-23) and suppose that Assumption 1 holds for the ground state densities of both quasi-1-dimensional periodic systems. More precisely, let $m_L(x, \boldsymbol{r})$ and $m_R(x, \boldsymbol{r})$ be nonnegative C_c^∞ functions with supports respectively in Γ_L and Γ_R such that $\int_{\mathbb{R}^3} m_L = 1$ and $\int_{\mathbb{R}^3} m_R = 1$. Assume that there exist $m_{\mathrm{sym},L}(|\boldsymbol{r}|), m_{\mathrm{sym},R}(|\boldsymbol{r}|) \in C_c^\infty(\mathbb{R}^2)$ such that,

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

Denoting by $Z_L, Z_R \in \mathbb{N}\backslash\{0\}$ the total charges of the nuclei per unit cells, the smeared periodic nuclear densities are respectively defined as

$$\mu_{\mathrm{per},L}(x, \boldsymbol{r}) := \sum_{n\in\mathbb{Z}} Z_L\, m_L(x - a_L n, \boldsymbol{r}), \quad \mu_{\mathrm{per},R}(x, \boldsymbol{r}) := \sum_{n\in\mathbb{Z}} Z_R\, m_R(x - a_R n, \boldsymbol{r}). \tag{3-1}$$

The periodic Green's functions with periods Γ_L and Γ_R are separately defined as

$$G_{a_L}(x, \boldsymbol{r}) = a_L^{-1} G\Big(\frac{x}{a_L}, \boldsymbol{r}\Big), \quad G_{a_R}(x, \boldsymbol{r}) = a_R^{-1} G\Big(\frac{x}{a_R}, \boldsymbol{r}\Big),$$

where $G(\cdot)$ is the periodic Green's function defined in (2-7). One can easily verify that

$$-\Delta G_{a_L}(x, \boldsymbol{r}) = 4\pi \sum_{n\in\mathbb{Z}} \delta_{(x,\boldsymbol{r})=(a_L n, \boldsymbol{0})} \in \mathscr{S}'(\mathbb{R}^3), \quad -\Delta G_{a_R}(x, \boldsymbol{r}) = 4\pi \sum_{n\in\mathbb{Z}} \delta_{(x,\boldsymbol{r})=(a_R n, \boldsymbol{0})} \in \mathscr{S}'(\mathbb{R}^3).$$

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 $\mu_{\mathrm{per},L}$ and $\mu_{\mathrm{per},R}$:

$$\gamma_{\mathrm{per},L} := \mathbb{1}_{(-\infty,\epsilon_L]}(H_{\mathrm{per},L}), \quad H_{\mathrm{per},L} := -\frac{\Delta}{2} + V_{\mathrm{per},L}, \quad V_{\mathrm{per},L} := (\rho_{\mathrm{per},L} - \mu_{\mathrm{per},L}) \star_{\Gamma_L} G_{a_L},$$
$$\gamma_{\mathrm{per},R} := \mathbb{1}_{(-\infty,\epsilon_R]}(H_{\mathrm{per},R}), \quad H_{\mathrm{per},R} := -\frac{\Delta}{2} + V_{\mathrm{per},R}, \quad V_{\mathrm{per},R} := (\rho_{\mathrm{per},R} - \mu_{\mathrm{per},R}) \star_{\Gamma_R} G_{a_R},$$

where the negative constants ϵ_L and ϵ_R are the Fermi levels of the quasi-1-dimensional systems. The junction of the quasi-1-dimensional systems is described by considering the following nuclear density configuration (see Figure 2):

$$\mu_J(x, \boldsymbol{r}) := \mathbb{1}_{x\le 0} \cdot \mu_{\mathrm{per},L}(x, \boldsymbol{r}) + \mathbb{1}_{x>0} \cdot \mu_{\mathrm{per},R}(x, \boldsymbol{r}) + \nu(x, \boldsymbol{r}), \tag{3-2}$$

where $\nu(x, \boldsymbol{r}) \in L^{6/5}(\mathbb{R}^3)$ describes how the junction switches between the underlying nuclear densities. The assumption $\nu \in L^{6/5}(\mathbb{R}^3)$ ensures that $D(\nu, \nu) < +\infty$. Recall that

$$D(f, g) = \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \frac{f(x)g(y)}{|x-y|}\,dx\,dy = \frac{1}{4\pi}\int_{\mathbb{R}^3} \frac{\overline{\hat{f}(k)}\hat{g}(k)}{|k|^2}\,dk$$

describes the Coulomb interactions in the whole space. Once one sets the nuclear configuration (3-2), electrons are allowed to move in the 3-dimensional space. The *infinite* rHF energy functional for the junction system associated with a test density matrix γ_J formally reads

$$\mathcal{E}(\gamma_J) = \mathrm{Tr}\big(-\tfrac{1}{2}\Delta\gamma_J\big) + \tfrac{1}{2}D(\rho_{\gamma_J} - \mu_J, \rho_{\gamma_J} - \mu_J). \tag{3-3}$$

Let us also introduce the Coulomb space $\mathcal{C}$ and its dual $\mathcal{C}'$ (Beppo-Levi space [Cancès et al. 2008]):

$$\mathcal{C} := \{\rho \in \mathscr{S}'(\mathbb{R}^3) \mid \hat{\rho} \in L^1_{\mathrm{loc}}(\mathbb{R}^3),\ D(\rho,\rho) < \infty\}, \quad \mathcal{C}' := \{V \in L^6(\mathbb{R}^3) \mid \nabla V \in (L^2(\mathbb{R}^3))^3\}. \tag{3-4}$$

Note that the ground state energy of the junction system, if it exists, is infinite and there is no periodicity in this system; hence usual techniques which essentially consist of considering the energy per unit volume [Catto et al. 2001; Cancès et al. 2008] are not applicable. We next define a reference system such that the difference between the junction system and the reference can be considered as a perturbation. This perturbative approach has been used in [Hainzl et al. 2005a; 2007; 2009; Cancès et al. 2008] in various contexts. The next section is devoted to the rigorous mathematical construction of the reference state and its rHF energy functional.

3B. ***Reference state for the junction system.*** In this section, we construct a reference Hamiltonian obtained by a linear combination of the periodic mean-field potentials $V_{\mathrm{per},L}$ and $V_{\mathrm{per},R}$. We prove the validity of this approach by showing that the density generated by this reference state is close to the linear combination of the periodic densities $\rho_{\mathrm{per},L}$ and $\rho_{\mathrm{per},R}$.

Hamiltonian of the reference state. We introduce a class of smoothed cut-off functions. For $\boldsymbol{x} \in \mathbb{R}^3$, consider

$$\mathcal{X} := \Big\{\chi \in C^2(\mathbb{R}^3) \,\Big|\, 0 \le \chi \le 1,\ \chi(\boldsymbol{x}) = 1 \text{ if } \boldsymbol{x} \in \Big(-\infty, -\frac{a_L}{2}\Big] \times \mathbb{R}^2,\ \chi(\boldsymbol{x}) = 0 \text{ if } \boldsymbol{x} \in \Big[\frac{a_R}{2}, +\infty\Big) \times \mathbb{R}^2\Big\}. \tag{3-5}$$

Fix $\chi \in \mathcal{X}$, let us introduce a reference potential

$$V_\chi := \chi^2 V_{\mathrm{per},L} + (1-\chi^2) V_{\mathrm{per},R}.$$

We will show in Section 3D that the choice of $\chi \in \mathcal{X}$ is irrelevant. By Theorem 2.7 and Lemma 2.10 we know that V_χ belongs to $L^p_{\mathrm{loc}}(\mathbb{R}, L^p(\mathbb{R}^2))$ for $1 < p \le \infty$, is continuous in all directions and tends to zero in the $\boldsymbol{r}$-direction. By the Kato–Rellich theorem (see for example [Helffer 2013, Theorem 9.10]), there exists a unique self-adjoint operator

$$H_\chi := -\tfrac{1}{2}\Delta + V_\chi \tag{3-6}$$

on $L^2(\mathbb{R}^3)$ with domain $H^2(\mathbb{R}^3)$ and form domain $H^1(\mathbb{R}^3)$. We next show that the essential spectrum of the reference Hamiltonian H_χ is the union of the essential spectra of $H_{\mathrm{per},L}$ and $H_{\mathrm{per},R}$, which implies that the reference system does not change essentially the unions of possible energy levels of quasiperiodic systems, and that there are no surface states which propagate along the junction surface in the $\boldsymbol{r}$-direction. Note that this is a priori not obvious as the cut-off function χ is $\boldsymbol{r}$-translation-invariant (hence not compact), therefore scattering states may occur at the junction surface and escape to infinity in the $\boldsymbol{r}$-direction. Standard techniques in scattering theory to prove this statement, such as Dirichlet decoupling [Deift and Simon 1976; Hempel et al. 2015], are not applicable in our situation since the junction surface is not compact.

Proposition 3.1 (spectral properties of the reference state H_χ). *For any $\chi \in \mathcal{X}$, the essential spectrum of H_χ defined in (3-6) satisfies*

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

In particular, $[0, +\infty) \subset \sigma_{\mathrm{ess}}(H_\chi)$ and $\sigma_{\mathrm{ess}}(H_\chi)$ does not depend on the shape of the cut-off function $\chi \in \mathcal{X}$ defined in (3-5).

The proof can be found in Section A3 of the Appendix. Note that Proposition 3.1 also implies that the reference system essentially preserves the scattering channels of the underlying quasi-1-dimensional systems, since the scattering involves the purely absolutely continuous spectrum of a Hamiltonian (see for example [Exner and Frank 2007; Bruneau et al. 2016a; 2016b]). However, this does not exclude the existence of embedded eigenvalues in the essential spectrum, which may cause additional scattering channels [Frank 2003; Frank and Shterenberg 2004]. We prove in Corollary 3.5.1 that the results in Proposition 3.1 still hold for the nonlinear junction.

Reference state as a spectral projector. Before constructing the reference state, let us discuss different regimes for junction system. From Theorem 2.7 we know that the chemical potentials (Fermi levels) ϵ_L and ϵ_R are negative. Introduce the energy interval $I_{\epsilon_F} := [\min(\epsilon_L, \epsilon_R), \max(\epsilon_L, \epsilon_R)]$. In view of Proposition 3.1, assume that the essential spectrum of H_χ below 0 is purely absolutely continuous, the nonequilibrium regime (Figure 3) corresponds to

$$\sigma_{\mathrm{ac}}(H_\chi) \cap I_{\epsilon_F} \neq \varnothing.$$

In this regime, steady state currents occur and the Landauer–Büttiker conductance can be calculated [Bruneau et al. 2015; 2016a; 2016b]. When $\mu_{\mathrm{per},L}$ and $\mu_{\mathrm{per},R}$ are identical, the junction system becomes

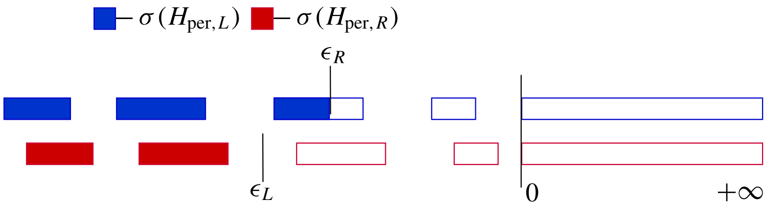

Figure 3. Spectrum of $H_{\text{per},L}$, $H_{\text{per},R}$ in the nonequilibrium regime.

periodic with different chemical potentials ϵ_L and ϵ_R on the left and right half-lines. In this case the Thouless conductance [Bruneau et al. 2015] can be defined and it is given by

$$C_T \frac{|\sigma_{\text{ac}}(H_\chi) \bigcap I_{\epsilon_F}|}{|I_{\epsilon_F}|} > 0,$$

for some positive constant C_T. However it is not the aim of this article to discuss steady state currents for nonequilibrium systems. We instead consider the equilibrium regime (see Figure 4) with the following assumption.

Assumption 2. *The chemical potentials ϵ_L and ϵ_R are in a common spectral gap (Σ_a, Σ_b) (equilibrium regime, see Figure 4), where Σ_a is the maximum of the filled bands of $H_{\text{per},L}$ and $H_{\text{per},R}$, and Σ_b is the minimum of the unfilled bands of $H_{\text{per},L}$ and $H_{\text{per},R}$.*

Assumption 2 guarantees that the Fermi level of the junction system lies in a spectral gap of H_χ in view of Proposition 3.1, which is a common hypothesis [Cancès et al. 2008; Hainzl et al. 2005a; 2009] for 3-dimensional periodic insulating and semiconducting systems. We make this assumption for simplicity. Note that with approaches proposed in [Frank et al. 2011; 2013; Cancès et al. 2020] it is possible to extend the results to metallic systems provided that the junction system is in its ground state and no steady state current occurs.

Let us without loss of generality choose the Fermi level $\epsilon_F = \max(\epsilon_L, \epsilon_R) = \sup I_{\epsilon_F}$ and define the reference state γ_χ as the spectral projector associated with the states of H_χ below ϵ_F:

$$\gamma_\chi := \mathbb{1}_{(-\infty,\epsilon_F)}(H_\chi). \tag{3-7}$$

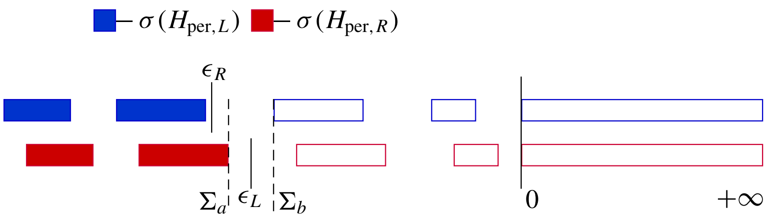

Figure 4. Spectrum of $H_{\text{per},L}$, $H_{\text{per},R}$ in the equilibrium regime.

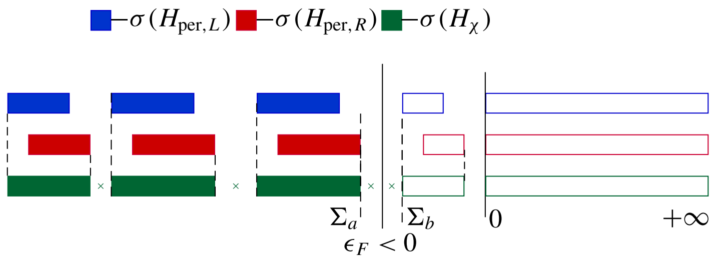

Figure 5. Spectrum of $H_{\mathrm{per},L}$, $H_{\mathrm{per},R}$ and H_χ below 0.

Note that H_χ can have discrete spectrum in the gap (Σ_a, Σ_b), with eigenvalues possibly accumulating at Σ_a and Σ_b, and ϵ_F can also be an eigenvalue of H_χ; see Figure 5. The definition of (3-7), however, excludes the possible bound states with energy ϵ_F.

The following proposition shows that the density ρ_χ of γ_χ is well-defined in $L^1_{\mathrm{loc}}(\mathbb{R}^3)$ and is close to the linear combination of the periodic densities $\rho_{\mathrm{per},L}$ and $\rho_{\mathrm{per},R}$, the difference decaying exponentially fast in the x-direction as $|x| \to \infty$.

Proposition 3.2 (exponential decay of density). *Under Assumption 2, the spectral projector γ_χ is locally trace class, so that its density ρ_χ is well-defined in $L^1_{\mathrm{loc}}(\mathbb{R}^3)$. Moreover,*

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

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

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

it holds

$$\int_{\mathbb{R}^3} \left| w_\alpha \big(\chi^2\rho_{\mathrm{per},L} + (1-\chi^2)\rho_{\mathrm{per},R} - \rho_\chi\big) w_\alpha \right| \le C e^{-t|\alpha|}.$$

The proof can be read in Section 4D.

Fictitious nuclear density of the reference state. The density ρ_χ associated with γ_χ is fixed once the Fermi level ϵ_F is chosen. We can therefore define a fictitious nuclear density μ_χ by imposing that the total electronic density $\rho_\chi - \mu_\chi$ generates the potential V_χ. The fictitious nuclear density μ_χ is given by

$$-\Delta V_\chi = 4\pi(\rho_\chi - \mu_\chi), \quad \mu_\chi := \rho_\chi - \big(\chi^2(\rho_{\mathrm{per},L} - \mu_{\mathrm{per},L}) + (1-\chi^2)(\rho_{\mathrm{per},R} - \mu_{\mathrm{per},R}) + \eta_\chi\big), \tag{3-8}$$

where η_χ has compact support in the x-direction:

$$\eta_\chi := -\frac{1}{4\pi}\big(\partial_x^2(\chi^2)(V_{\mathrm{per},L} - V_{\mathrm{per},R}) + 2\partial_x(\chi^2)\partial_x(V_{\mathrm{per},L} - V_{\mathrm{per},R})\big). \tag{3-9}$$

Let us emphasize that the Poisson's equation (3-8) is defined on the whole space $\mathbb{R}^3$.

The nuclear density of the junction is a fictitious nuclear density plus a perturbation. Once we have defined fictitious nuclear density, we can treat the difference between the real nuclear density of the junction system μ_J and the fictitious nuclear density μ_χ as a perturbative nuclear density. By doing so we can define a finite renormalized energy with respect to the perturbative nuclear density. Note that this idea is similar to the definition of the defect state in [Cancès et al. 2008] for defects in crystals, and the polarization of the vacuum in the Bogoliubov–Dirac–Fock model [Hainzl et al. 2005a; 2007; 2009]. Introduce

$$\nu_\chi := \mu_J - \mu_\chi = (\mathbb{1}_{x\le 0} - \chi^2)(\mu_{\mathrm{per},L} - \mu_{\mathrm{per},R}) + (\chi^2\rho_{\mathrm{per},L} + (1-\chi^2)\rho_{\mathrm{per},R} - \rho_\chi) + \eta_\chi + \upsilon. \quad (3\text{-}10)$$

In order to guarantee that the perturbative state has a finite Coulomb energy, we need $D(\nu_\chi,\nu_\chi) < +\infty$. A sufficient condition is that ν_χ belongs to $L^{6/5}(\mathbb{R}^3)$. This motivates the following L^p-estimate on η_χ.

Lemma 3.3. *The function η_χ defined in (3-9) belongs to $L^p(\mathbb{R}^3)$ for $1 < p < 6$.*

The proof can be read in Section 4E. In view of Lemma 3.3 and Proposition 3.2, together with the fact that $(\mathbb{1}_{x\le 0} - \chi^2)(\mu_{\mathrm{per},L} - \mu_{\mathrm{per},R})$ has compact support and υ belongs to $L^{6/5}(\mathbb{R}^3)$, it is easy to see that ν_χ belongs to $L^{6/5}(\mathbb{R}^3)$, and hence to the Coulomb space $\mathcal{C}$ defined in (3-4). This means that the perturbative state generated by the nuclear density ν_χ has finite Coulomb energy.

Remark 3.4. The integrability of V_{per} provided by Lemma 2.10 is crucial to deduce Lemma 3.3.

3C. ***Definition of the perturbative state.*** In this section we define a perturbative state associated with the perturbative density ν_χ following the ideas developed in [Cancès et al. 2008]. We formally derive the rHF energy difference between the junction state γ_J and the reference state γ_χ by writing $\gamma_J = \gamma_\chi + Q_\chi$ with Q_χ a trial density state. In view of (3-3), we formally have

$$\begin{aligned}
&\mathcal{E}(\gamma_J) - \mathcal{E}(\gamma_\chi)\\
&= \mathrm{Tr}\big(-\tfrac12\Delta(\gamma_\chi + Q_\chi)\big) + \tfrac12 D(\rho_J - \mu_J, \rho_J - \mu_J) - \mathrm{Tr}\big(-\tfrac12\Delta\gamma_\chi\big) - \tfrac12 D(\rho_\chi - \mu_\chi, \rho_\chi - \mu_\chi)\\
&= \mathrm{Tr}(-\tfrac12\Delta Q_\chi) + D(\rho_\chi - \mu_\chi, \rho_{Q_\chi}) - D(\rho_{Q_\chi}, \nu_\chi) + \tfrac12 D(\rho_{Q_\chi}, \rho_{Q_\chi}) - D(\rho_\chi - \mu_\chi, \nu_\chi) + \tfrac12 D(\nu_\chi, \nu_\chi)\\
&= \mathrm{Tr}(H_\chi Q_\chi) - D(\rho_{Q_\chi}, \nu_\chi) + \tfrac12 D(\rho_{Q_\chi}, \rho_{Q_\chi}) - D(\rho_\chi - \mu_\chi, \nu_\chi) + \tfrac12 D(\nu_\chi, \nu_\chi). \qquad (3\text{-}11)
\end{aligned}$$

We next give a mathematical definition of the terms in the last equality of (3-11). We expect Q_χ to be a perturbation of the reference state γ_χ. More precisely, we expect Q_χ to be Hilbert–Schmidt. This is usually called the Shale–Stinespring condition [1965]; see [Lewin 2009; Solovej 2005] for a detailed discussion. Moreover, we also expect the kinetic energy of Q_χ to be finite. Let Π be an orthogonal projector on the Hilbert space $\mathfrak{H}$ such that both Π and $\Pi^\perp := 1 - \Pi$ have infinite ranks. A self-adjoint compact operator A on $\mathfrak{H}$ is said to be Π-trace class if $A \in \mathfrak{S}_2(\mathfrak{H})$ and both $\Pi A \Pi$ and $\Pi^\perp A \Pi^\perp$ are in $\mathfrak{S}_1(\mathfrak{H})$. For an operator A we define its Π-trace as

$$\mathrm{Tr}_\Pi(A) := \mathrm{Tr}(\Pi A \Pi) + \mathrm{Tr}(\Pi^\perp A \Pi^\perp),$$

and denote by $\mathfrak{S}_1^\Pi(\mathfrak{H})$ the associated set of Π-trace class operators. Since the reference state γ_χ defined in (3-7) is an orthogonal projector on $L^2(\mathbb{R}^3)$, we can define associated γ_χ-trace class operators. For any trial density matrix Q_χ, let us define by $Q_\chi^{++} := \gamma_\chi^\perp Q_\chi \gamma_\chi^\perp$ and $Q_\chi^{--} := \gamma_\chi Q_\chi \gamma_\chi$, and introduce a Banach space of operators with finite γ_χ-trace and finite kinetic energy as follows:

$$\mathcal{Q}_\chi := \big\{ Q_\chi \in \mathfrak{S}_1^{\gamma_\chi}(L^2(\mathbb{R}^3)) \;\big|\; Q_\chi^* = Q_\chi,\ |\nabla| Q_\chi \in \mathfrak{S}_2(L^2(\mathbb{R}^3)),\\ |\nabla| Q_\chi^{++} |\nabla| \in \mathfrak{S}_1(L^2(\mathbb{R}^3)),\ |\nabla| Q_\chi^{--} |\nabla| \in \mathfrak{S}_1(L^2(\mathbb{R}^3)) \big\},$$

equipped with its natural norm

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

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

$$\mathcal{K}_\chi := \{ Q_\chi \in \mathcal{Q}_\chi \mid -\gamma_\chi \le Q_\chi \le 1 - \gamma_\chi \}.$$

Note that $\mathcal{K}_\chi$ is not empty since it contains at least 0. Note also that $\mathcal{K}_\chi$ is the convex hull of states in $\mathcal{Q}_\chi$ of the special form $\gamma - \gamma_\chi$, where γ is an orthogonal projector [Cancès et al. 2008]. Furthermore, for any $Q_\chi \in \mathcal{K}_\chi$ a simple algebraic calculation shows that

$$Q_\chi^{++} \ge 0, \quad Q_\chi^{--} \le 0, \quad 0 \le Q_\chi^2 \le Q_\chi^{++} - Q_\chi^{--}.$$

As mentioned in the previous section, the Fermi level ϵ_F can be an eigenvalue of H_χ. Consider $N \in \mathbb{N}^*$ such that $\epsilon_F \in (\Sigma_{N,\chi}, \Sigma_{N+1,\chi}]$, where $\Sigma_{N,\chi} < \Sigma_{N+1,\chi}$ are two eigenvalues of H_χ in the gap (Σ_a, Σ_b), and let $\Sigma_{N,\chi} = \Sigma_a$ and $\Sigma_{N+1,\chi} = \Sigma_b$ whenever there is no such element. For any $\kappa \in (\Sigma_{N,\chi}, \epsilon_F)$, let us introduce the following rHF kinetic energy of a state $Q_\chi \in \mathcal{Q}_\chi$:

$$\operatorname{Tr}_{\gamma_\chi}(H_\chi Q_\chi) := \operatorname{Tr}\big(|H_\chi - \kappa|^{1/2}(Q_\chi^{++} - Q_\chi^{--})|H_\chi - \kappa|^{1/2}\big) + \kappa \operatorname{Tr}_{\gamma_\chi}(Q_\chi).$$

By [Cancès et al. 2008, Corollary 1], the above expression is independent of $\kappa \in (\Sigma_{N,\chi}, \epsilon_F)$. In view of the last line of (3-11) we introduce the following minimization problem

$$E_{\kappa,\chi} = \inf_{Q_\chi \in \mathcal{K}_\chi} \{ \mathcal{E}_\chi(Q_\chi) - \kappa \operatorname{Tr}_{\gamma_\chi}(Q_\chi) \}, \tag{3-12}$$

where

$$\mathcal{E}_\chi(Q_\chi) := \operatorname{Tr}_{\gamma_\chi}(H_\chi Q_\chi) - D(\rho_{Q_\chi}, \nu_\chi) + \tfrac{1}{2} D(\rho_{Q_\chi}, \rho_{Q_\chi}). \tag{3-13}$$

3D. *Properties of the junction system.* The following result shows that the minimization problem (3-12) is well-posed and admits minimizers.

Proposition 3.5 (existence of the perturbative ground state). *Assume that Assumption 2 holds. Then there exist minimizers for the problem (3-12). There may be several minimizers, but they all share the same density. Moreover, any minimizer $\bar{Q}_\chi$ of (3-12) satisfies the following self-consistent equation*:

$$\begin{cases} \bar{Q}_\chi = \mathbb{1}_{(-\infty,\epsilon_F)}(H_{\bar{Q}_\chi}) - \gamma_\chi + \delta_\chi, \\ H_{\bar{Q}_\chi} = H_\chi + (\rho_{\bar{Q}_\chi} - \nu_\chi) \star |\cdot|^{-1}, \end{cases} \tag{3-14}$$

where δ_χ is a finite-rank self-adjoint operator satisfying $0 \le \delta_\chi \le 1$ *and* $\operatorname{Ran}(\delta_\chi) \subseteq \operatorname{Ker}(H_{\bar{Q}_\chi} - \epsilon_F)$.

The proof is a direct adaptation of several results obtained in [Cancès et al. 2008, Proposition 1, Lemma 2, Corollary 1, Corollary 2 and Theorem 2]. A short summary of main arguments can also be read in [Cao 2019b, Proposition 3.5]. Note that $(\rho_{\overline{Q}_\chi} - \nu_\chi) \star |\cdot|^{-1} \in L^6(\mathbb{R}^3)$ by [Cancès and Stoltz 2012, Lemma 16]; therefore $(1-\Delta)^{-1}(\rho_{\overline{Q}_\chi} - \nu_\chi) \star |\cdot|^{-1}$ belongs to $\mathfrak{S}_6$ by the Kato–Seiler–Simon inequality (4-1). Hence $(\rho_{\overline{Q}_\chi} - \nu_\chi) \star |\cdot|^{-1}$ is $-\Delta$-compact and thus H_χ-compact by the boundedness of V_χ, leaving the essential spectrum unchanged. Therefore in view of Proposition 3.1, the following corollary holds.

Corollary 3.5.1. *For any $\chi \in \mathcal{X}$ and $H_{\overline{Q}_\chi}$ a solution of (3-14), it holds*

$$\sigma_{\mathrm{ess}}(H_{\overline{Q}_\chi}) = \sigma_{\mathrm{ess}}(H_{\mathrm{per},L}) \cup \sigma_{\mathrm{ess}}(H_{\mathrm{per},R}), \qquad \sigma_{\mathrm{ess}}(H_{\overline{Q}_\chi}) \cap (-\infty, 0] \subseteq \sigma_{\mathrm{ac}}(H_{\overline{Q}_\chi}).$$

In particular, $[0,+\infty) \subset \sigma_{\mathrm{ess}}(H_{\overline{Q}_\chi})$ and $\sigma_{\mathrm{ess}}(H_{\overline{Q}_\chi})$ does not depend on the shape of the cut-off function $\chi \in \mathcal{X}$ defined in (3-5).

The result of Proposition 3.5 can be interpreted as follows: given a cut-off function χ belonging to the class $\mathcal{X}$ defined in (3-5), we can construct a reference state γ_χ and a perturbative ground state $\overline{Q}_\chi$, the sum of which forms the ground state of the junction system. However it is artificial to introduce cut-off functions χ since there are infinitely many possible choices. In view of (3-2), the ground state of the junction system should not depend on the choice of cut-off functions. The following theorem shows that the electronic density of the junction system is indeed independent of the choice of the cut-off function χ.

Theorem 3.6 (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 χ, where ρ_χ is the density associated with the spectral projector γ_χ defined in (3-7), and ρ_{Q_χ} is the unique density associated with the solution Q_χ of the minimization problem (3-14).*

The proof can be read in Section 4F. Theorem 3.6 and Proposition 3.5 together imply that:

Corollary 3.6.1. *The ground state of the junction system (3-2) is of the form*

$$\mathbb{1}_{(-\infty,\epsilon_F)}(H_\chi + (\rho_{\overline{Q}_\chi} - \nu_\chi) \star |\cdot|^{-1}) + \delta_\chi, \quad 0 \le \delta_\chi \le 1, \quad \mathrm{Ran}(\delta_\chi) \subseteq \mathrm{Ker}(H_\chi + (\rho_{\overline{Q}_\chi} - \nu_\chi) \star |\cdot|^{-1} - \epsilon_F),$$

and its density is independent of the choice of χ.

Note that an extension to junctions of 2-dimensional materials may be done by similar constructions as above; see [Cao 2019a] for more details.

4. Proofs of the results

In order to simplify the notation, in Sections 4A–4C when treating the quasi-1-dimensional periodic system we denote by $\mathfrak{S}_p$ the Schatten class $\mathfrak{S}_p(L^2_{\mathrm{per},x}(\Gamma))$ for $1 \le p \le +\infty$. Unless otherwise specified, starting from Section 4D we use $\mathfrak{S}_p$ instead of $\mathfrak{S}_p(L^2(\mathbb{R}^3))$ for the proofs of the junction system. First of all, let us recall the following Kato–Seiler–Simon (KSS) inequality:

Lemma 4.1 [Seiler and Simon 1975, Lemma 2.1]. *Let $2 \le p \le \infty$. For g, f belonging to $L^p(\mathbb{R}^3)$, the following inequality holds*:

$$\|f(-\mathrm{i}\nabla)g(x)\|_{\mathfrak{S}_p(L^2(\mathbb{R}^3))} \le (2\pi)^{-3/p}\|g\|_{L^p(\mathbb{R}^3)}\|f\|_{L^p(\mathbb{R}^3)}. \tag{4-1}$$

4A. ***Proof of Lemma 2.5.*** We prove this lemma by an explicit construction of a density matrix belonging to $\mathcal{F}_\Gamma$. Consider a cut-off function $\psi \in C_c^\infty(\Gamma)$ such that $0 \le \psi \le 1$ and $\int_\Gamma \psi^2 = 1$, and define $\psi_{\mathrm{per}} = \sum_{n\in\mathbb{N}} \psi(\cdot - n)$. Let $\omega \ge 0$ be a parameter to be made precise later. Define

$$\gamma_\omega = \mathbb{1}_{[0,\omega]}(-\Delta)\psi_{\mathrm{per}}^2\mathbb{1}_{[0,\omega]}(-\Delta). \tag{4-2}$$

It is easy to see that $0 \le \gamma_\omega \le 1$, and that $\tau_k^x\gamma_\omega = \gamma_\omega\tau_k^x$ for all $k \in \mathbb{Z}$ by construction. It is also easy to see that the density of γ_ω is

$$\rho_{\gamma_\omega} = \frac{1}{(2\pi)^3}\int_{|k^2|\le\omega} dk = (6\pi)^{-2}\omega^{3/2}\psi_{\mathrm{per}}^2,$$

which is smooth and Γ-periodic. Moreover, it holds $\int_\Gamma \rho_{\gamma_\omega} = (6\pi)^{-2}\omega^{2/3}$. The kinetic energy per unit cell of γ_ω can be written as

$$\mathrm{Tr}_{L^2_{\mathrm{per},x}(\Gamma)}\big(|\nabla|\mathbb{1}_{[0,\omega]}(-\Delta)\psi_{\mathrm{per}}^2\mathbb{1}_{[0,\omega]}(-\Delta)|\nabla|\big) = \frac{1}{(2\pi)^3}\int_{|k|^2\le\omega}|k|^2\,dk = \frac{1}{10\pi^2}\omega^{5/2}.$$

Hence for all finite ω, we have γ_ω belongs to $\mathcal{P}_{\mathrm{per},x}$. Let us now show that there exists $\omega_* \ge 0$ such that $\rho_{\gamma_{\omega_*}} - \mu_{\mathrm{per}} \in \mathcal{C}_\Gamma$. It is easy to see that there exists $\omega_* > 0$ such that

$$\int_\Gamma \rho_{\gamma_{\omega_*}} = (6\pi)^{-2}\omega_*^{2/3} = \int_\Gamma \mu_{\mathrm{per}}. \tag{4-3}$$

This condition is equivalent to $\mathscr{F}(\rho_{\gamma_{\omega_*}} - \mu_{\mathrm{per}})(0, \mathbf{0}) = 0$. As $\boldsymbol{k} \mapsto \mathscr{F}(\rho_{\gamma_{\omega_*}} - \mu_{\mathrm{per}})(0, \boldsymbol{k})$ is $C^1(\mathbb{R}^2)$ and bounded, the function $\boldsymbol{k} \mapsto |\boldsymbol{k}|^{-1}\mathscr{F}(\rho_{\gamma_{\omega_*}} - \mu_{\mathrm{per}})(0, \boldsymbol{k})$ is in $L^2_{\mathrm{loc}}(\mathbb{R}^2)$. In view of this, there exists a positive constant C such that

$$\begin{aligned}
&\sum_{n\in\mathbb{Z}}\int_{\mathbb{R}^2}\frac{|\mathscr{F}(\rho_{\gamma_{\omega_*}} - \mu_{\mathrm{per}})(n, \boldsymbol{k})|^2}{|\boldsymbol{k}|^2 + 4\pi^2n^2}\,d\boldsymbol{k}\\
&\le \int_{|\boldsymbol{k}|\le 2\pi}\frac{|\mathscr{F}(\rho_{\gamma_{\omega_*}} - \mu_{\mathrm{per}})(0, \boldsymbol{k})|^2}{|\boldsymbol{k}|^2}\,d\boldsymbol{k}\\
&\qquad + \frac{1}{4\pi^2}\bigg(\int_{|\boldsymbol{k}|>2\pi}|\mathscr{F}(\rho_{\gamma_{\omega_*}} - \mu_{\mathrm{per}})(0, \boldsymbol{k})|^2\,d\boldsymbol{k} + \sum_{n\in\mathbb{Z}\setminus\{0\}}\int_{\mathbb{R}^2}|\mathscr{F}(\rho_{\gamma_{\omega_*}} - \mu_{\mathrm{per}})(n, \boldsymbol{k})|^2\,d\boldsymbol{k}\bigg)\\
&\le C + \frac{1}{4\pi^2}\int_\Gamma|\rho_{\gamma_{\omega_*}} - \mu_{\mathrm{per}}|^2 < +\infty.
\end{aligned} \tag{4-4}$$

In view of the definition of the Coulomb energy (2-13), we can therefore conclude that

$$D_\Gamma(\rho_{\gamma_{\omega_*}} - \mu_{\mathrm{per}}, \rho_{\gamma_{\omega_*}} - \mu_{\mathrm{per}}) < +\infty.$$

This concludes the proof that $\gamma_{\omega_*} \in \mathcal{F}_\Gamma$. Hence $\mathcal{F}_\Gamma$ is not empty. As any density ρ_γ associated with $\gamma \in \mathcal{P}_{\mathrm{per},x}$ is integrable, we can conclude that (2-16) holds in view of Remark 2.4.

4B. ***Proof of Theorem 2.6.*** We prove the existence of minimizers and the uniqueness of the density of minimizers for the problem (2-17) by considering a minimizing sequence of the energy functional, and show that there is no loss of compactness. This approach is rather classical for rHF-type models [Catto et al. 2001; Cancès et al. 2008; 2013; 2020]. But in our case we need to be careful as electrons might escape to infinity in the $\boldsymbol{r}$-direction. We show that this is impossible thanks to the Coulomb interactions.

First of all, it is convenient to introduce the following Banach space of operators which are $\mathbb{Z}$-translation-invariant in the x-direction:

$$\mathfrak{S}^x_{1,\mathrm{per}}(\Gamma) := \{\gamma \in \mathcal{S}(L^2(\mathbb{R}^3)) \mid \tau^x_k \gamma = \gamma \tau^x_k \text{ for all } k \in \mathbb{Z},\ \underline{\mathrm{Tr}}_{L^2(\Gamma)}(|\gamma|) := \mathrm{Tr}_{L^2(\mathbb{R}^3)}(\mathbb{1}_\Gamma |\gamma| \mathbb{1}_\Gamma) < +\infty\},$$

equipped with the norm $\|\gamma\|_{\mathfrak{S}^x_{1,\mathrm{per}}(\Gamma)} := \underline{\mathrm{Tr}}_{L^2(\Gamma)}(|\gamma|)$. In view of (2-1), it is clear that for any operator $\gamma \in \mathcal{F}_\Gamma$, it holds that

$$\mathrm{Tr}_{L^2(\mathbb{R}^3)}(\mathbb{1}_\Gamma \gamma \mathbb{1}_\Gamma) = \int_\Gamma \rho_\gamma = \frac{1}{2\pi}\int_{\Gamma^*}\left(\int_\Gamma \rho_{\gamma_\xi}\right) d\xi = \frac{1}{2\pi}\int_{\Gamma^*} \mathrm{Tr}_{L^2_{\mathrm{per},x}(\Gamma)}(\gamma_\xi)\, d\xi.$$

Therefore any operator $0 \le \gamma \le 1$ belongs to $\mathcal{F}_\Gamma$ if and only if $\gamma \in \mathfrak{S}^x_{1,\mathrm{per}}(\Gamma)$, $\sqrt{-\Delta}\gamma\sqrt{-\Delta} \in \mathfrak{S}^x_{1,\mathrm{per}}(\Gamma)$ and $\rho_\gamma - \mu_{\mathrm{per}} \in \mathcal{C}_\Gamma$.

For any $\gamma \in \mathfrak{S}^x_{1,\mathrm{per}}(\Gamma)$, define $\underline{\mathrm{Tr}}_{L^2(\Gamma)}\big(-\frac{1}{2}\Delta\gamma\big) := \frac{1}{2}\mathrm{Tr}_{L^2(\mathbb{R}^3)}(\mathbb{1}_\Gamma\sqrt{-\Delta}\gamma\sqrt{-\Delta}\mathbb{1}_\Gamma)$. Consider a minimizing sequence γ_n of the energy functional

$$\mathcal{E}_{\mathrm{per},x}(\gamma) = \underline{\mathrm{Tr}}_{L^2(\Gamma)}\big(-\tfrac{1}{2}\Delta\gamma\big) + \tfrac{1}{2} D_\Gamma(\rho_\gamma - \mu_{\mathrm{per}}, \rho_\gamma - \mu_{\mathrm{per}})$$

on $\mathcal{F}_\Gamma$. Therefore there exists $C > 0$ such that for all $n \ge 1$

$$0 \le \underline{\mathrm{Tr}}_{L^2(\Gamma)}\big(-\tfrac{1}{2}\Delta\gamma_n\big) \le C, \quad 0 \le D_\Gamma(\rho_{\gamma_n} - \mu_{\mathrm{per}}, \rho_{\gamma_n} - \mu_{\mathrm{per}}) \le C. \tag{4-5}$$

By Lemma 2.5, we also have

$$\underline{\mathrm{Tr}}_{L^2(\Gamma)}(\gamma_n) = \int_\Gamma \mu_{\mathrm{per}}. \tag{4-6}$$

In view of (4-5) and (4-6), we deduce that there exist (up to extraction) γ and T belonging to $\mathfrak{S}^x_{1,\mathrm{per}}(\Gamma)$ such that $\gamma_n \overset{*}{\rightharpoonup} \gamma \in \mathfrak{S}^x_{1,\mathrm{per}}(\Gamma)$ and $\sqrt{-\Delta}\gamma_n\sqrt{-\Delta} \overset{*}{\rightharpoonup} T \in \mathfrak{S}^x_{1,\mathrm{per}}(\Gamma)$. Besides, the bounds (4-5) also imply that $\rho_{\gamma_n} - \mu_{\mathrm{per}} \rightharpoonup \tilde{\rho}_\gamma - \mu_{\mathrm{per}}$ weakly in $\mathcal{C}_\Gamma$, and hence in $\mathcal{D}'(\mathbb{R}^3)$ (see [Cao 2019a, Lemma 3.21, page 111] for details), the space of distributions.

The identification of $T \equiv \sqrt{-\Delta}\gamma\sqrt{-\Delta}$ is straightforward by testing these operators against operators with compact support and by the uniqueness of the weak limit in $\mathfrak{S}^x_{1,\mathrm{per}}(\Gamma)$. Let us prove that $\rho_\gamma \equiv \tilde{\rho}_\gamma \in \mathcal{D}'(\mathbb{R}^3)$: since $\gamma_n \overset{*}{\rightharpoonup} \gamma \in \mathfrak{S}^x_{1,\mathrm{per}}(\Gamma)$ and $\sqrt{-\Delta}\gamma_n\sqrt{-\Delta}$ is bounded in $\mathfrak{S}^x_{1,\mathrm{per}}(\Gamma)$, the density ρ_{γ_n} is therefore bounded in $L^1_{\mathrm{per},x}(\Gamma)$ and $\nabla\sqrt{\rho_{\gamma_n}}$ is bounded in $L^2_{\mathrm{per},x}(\Gamma)$ by the Hoffmann-Ostenhof inequality (2-12). Therefore ρ_{γ_n} converges weakly in $L^r_{\mathrm{per},x}(\Gamma)$ for $1 < r \le 3$, and strongly locally in $L^q(\mathbb{R}^3)$ to ρ_γ for $1 \le q < 3$; hence $\rho_\gamma \equiv \tilde{\rho}_\gamma \in \mathcal{D}'(\mathbb{R}^3)$.

Thus the uniform bound (4-5) together with the weak convergence of $\sqrt{-\Delta}\gamma_n\sqrt{-\Delta} \overset{*}{\rightharpoonup} \sqrt{-\Delta}\gamma\sqrt{-\Delta} \in \mathfrak{S}^x_{1,\mathrm{per}}(\Gamma)$ implies

$$\underline{\mathrm{Tr}}_{L^2(\Gamma)}\big(-\tfrac{1}{2}\Delta\gamma\big) \le \liminf_{n\to\infty} \underline{\mathrm{Tr}}_{L^2(\Gamma)}\big(-\tfrac{1}{2}\Delta\gamma_n\big). \tag{4-7}$$

The inequality (4-7) also implies $\sqrt{\rho_\gamma} \in H^1_{\mathrm{per},x}(\Gamma)$ by the Hoffmann-Ostenhof inequality (2-12). Hence $\rho_\gamma \in L^p_{\mathrm{per},x}(\Gamma)$ for $1 \le p \le 3$.

Remark 4.2 (charge conservation in the limit). Since $\rho_\gamma - \mu_{\mathrm{per}}$ is an element in $\mathcal{C}_\Gamma$, this implies that the charge is neutral by Remark 2.4. That is, $\int_\Gamma \rho_\gamma = \int_\Gamma \mu_{\mathrm{per}}$.

As $D_\Gamma(\cdot\,,\cdot)$ defines an inner product on $\mathcal{C}_\Gamma$, by the weak convergence of $\rho_{\gamma_n} - \mu_{\mathrm{per}}$ to $\rho_\gamma - \mu_{\mathrm{per}}$ in $\mathcal{C}_\Gamma$ we obtain

$$D_\Gamma(\rho_\gamma - \mu_{\mathrm{per}}, \rho_\gamma - \mu_{\mathrm{per}}) \le \liminf_{n\to\infty} D_\Gamma(\rho_{\gamma_n} - \mu_{\mathrm{per}}, \rho_{\gamma_n} - \mu_{\mathrm{per}}). \tag{4-8}$$

In view of (4-7) and (4-8), we conclude that

$$\mathcal{E}_{\mathrm{per},x}(\gamma) \le \liminf_{n\to\infty} \mathcal{E}_{\mathrm{per},x}(\gamma_n),$$

which shows that the state γ is a minimizer of the problem (2-17).

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

$$\mathcal{E}_{\mathrm{per},x}\big(\tfrac{1}{2}(\bar{\gamma}_1 + \bar{\gamma}_2)\big) = \tfrac{1}{2}\mathcal{E}_{\mathrm{per},x}(\bar{\gamma}_1) + \tfrac{1}{2}\mathcal{E}_{\mathrm{per},x}(\bar{\gamma}_2) - \tfrac{1}{4} D_\Gamma(\rho_{\bar{\gamma}_1} - \rho_{\bar{\gamma}_2}, \rho_{\bar{\gamma}_1} - \rho_{\bar{\gamma}_2}),$$

which shows that $D_\Gamma(\rho_{\bar{\gamma}_1} - \rho_{\bar{\gamma}_2}, \rho_{\bar{\gamma}_1} - \rho_{\bar{\gamma}_2}) \equiv 0$; hence all the minimizers of the problem (2-17) share the same density.

4C. *Proof of Theorem 2.7.* We first define a mean-field Hamiltonian associated with the problem (2-17), and then show that the Fermi level is always negative. Moreover, the minimizer of (2-17) is uniquely given by the spectral projector of the mean-field Hamiltonian. In the end we show that the density of the minimizer decays exponentially fast in the $\boldsymbol{r}$-direction.

Properties of the mean-field potential and Hamiltonian. We begin with the definition of a mean-field potential and a mean-field Hamiltonian, and next study the spectrum of the mean-field Hamiltonian. Consider a minimizer γ_{per} of (2-17) with the unique density $\rho_{\gamma_{\mathrm{per}}} \in L^p_{\mathrm{per},x}(\Gamma)$, where $1 \le p \le 3$. Define the mean-field potential

$$V_{\mathrm{per}} := q_{\mathrm{per}} \star_\Gamma G, \qquad q_{\mathrm{per}} := \rho_{\gamma_{\mathrm{per}}} - \mu_{\mathrm{per}},$$

which is the solution of Poisson's equation $-\Delta V_{\mathrm{per}} = 4\pi q_{\mathrm{per}}$. Let us prove that V_{per} belongs to $L^p_{\mathrm{per},x}(\Gamma)$ for $2 < p \le +\infty$. As μ_{per} is smooth and has compact support in the $\boldsymbol{r}$-direction and $\rho_{\gamma_{\mathrm{per}}}$ belongs to $L^p_{\mathrm{per},x}(\Gamma)$ for $1 \le p \le 3$; hence $\mathscr{F} q_{\mathrm{per}}(0,\cdot)$ belongs to $L^2(\mathbb{R}^2) \cap L^\infty(\mathbb{R}^2) \cap C^0(\mathbb{R}^2)$ by classical Fourier theory; see for example [Reed and Simon 1975]. Moreover, as $\int_\Gamma |\boldsymbol{r}|\rho_{\gamma_{\mathrm{per}}}(x,\boldsymbol{r}) < +\infty$ by (2-18),

$$\begin{aligned}\|\partial_{\boldsymbol{k}} \mathscr{F} q_{\mathrm{per}}(0,\boldsymbol{k})\|_{L^\infty(\mathbb{R}^2)} &= \left|\int_\Gamma \mathrm{e}^{-\mathrm{i}\boldsymbol{r}\cdot\boldsymbol{k}} \boldsymbol{r}\cdot q_{\mathrm{per}}(x,\boldsymbol{r})\,dx\,d\boldsymbol{r}\right| \\ &\le \left|\int_\Gamma |\boldsymbol{r}|\,|\rho_{\gamma_{\mathrm{per}}} + \mu_{\mathrm{per}}|(x,\boldsymbol{r})\,dx\,d\boldsymbol{r}\right| < +\infty. \end{aligned}\tag{4-9}$$

This implies that $\mathscr{F}q_{\text{per}}(0,\boldsymbol{k})$ is $C^1(\mathbb{R}^2)$ and bounded. Note also that $\mathscr{F}q_{\text{per}}(0,\mathbf{0})=0$ by the charge neutrality and that $\mathscr{F}q_{\text{per}}(0,\cdot)$ belongs to $L^2(\mathbb{R}^2)\cap L^\infty(\mathbb{R}^2)\cap C^0(\mathbb{R}^2)$; hence, for $1\le\alpha<2$,

$$\begin{aligned}\int_{\mathbb{R}^2}|\mathscr{F}V_{\text{per}}(0,\boldsymbol{k})|^\alpha\,d\boldsymbol{k}&=\int_{\mathbb{R}^2}\frac{|\mathscr{F}q_{\text{per}}(0,\boldsymbol{k})|^\alpha}{|\boldsymbol{k}|^{2\alpha}}\,d\boldsymbol{k}\\&\le\int_{|\boldsymbol{k}|<1}\frac{|\mathscr{F}q_{\text{per}}(0,\boldsymbol{k})|^\alpha}{|\boldsymbol{k}|^{2\alpha}}\,d\boldsymbol{k}+\left(\int_{|\boldsymbol{k}|\ge1}|\mathscr{F}q_{\text{per}}(0,\boldsymbol{k})|^{2\alpha}\,d\boldsymbol{k}\right)^{1/2}\left(\int_{|\boldsymbol{k}|\ge1}\frac{1}{|\boldsymbol{k}|^{4\alpha}}\,d\boldsymbol{k}\right)^{1/2}\\&<+\infty.\end{aligned}\tag{4-10}$$

Note that the mixed Fourier transform $\mathscr{F}$ is an isometry from $L^2_{\text{per},x}(\Gamma)$ to $\ell^2(\mathbb{Z},L^2(\mathbb{R}^2))$ by (2-4). On the other hand,

$$\text{for all }\phi\in\ell^1(\mathbb{Z},L^1(\mathbb{R}^2)),\quad\|\mathscr{F}^{-1}\phi\|_{L^\infty(\Gamma)}=\sup_{x\in\Gamma}\left|\frac{1}{2\pi}\sum_{n\in\mathbb{Z}}\int_{\mathbb{R}^2}\phi_n(\boldsymbol{k})\,\mathrm{e}^{\mathrm{i}(2\pi nx+\boldsymbol{k}\cdot\boldsymbol{r})}\,d\boldsymbol{k}\right|\le\frac{1}{2\pi}\|\phi\|_{\ell^1(\mathbb{Z},L^1(\mathbb{R}^2))}.$$

By the Riesz–Thorin interpolation theorem (see for example [Reed and Simon 1975; Lieb and Loss 2001, Theorem 5.7]), we can deduce a Hausdorff–Young inequality for $\mathscr{F}^{-1}$: for $1\le\alpha\le2$ there exists a constant C_α depending on α such that

$$\text{for all }\phi\in\ell^\alpha(\mathbb{Z},L^\alpha(\mathbb{R}^2)),\quad\|\mathscr{F}^{-1}\phi\|_{L^{\alpha'}_{\text{per},x}(\Gamma)}\le C_\alpha\|\phi\|_{\ell^\alpha(\mathbb{Z},L^\alpha(\mathbb{R}^2))},\tag{4-11}$$

where $\alpha':=\alpha/(\alpha-1)$. Hence in view of (4-10) and (4-11), for $1\le\alpha<2$ and $2<\alpha'=\alpha/(\alpha-1)\le+\infty$ there exist positive constants $C_{\alpha,1}$, $C_{\alpha,2}$ and $C'_{\alpha,2}$ such that

$$\begin{aligned}\|V_{\text{per}}\|^\alpha_{L^{\alpha'}_{\text{per},x}(\Gamma)}\le C^\alpha_\alpha\|\mathscr{F}V_{\text{per}}\|^\alpha_{\ell^\alpha(\mathbb{Z},L^\alpha(\mathbb{R}^2))}&=\frac{C^\alpha_\alpha}{2\pi}\sum_{n\in\mathbb{Z}}\int_{\mathbb{R}^2}|\mathscr{F}V_{\text{per}}(n,\boldsymbol{k})|^\alpha\,d\boldsymbol{k}\\&=\frac{C^\alpha_\alpha}{2\pi}\int_{\mathbb{R}^2}|\mathscr{F}V_{\text{per}}(0,\boldsymbol{k})|^\alpha\,d\boldsymbol{k}+\frac{C^\alpha_\alpha}{2\pi}\sum_{n\neq0}\int_{\mathbb{R}^2}\frac{|\mathscr{F}q_{\text{per}}(n,\boldsymbol{k})|^\alpha}{(4\pi n^2+|\boldsymbol{k}|^2)^\alpha}\,d\boldsymbol{k}\\&\le C_{\alpha,1}+\frac{C^\alpha_\alpha}{2\pi}\left(\sum_{n\neq0}\int_{\mathbb{R}^2}|\mathscr{F}q_{\text{per}}(n,\boldsymbol{k})|^{2\alpha}\,d\boldsymbol{k}\right)^{1/2}\left(\sum_{n\neq0}\int_{\mathbb{R}^2}\frac{1}{(4\pi n^2+|\boldsymbol{k}|^2)^{2\alpha}}\,d\boldsymbol{k}\right)^{1/2}\\&\le C_{\alpha,1}+C_{\alpha,2}\|\mathscr{F}q_{\text{per}}\|^\alpha_{\ell^{2\alpha}(\mathbb{Z},L^{2\alpha}(\mathbb{R}^2))}\le C_{\alpha,1}+C'_{\alpha,2}\|q_{\text{per}}\|^\alpha_{L^q_{\text{per},x}(\Gamma)}<+\infty,\end{aligned}\tag{4-12}$$

where the last step we have used estimates similar to (4-11) for $\mathscr{F}$ and the fact that q_{per} belongs to $L^q_{\text{per},x}(\Gamma)$ for $\frac{4}{3}<q:=2\alpha/(2\alpha-1)\le2$. Therefore V_{per} belongs to $L^p_{\text{per},x}(\Gamma)$ for $2<p\le+\infty$. By the elliptic regularity we know that V_{per} belongs to the Sobolev space $W^{2,p}_{\text{per},x}(\Gamma)$ for $2<p\le3$, where $W^{2,p}_{\text{per},x}(\Gamma)$ is the space of functions, together with their gradients and hessians, belonging to $L^p_{\text{per},x}(\Gamma)$. Approximating V_{per} by functions in $\mathcal{D}_{\text{per},x}(\Gamma)$, we also deduce that V_{per} tends to 0 when $|\boldsymbol{r}|$ tends to infinity. The mean-field potential V_{per} defines a $-\Delta$-bounded operator on $L^2(\mathbb{R}^3)$ with relative bound zero; hence by the Kato–Rellich theorem (see for example [Helffer 2013, Theorem 9.10]) we know that $H_{\text{per}}=-\frac{1}{2}\Delta+V_{\text{per}}$ uniquely defines a self-adjoint operator on $L^2(\mathbb{R}^3)$ with domain $H^2(\mathbb{R}^3)$ and form

domain $H^1(\mathbb{R}^3)$. As H_{per} is $\mathbb{Z}$-translation-invariant in the x-direction,

$$H_{\text{per}} = \mathscr{B}^{-1}\left(\int_{\Gamma^*} H_{\text{per},\xi}\,\frac{d\xi}{2\pi}\right)\mathscr{B}, \qquad H_{\text{per},\xi} := -\tfrac{1}{2}\Delta_\xi + V_{\text{per}}.$$

Note that the decomposed Hamiltonian $H_{\text{per},\xi}$ does not have a compact resolvent as Γ is not a bounded domain. It is easy to see that $\sigma(-\Delta_\xi) = \sigma_{\text{ess}}(-\Delta_\xi) = [0, +\infty)$. On the other hand, by the inequality (2-6) we have

$$\|V_{\text{per}}(1-\Delta_\xi)^{-1}\|_{\mathfrak{S}_2} \le \frac{1}{2\pi}\|V_{\text{per}}\|_{L^2_{\text{per},x}(\Gamma)}\left(\sum_{n\in\mathbb{Z}}\int_{\mathbb{R}^2}\frac{1}{((2\pi n+\xi)^2+|\boldsymbol{k}|^2+1)^2}\,d\boldsymbol{k}\right)^{1/2} < +\infty.$$

In particular V_{per} is a compact perturbation of $-\Delta_\xi$, and therefore introduces at most countably many eigenvalues below 0 which are bounded from below by $-\|V_{\text{per}}\|_{L^\infty}$. Denote by $\{\lambda_n(\xi)\}_{1\le n\le N_H}$ these (negative) eigenvalues for $N_H \in \mathbb{N}^*$ (N_H can be finite or infinite). Then for all $\xi \in \Gamma^*$,

$$\sigma_{\text{ess}}(H_{\text{per},\xi}) = \sigma_{\text{ess}}(-\Delta_\xi) = [0, +\infty), \qquad \sigma_{\text{disc}}(H_{\text{per},\xi}) = \bigcup_{1\le n\le N_H}\lambda_n(\xi).$$

In view of the decomposition (2-19), a result of [Reed and Simon 1978, Theorem XIII.85] gives the spectral decomposition

$$\sigma_{\text{ess}}(H_{\text{per}}) \supseteq \bigcup_{\xi\in\Gamma^*}\sigma_{\text{ess}}(H_{\text{per},\xi}) = [0, +\infty), \qquad \sigma_{\text{disc}}(H_{\text{per}}) \subseteq \bigcup_{\xi\in\Gamma^*}\sigma_{\text{disc}}(H_{\text{per},\xi}) = \bigcup_{\xi\in\Gamma^*}\bigcup_{1\le n\le N_H}\lambda_n(\xi).$$

We also obtain from [Reed and Simon 1978, Theorem XIII.85(e)] that

$$\lambda \in \sigma_{\text{disc}}(H_{\text{per}}) \quad\Longleftrightarrow\quad \{\xi\in\Gamma^* \mid \lambda \in \sigma_{\text{disc}}(H_{\text{per},\xi})\} \text{ has nontrivial Lebesgue measure.}$$

By the regular perturbation theory of the point spectra [Kato 1966] (see also [Reed and Simon 1978, Section XII.2]) and the approach of Thomas [1973, Lemma 1], we know that the eigenvalues $\lambda_n(\xi)$ below 0 are analytical functions of ξ and cannot be constant, so that $\{\xi\in\Gamma^* \mid \lambda\in\sigma_{\text{disc}}(H_{\text{per},\xi})\}$ has trivial Lebesgue measure, and the essential spectrum of H_{per} below 0 is purely absolutely continuous. As a conclusion,

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

The Fermi level is always negative. Let us prove that the inequality $N_H = F(0) \ge \int_\Gamma \mu_{\text{per}}$ always holds. The physical meaning of this statement is that the Fermi level of the quasi-1-dimensional system at ground state is always negative when the mean-field potential tends to 0 in the $\boldsymbol{r}$-direction. We prove this by contradiction: Assume that $F(0) < \int_\Gamma \mu_{\text{per}}$. Then we can always construct (infinitely many) states belonging to $\mathcal{F}_\Gamma$ with positive energies arbitrarily close to 0 and they decrease the ground state energy of the problem (2-17).

Let us first define a spectral projector representing all the states of H_{per} below 0: for any $\xi\in\Gamma^*$ and $H_{\text{per},\xi}$ defined in (2-19), define

$$\gamma_{\text{per}}^- := \mathbb{1}_{(-\infty,0]}(H_{\text{per}}), \qquad \gamma_{\text{per},\xi}^- := \mathbb{1}_{(-\infty,0]}(H_{\text{per},\xi}).$$

Therefore,

$$N_H = F(0) = \frac{1}{|\Gamma^*|}\int_{\Gamma^*} \mathrm{Tr}_{L^2_{\mathrm{per},x}(\Gamma)}(\gamma^-_{\mathrm{per},\xi})\,d\xi = \int_\Gamma \rho_{\gamma^-_{\mathrm{per}}}. \tag{4-13}$$

The inequality $F(0) < \int_\Gamma \mu_{\mathrm{per}}$ implies

$$Z_{\mathrm{diff}} := \int_\Gamma \mu_{\mathrm{per}} - N_H = \int_\Gamma \mu_{\mathrm{per}} - \int_\Gamma \rho_{\gamma^-_{\mathrm{per}}} \quad \in \mathbb{N}^*. \tag{4-14}$$

The condition (4-14) implies in particular that $N_H < +\infty$, i.e., that there are at most finitely many states below 0. Let us construct states of H_{per} with positive energies. These states belonging to $L^2(\mathbb{R}^3)$ approximate the plane waves of H_{per} traveling in the $\boldsymbol{r}$-direction. For $R > 0$, recall that $\mathfrak{B}_R$ is the ball in $\mathbb{R}^3$ centered at 0. Consider a smooth function $t(x, \boldsymbol{r})$ supported in $\mathfrak{B}_1$, equal to 1 in $\mathfrak{B}_{1/2}$ and such that $\|t\|_{L^2(\mathbb{R}^3)} = 1$. For $n \in \mathbb{N}^*$, let us define

$$\psi_n(x, \boldsymbol{r}) := n^{-3/2} t\left(\frac{(x, \boldsymbol{r}) - (n^2, (n^2, n^2))}{n}\right).$$

It is easy to see that ψ_n belongs to $L^2(\mathbb{R}^3)$, converges weakly to 0 when n tends to infinity and $\|\psi_n\|_{L^2(\mathbb{R}^3)} = 1$. Moreover, as V_{per} tends to 0 in the $\boldsymbol{r}$-direction, for any $\epsilon > 0$ there exists an integer N_ϵ such that $|V_{\mathrm{per}}(\,\cdot\,, (n^2, n^2))| \le \epsilon$ when $n \ge N_\epsilon$. Denote by $\{\psi_{n,\xi}\}_{n\in\mathbb{N}^*,\xi\in\Gamma^*}$ the Bloch decomposition $\mathscr{B}$ in the x-direction (see Section 2A for the definition) of $\{\psi_n\}_{n\in\mathbb{N}^*}$ which belong to $L^2_{\mathrm{per},x}(\Gamma)$. For $n \ge N_\epsilon$, it holds

$$\begin{aligned}\|H_{\mathrm{per}}\psi_n\|^2_{L^2(\mathbb{R}^3)} &= \frac{1}{2\pi}\int_{\Gamma^*} \|H_{\mathrm{per},\xi}\psi_{n,\xi}\|^2_{L^2_{\mathrm{per},x}(\Gamma)}\,d\xi \\ &= \left\| -n^{-7/2}\Delta t\left(\frac{\cdot - (n^2, (n^2, n^2))}{n}\right) + V_{\mathrm{per}}\psi_n \right\|^2_{L^2(\mathbb{R}^3)} \le 2\left(\frac{1}{n^4} + \epsilon^2\right).\end{aligned} \tag{4-15}$$

Note that $\gamma^-_{\mathrm{per},\xi} H_{\mathrm{per},\xi} = \sum_{n=1}^{N_H} P_{\{\lambda_n(\xi)\}}(H_{\mathrm{per},\xi})$ is a compact operator, where $P_{\{\cdot\}}(H_{\mathrm{per},\xi})$ is the spectral projector of $H_{\mathrm{per},\xi}$. There exists an orthonormal basis $\{e_{n,\xi}\}_{n\ge 1}$ of $L^2_{\mathrm{per},x}(\Gamma)$ with elements in $H^1_{\mathrm{per},x}(\Gamma)$ such that $\gamma^-_{\mathrm{per},\xi} H_{\mathrm{per},\xi} e_{n,\xi} = \lambda_n(\xi) e_{n,\xi}$ for $1 \le n \le N_H$, and $\gamma^-_{\mathrm{per},\xi} H_{\mathrm{per},\xi} e_{n,\xi} \equiv 0$ for $n > N_H$. Let us construct test density matrices composed by all the states of H_{per} with negative energies and some states with positive energies. More precisely, for $N_0 \in \mathbb{N}^*$ to be made precise later, consider a test density matrix

$$\gamma_{N_0} = \mathscr{B}^{-1}\left(\int_{\Gamma^*} \gamma_{N_0,\xi}\,\frac{d\xi}{2\pi}\right)\mathscr{B},$$

where

$$\begin{aligned}\gamma_{N_0,\xi} &:= \gamma^-_{\mathrm{per},\xi} + \sum_{n=N_0+1}^{N_0+Z_{\mathrm{diff}}} (1 - \gamma^-_{\mathrm{per},\xi})|\psi_{n,\xi}\rangle\langle\psi_{n,\xi}| \\ &= \sum_{n=1}^{+\infty} \gamma^-_{\mathrm{per},\xi}|e_{n,\xi}\rangle\langle e_{n,\xi}| + \sum_{n=N_0+1}^{N_0+Z_{\mathrm{diff}}} (1 - \gamma^-_{\mathrm{per},\xi})|\psi_{n,\xi}\rangle\langle\psi_{n,\xi}|.\end{aligned}$$

Lemma 4.3. *For any $N_0 \in \mathbb{N}^*$, the state γ_{N_0} belongs to the admissible set $\mathcal{F}_\Gamma$.*

Proof. It is easy to see that $0 \le \gamma_{N_0} \le 1$. Note also that $\operatorname{Ran}(\gamma^-_{\mathrm{per},\xi}) = \operatorname{Span}\{e_{n,\xi}\}_{1\le n\le N_H}$ for all $\xi \in \Gamma^*$. The density of γ_{N_0} can be written as

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

The density $\rho_{\gamma_{N_0}}$ belongs to $L^p_{\mathrm{per}}(\Gamma)$ for $1 \le p \le 3$ as $\{e_{n,\xi}\}_{n\ge1}$ and $\{\psi_{n,\xi}\}_{n\ge1}$ belong to $H^1_{\mathrm{per},x}(\Gamma)$. Additionally, in view of (4-13),

$$\begin{aligned}\int_\Gamma \rho_{\gamma_{N_0}} &= \frac{1}{2\pi}\int_{\Gamma^*}\operatorname{Tr}_{L^2_{\mathrm{per},x}(\Gamma)}(\gamma^-_{\mathrm{per},\xi})\,d\xi + \frac{1}{2\pi}\sum_{n=N_0+1}^{N_0+Z_{\mathrm{diff}}}\int_\Gamma\int_{\Gamma^*}|\psi_{n,\xi}|^2\,d\xi \\ &= N_H + \sum_{n=N_0+1}^{N_0+Z_{\mathrm{diff}}}\int_{\mathbb{R}^3}|\psi_n|^2 = N_H + Z_{\mathrm{diff}} = \int_\Gamma \mu_{\mathrm{per}}. \end{aligned} \tag{4-16}$$

A simple calculation shows that $|\nabla|\gamma_{N_0,\xi}|\nabla|$ is trace-class on $L^2_{\mathrm{per},x}(\Gamma)$. Hence γ_{N_0} belongs to $\mathcal{P}_{\mathrm{per},x}$. Let us show that $\rho_{\gamma_{N_0}} - \mu_{\mathrm{per}}$ belongs to $\mathcal{C}_\Gamma$. Following calculations similar to the ones leading to (4-4), we only need to prove that $\boldsymbol{k} \mapsto |\boldsymbol{k}|^{-1}\mathscr{F}(\rho_{\gamma_{N_0}} - \mu_{\mathrm{per}})(0,\boldsymbol{k})$ is square-integrable near $\boldsymbol{k} = \boldsymbol{0}$ since $\rho_{\gamma_{N_0}} - \mu_{\mathrm{per}}$ belongs to $L^2_{\mathrm{per},x}(\Gamma)$. Note that

$$\mathscr{F}(\rho_{\gamma_{N_0}} - \mu_{\mathrm{per}})(0,\boldsymbol{0}) = \int_\Gamma \rho_{\gamma_{N_0}} - \mu_{\mathrm{per}} = 0$$

and

$$\begin{aligned}|\partial_{\boldsymbol{k}}\mathscr{F}(\rho_{\gamma_{N_0}} - \mu_{\mathrm{per}})(0,\boldsymbol{0})| &= \left|\int_\Gamma \boldsymbol{r}(\rho_{\gamma_{N_0}} - \mu_{\mathrm{per}})(x,\boldsymbol{r})\,dx\,d\boldsymbol{r}\right| \\ &\le \frac{1}{2\pi}\sum_{n=1}^{N_H}\int_{\Gamma^*}\int_\Gamma |\boldsymbol{r}|\,|e_{n,\xi}|^2(x,\boldsymbol{r})\,dx\,d\boldsymbol{r}\,d\xi \\ &\qquad + \sum_{n=N_0+1}^{N_0+Z_{\mathrm{diff}}}\int_{\mathbb{R}^3}|\boldsymbol{r}|\,|\psi_n|^2(x,\boldsymbol{r})\,dx\,d\boldsymbol{r} + \int_\Gamma |\boldsymbol{r}|\mu_{\mathrm{per}}(x,\boldsymbol{r})\,dx\,d\boldsymbol{r} < +\infty,\end{aligned}$$

where we have used the fact that the eigenfunctions of $H_{\mathrm{per},\xi}$ associated with negative eigenvalues decay exponentially (see [Hislop and Sigal 1996, Theorem 3.4] and [Combes and Thomas 1973, Theorem 1]) so that $\int_\Gamma |\boldsymbol{r}|\,|e_{n,\xi}|^2(x,\boldsymbol{r})\,dx\,d\boldsymbol{r} < +\infty$ for $1 \le n \le N_H$ and $\xi \in \Gamma^*$, and the fact that $\{\psi_n\}_{N_0+1\le n\le N_0+Z_{\mathrm{diff}}}$ have compact support in the $\boldsymbol{r}$-direction by definition. Therefore $\mathscr{F}(\rho_{\gamma_{N_0}} - \mu_{\mathrm{per}})(0,\boldsymbol{k})$ is C^1 near $\boldsymbol{k} = \boldsymbol{0}$. The conclusion then follows by arguments similar to those leading to (4-4) in Section 4A. □

Lemma 4.3 implies that we can construct many admissible states in $\mathcal{F}_\Gamma$ by varying N_0. Let us show that we can always find N_0 such that γ_{N_0} decreases the ground state energy of (2-17) if $N_H < \int_\Gamma \mu_{\mathrm{per}}$.

Given a minimizer $\bar\gamma$ of (2-17), simple expansion of the energy functional around minimal shows that $\bar\gamma$ also minimizes the functional (see [Cancès et al. 2008])

$$\gamma \mapsto \int_{\Gamma^*}\operatorname{Tr}_{L^2_{\mathrm{per},x}(\Gamma)}(H_{\mathrm{per},\xi}\gamma_\xi)\,d\xi$$

on $\mathcal{F}_\Gamma$. Therefore, given $N_0 \in \mathbb{N}^*$ we have

$$
\begin{aligned}
0 &\le \int_{\Gamma^*} \mathrm{Tr}_{L^2_{\mathrm{per},x}(\Gamma)}(H_{\mathrm{per},\xi}(\gamma_{N_0,\xi} - \bar{\gamma}_\xi))\, d\xi \\
&= \int_{\Gamma^*} \mathrm{Tr}_{L^2_{\mathrm{per},x}(\Gamma)}(\gamma^-_{\mathrm{per},\xi} H_{\mathrm{per},\xi}(\gamma_{N_0,\xi} - \bar{\gamma}_\xi))\, d\xi + \int_{\Gamma^*} \mathrm{Tr}_{L^2_{\mathrm{per},x}(\Gamma)}((1-\gamma^-_{\mathrm{per},\xi}) H_{\mathrm{per},\xi}(\gamma_{N_0,\xi} - \bar{\gamma}_\xi))\, d\xi \\
&= M + \int_{\Gamma^*} \mathrm{Tr}_{L^2_{\mathrm{per},x}(\Gamma)}((1-\gamma^-_{\mathrm{per},\xi}) H_{\mathrm{per},\xi}\gamma_{N_0,\xi})\, d\xi - \int_{\Gamma^*} \mathrm{Tr}_{L^2_{\mathrm{per},x}(\Gamma)}((1-\gamma^-_{\mathrm{per},\xi}) H_{\mathrm{per},\xi}\bar{\gamma}_\xi)\, d\xi, \qquad (4\text{-}17)
\end{aligned}
$$

where, since $0 \le \bar{\gamma}_\xi \le 1$ and $\{\lambda_n(\,\cdot\,)\}_{1\le n\le N_H} < 0$,

$$
\begin{aligned}
M &:= \int_{\Gamma^*} \mathrm{Tr}_{L^2_{\mathrm{per},x}(\Gamma)}(\gamma^-_{\mathrm{per},\xi} H_{\mathrm{per},\xi}(\gamma_{N_0,\xi} - \bar{\gamma}_\xi))\, d\xi = \int_{\Gamma^*} \sum_{n=1}^{N_H} \lambda_n(\xi) \langle e_{n,\xi} | 1 - \gamma^-_{\mathrm{per},\xi}\bar{\gamma}_\xi | e_{n,\xi}\rangle\, d\xi \\
&= \int_{\Gamma^*} \sum_{n=1}^{N_H} \lambda_n(\xi) \langle e_{n,\xi} | 1 - \bar{\gamma}_\xi | e_{n,\xi}\rangle\, d\xi \le 0. \qquad (4\text{-}18)
\end{aligned}
$$

In view of (4-15) and by a Cauchy–Schwarz inequality, we deduce that, for $N_0 \ge N_\epsilon$,

$$
\begin{aligned}
&\int_{\Gamma^*} \mathrm{Tr}_{L^2_{\mathrm{per},x}(\Gamma)}((1-\gamma^-_{\mathrm{per},\xi}) H_{\mathrm{per},\xi}\gamma_{N_0,\xi})\, d\xi \\
&\qquad = \int_{\Gamma^*} \sum_{n=N_0+1}^{N_0+Z_{\mathrm{diff}}} \sum_{m=1}^{+\infty} \langle e_{m,\xi} | H_{\mathrm{per},\xi} | \psi_{n,\xi}\rangle \langle \psi_{n,\xi} | e_{m,\xi}\rangle\, d\xi \\
&\qquad \le \int_{\Gamma^*} \sum_{n=N_0+1}^{N_0+Z_{\mathrm{diff}}} \biggl(\sum_{m=1}^{+\infty} |\langle \psi_{n,\xi} | e_{m,\xi}\rangle|^2\biggr)^{1/2} \biggl(\sum_{m=1}^{+\infty} |\langle e_{m,\xi} | H_{\mathrm{per},\xi} | \psi_{n,\xi}\rangle|^2\biggr)^{1/2} d\xi \\
&\qquad = \int_{\Gamma^*} \sum_{n=N_0+1}^{N_0+Z_{\mathrm{diff}}} \|\psi_{n,\xi}\|_{L^2_{\mathrm{per},x}(\Gamma)} \|H_{\mathrm{per},\xi}\psi_{n,\xi}\|_{L^2_{\mathrm{per},x}(\Gamma)}\, d\xi \\
&\qquad \le 2\pi \sum_{n=N_0+1}^{N_0+Z_{\mathrm{diff}}} \biggl(\frac{1}{2\pi}\int_{\Gamma^*} \|\psi_{n,\xi}\|^2_{L^2_{\mathrm{per},x}(\Gamma)}\, d\xi\biggr)^{1/2} \biggl(\frac{1}{2\pi}\int_{\Gamma^*} \|H_{\mathrm{per},\xi}\psi_{n,\xi}\|^2_{L^2_{\mathrm{per},x}(\Gamma)}\, d\xi\biggr)^{1/2} \\
&\qquad \le 2\sqrt{2}\pi \sum_{n=N_0+1}^{N_0+Z_{\mathrm{diff}}} \biggl(\frac{1}{n^4} + \epsilon^2\biggr)^{1/2} \le 2\sqrt{2}\pi\, Z_{\mathrm{diff}} \biggl(\frac{1}{N_0^4} + \epsilon^2\biggr)^{1/2}. \qquad (4\text{-}19)
\end{aligned}
$$

Moreover, by the definition of γ^-_{per},

$$
\begin{aligned}
&\int_{\Gamma^*} \mathrm{Tr}_{L^2_{\mathrm{per},x}(\Gamma)}((1-\gamma^-_{\mathrm{per},\xi}) H_{\mathrm{per},\xi}\bar{\gamma}_\xi) \\
&\qquad = \int_{\Gamma^*} \mathrm{Tr}_{L^2_{\mathrm{per},x}(\Gamma)}\bigl(|H_{\mathrm{per},\xi}|^{1/2}(1-\gamma^-_{\mathrm{per},\xi})\bar{\gamma}_\xi(1-\gamma^-_{\mathrm{per},\xi})|H_{\mathrm{per},\xi}|^{1/2}\bigr) \ge 0. \qquad (4\text{-}20)
\end{aligned}
$$

We distinguish in the inequality (4-18) the cases $M \equiv 0$ or $M < 0$. When $M \equiv 0$, the inequality (4-18) implies that $\bar{\gamma}_\xi \gamma^-_{\mathrm{per},\xi} = \gamma^-_{\mathrm{per},\xi}$ for almost all $\xi \in \Gamma^*$. In view of the inequalities (4-19) and (4-20), the inequality (4-17) implies

$$\text{for all } N_0 \geq N_\epsilon, \quad 0 \leq \int_{\Gamma^*} \mathrm{Tr}_{L^2_{\mathrm{per},x}(\Gamma)}((1-\gamma^-_{\mathrm{per},\xi})H_{\mathrm{per},\xi}\bar{\gamma}_\xi)\,d\xi \leq 2\sqrt{2}\pi\, Z_{\mathrm{diff}}\Big(\frac{1}{N_0^4}+\epsilon^2\Big)^{1/2}. \tag{4-21}$$

By letting N_0 tend to infinity, it is easy to deduce that $(1-\gamma^-_{\mathrm{per},\xi})\bar{\gamma}_\xi = 0$ for almost all $\xi \in \Gamma^*$. Together with the fact that $\bar{\gamma}_\xi \gamma^-_{\mathrm{per},\xi} = \gamma^-_{\mathrm{per},\xi}$ we deduce that $\bar{\gamma}_\xi \equiv \gamma^-_{\mathrm{per},\xi}$ for almost all $\xi \in \Gamma^*$. In view of (4-13) and (4-14), by the charge neutrality we obtain that

$$Z_{\mathrm{diff}} = \int_\Gamma \mu_{\mathrm{per}} - N_H = \int_\Gamma \rho_{\bar{\gamma}} - N_H = \frac{1}{|\Gamma^*|}\int_{\Gamma^*} \mathrm{Tr}_{L^2_{\mathrm{per},x}(\Gamma)}(\gamma^-_{\mathrm{per},\xi})\,d\xi - N_H \equiv 0.$$

Hence $\int_\Gamma \mu_{\mathrm{per}} = N_H = F(0)$. This also implies that the minimizer of the problem (2-17) is equal to γ^-_{per} when $N_H = F(0) = \int_\Gamma \mu_{\mathrm{per}}$ and $Z_{\mathrm{diff}} \equiv 0$. When $M < 0$ and $Z_{\mathrm{diff}} \neq 0$, we can always find $\epsilon > 0$ and $N_0 \geq N_\epsilon$ such that

$$2\sqrt{2}\pi\, Z_{\mathrm{diff}}\Big(\frac{1}{N_0^4}+\epsilon^2\Big)^{1/2} \leq -\frac{M}{2}.$$

In view of the inequalities (4-19) and (4-20), the inequality (4-17) implies

$$\text{for all } N_0 \geq N_\epsilon, \quad 0 \leq \int_{\Gamma^*} \mathrm{Tr}_{L^2_{\mathrm{per},x}(\Gamma)}((1-\gamma^-_{\mathrm{per},\xi})H_{\mathrm{per},\xi}\bar{\gamma}_\xi)\,d\xi \leq \frac{M}{2} < 0,$$

which leads to a contradiction. We can finally conclude that $F(0) \geq \int_\Gamma \mu_{\mathrm{per}}$, so that the Fermi level of the quasi-1-dimensional system is always nonpositive. In the following paragraph we show that the Fermi level can be chosen to be strictly negative.

Form of the minimizer and decay of the density of minimizers. We have already shown that if $N_H = F(0) \equiv \int_\Gamma \mu_{\mathrm{per}}$ then the 1-dimensional system has a unique minimizer which is equal to γ^-_{per}. This also implies that for almost all $\xi \in \Gamma^*$, the operator $H_{\mathrm{per},\xi}$ has N_H strictly negative eigenvalues below 0; therefore we can always choose the Fermi level $\epsilon_F \in (\max_{\xi\in\Gamma^*}\lambda_{N_H}(\xi), 0)$. If $F(0) > \int_\Gamma \mu_{\mathrm{per}}$, it is clear that there exists $\epsilon_F < 0$ such that $F(\epsilon_F) = \int_\Gamma \mu_{\mathrm{per}}$ as $F(\kappa)$ is a nondecreasing function on $(-\infty, 0]$ with range in $[0, F(0)]$. The form of the minimizer and the uniqueness is a direct adaptation of [Cancès et al. 2008, Theorem 1] by using a spectral projector decomposition similar to (A.2) of that theorem; that is, the unique minimizer can be written as

$$\gamma_{\mathrm{per}} = \mathbb{1}_{(-\infty,\epsilon_F]}(H_{\mathrm{per}}) = \mathscr{B}^{-1}\Big(\int_{\Gamma^*} \gamma_{\mathrm{per},\xi}\,\frac{d\xi}{2\pi}\Big)\mathscr{B} = \mathscr{B}^{-1}\Big(\int_{\Gamma^*}\sum_{n=1}^{N_H} \mathbb{1}(\lambda_n(\xi)\leq\epsilon_F)|e_{n,\xi}\rangle\langle e_{n,\xi}|\Big)\mathscr{B}, \tag{4-22}$$

where $\gamma_{\mathrm{per},\xi} := \mathbb{1}_{(-\infty,\epsilon_F]}(H_{\mathrm{per},\xi})$. The Fermi level $\epsilon_F < 0$ can be considered as the Lagrange multiplier associated with the charge neutrality condition

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

Once the unique minimizer is shown to be a spectral projector, we can use the exponential decay property of the eigenfunctions of $H_{\mathrm{per},\xi}$ in the $\boldsymbol{r}$-direction via the Combes–Thomas estimate [1973, Theorem 1]:

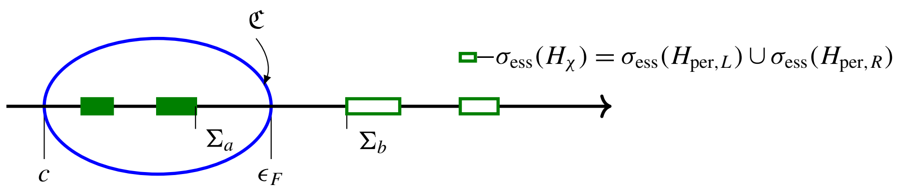

Figure 6. The essential spectrum of H_χ, $H_{\text{per},L}$ and $H_{\text{per},R}$, and the contour $\mathfrak{C}$.

for almost all $\xi \in \Gamma^*$, there exist positive constants $C(\xi)$ and $\alpha(\xi)$ such that

$$\text{for all } (x, \boldsymbol{r}) \in \Gamma, \text{ for all } 1 \le n \le N_H, \quad |e_{n,\xi}(x, \boldsymbol{r})| \le C(\xi) e^{-\alpha(\xi)|\boldsymbol{r}|}.$$

On the other hand, the fact that $\int_\Gamma \mu_{\text{per}} = F(\epsilon_F) < +\infty$ implies that there exist only finitely many states of $H_{\text{per},\xi}$ below ϵ_F for all $\xi \in \Gamma^*$. Therefore there exist positive constants C_{ϵ_F} and α_{ϵ_F} such that

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

Note that this exponential decay property coincides with Assumption 1 that $\int_\Gamma |\boldsymbol{r}| \rho_{\gamma_{\text{per}}}(x, \boldsymbol{r}) \, dx \, d\boldsymbol{r} < +\infty$.

4D. ***Proof of Proposition 3.2.*** In view of Proposition 3.1, consider a contour $\mathfrak{C}$ in the complex plane enclosing the spectrum of H_χ below the Fermi level ϵ_F without intersecting it, crossing the real axis at $c < \inf\{-\|V_{\text{per},L}\|_{L^\infty}, -\|V_{\text{per},R}\|_{L^\infty}\}$ (See Figure 6). This is possible even if ϵ_F is an eigenvalue: one can always slightly move the curve $\mathfrak{C}$ below ϵ_F in order bypass ϵ_F but still enclose all the spectrum of H_χ below ϵ_F. Let us introduce the following estimates, which are useful to characterize the decay property of densities. Since V_χ belongs to $L^\infty(\mathbb{R}^3)$, the following lemma is a direct adaption of [Cancès et al. 2008, Lemma 1]:

Lemma 4.4. *Under Assumption 2, there exist two positive constants c_1, c_2 such that,*

$$\textit{for all } \zeta \in \mathfrak{C}, \quad c_1(1 - \Delta) \le |H_\chi - \zeta| \le c_2(1 - \Delta)$$

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

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

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

Let us turn to the proof of Proposition 3.2. First of all let us show that γ_χ is locally trace class. Consider $\varrho \in C_c^\infty(\mathbb{R}^3)$. Note that γ_χ is a spectral projector. In view of Lemma 4.4, by Cauchy's resolvent formula and the Kato–Seiler–Simon inequality (4-1), there exists a positive constant C_χ such that

$$\|\varrho\gamma_\chi\varrho\|_{\mathfrak{S}_1} = \|\varrho\gamma_\chi\gamma_\chi\varrho\|_{\mathfrak{S}_1} = \|\varrho\gamma_\chi\|_{\mathfrak{S}_2}^2 = \left\| \varrho \oint_{\mathfrak{C}} \frac{1}{2i\pi} \frac{1}{\zeta - H_\chi} \, d\zeta \right\|_{\mathfrak{S}_2}^2 \le C_\chi \left\| \varrho \frac{1}{1 - \Delta} \right\|_{\mathfrak{S}_2}^2 \le \frac{C_\chi}{4\pi} \|\varrho\|_{L^2(\mathbb{R}^3)}^2.$$

This implies that γ_χ is locally trace class so that its density ρ_χ is well-defined in $L^1_{\mathrm{loc}}(\mathbb{R}^3)$. Let us prove that $\chi^2\rho_{\mathrm{per},L}+(1-\chi^2)\rho_{\mathrm{per},R}-\rho_\chi$ belongs to $L^p(\mathbb{R}^3)$ for $1<p\le 2$. It is difficult to directly compare the difference of $\chi^2\rho_{\mathrm{per},L}+(1-\chi^2)\rho_{\mathrm{per},R}$ and ρ_χ. We construct to this end a density operator γ_d whose density ρ_d is equal to $\chi^2\rho_{\mathrm{per},L}+(1-\chi^2)\rho_{\mathrm{per},R}-\rho_\chi$:

$$\gamma_d := \gamma_{d,1}+\gamma_{d,2},\quad \gamma_{d,1} := \chi(\gamma_{\mathrm{per},L}-\gamma_\chi)\chi,\quad \gamma_{d,2} := \sqrt{1-\chi^2}(\gamma_{\mathrm{per},R}-\gamma_\chi)\sqrt{1-\chi^2}. \tag{4-23}$$

Note that if $\gamma_d\in\mathfrak{S}_1$, then $\mathrm{Tr}_{L^2(\mathbb{R}^3)}(\gamma_d)=\chi^2\rho_{\mathrm{per},L}+(1-\chi^2)\rho_{\mathrm{per},R}-\rho_\chi$.

The density ρ_d is in $L^p(\mathbb{R}^3)$ for $1<p\le 2$. The proof that $\rho_d\in L^p(\mathbb{R}^3)$ relies on duality arguments: setting $q=p/(p-1)\in[2,+\infty)$, we prove that for any $W\in L^q(\mathbb{R}^3)$ there exists some $K_q>0$ such that $|\mathrm{Tr}_{L^2(\mathbb{R}^3)}(\gamma_d W)|\le K_q\|W\|_{L^q}$. By Cauchy's formula we have

$$\begin{aligned}\gamma_{d,1} &= \frac{1}{2\pi\mathrm{i}}\oint_{\mathfrak{C}}\chi\left(\frac{1}{z-H_{\mathrm{per},L}}-\frac{1}{\zeta-H_\chi}\right)\chi\,d\zeta,\\ \gamma_{d,2} &= \frac{1}{2\pi\mathrm{i}}\oint_{\mathfrak{C}}\sqrt{1-\chi^2}\left(\frac{1}{\zeta-H_{\mathrm{per},R}}-\frac{1}{\zeta-H_\chi}\right)\sqrt{1-\chi^2}\,d\zeta.\end{aligned} \tag{4-24}$$

Let us prove that there exists $K_q^1>0$ such that

$$|\mathrm{Tr}_{L^2(\mathbb{R}^3)}(\gamma_{d,1}W)|\le K_q^1\|W\|_{L^q}.$$

It is easily shown that a similar inequality holds for $\gamma_{d,2}$. Define $V_d:=(1-\chi^2)(V_{\mathrm{per},L}-V_{\mathrm{per},R})\in L^\infty(\mathbb{R}^3)$. Note that the function $V_d\chi$ has compact support in the x-direction and that $V_d\chi$ belongs to $L^r(\mathbb{R}^3)$ for $1<r\le+\infty$ by Theorem 2.7. For any $\zeta\in\mathfrak{C}$, the integrand of $\gamma_{d,1}$ can be written as

$$D(\zeta):=\chi\left(\frac{1}{\zeta-H_{\mathrm{per},L}}-\frac{1}{\zeta-H_\chi}\right)\chi=\chi\frac{1}{\zeta-H_{\mathrm{per},L}}V_d\frac{1}{\zeta-H_\chi}\chi.$$

Note that since χ is translation-invariant in the $\boldsymbol{r}$-direction, it is not in any L^p space in $\mathbb{R}^3$, which prevents us from using the standard techniques such as calculating the commutator $[-\Delta,\chi]$ to give Schatten class estimates on $\gamma_{d,1}$. By writing $1=\gamma_{\mathrm{per},L}+\gamma_{\mathrm{per},L}^\perp$ and $1=\gamma_\chi+\gamma_\chi^\perp$, the following decomposition holds:

$$D(\zeta)=\chi\frac{\gamma_{\mathrm{per},L}}{\zeta-H_{\mathrm{per},L}}V_d\frac{1}{\zeta-H_\chi}\chi+\chi\frac{\gamma_{\mathrm{per},L}^\perp}{\zeta-H_{\mathrm{per},L}}V_d\frac{\gamma_\chi}{\zeta-H_\chi}\chi+\chi\frac{\gamma_{\mathrm{per},L}^\perp}{\zeta-H_{\mathrm{per},L}}V_d\frac{\gamma_\chi^\perp}{\zeta-H_\chi}\chi. \tag{4-25}$$

By the residue theorem,

$$\int_{\mathfrak{C}}\chi\frac{\gamma_{\mathrm{per},L}^\perp}{\zeta-H_{\mathrm{per},L}}V_d\frac{\gamma_\chi^\perp}{\zeta-H_\chi}\chi\,d\zeta\equiv 0. \tag{4-26}$$

To estimate other terms in (4-25) we rely on the following lemma:

Lemma 4.5. *For any $1<p\le 2$, there exist positive constants $d_{p,1}$ and $d_{p,2}$, such that,*

$$\text{for all } \zeta\in\mathfrak{C},\quad \left\|\chi\frac{\gamma_{\mathrm{per},L}}{\zeta-H_{\mathrm{per},L}}V_d\right\|_{\mathfrak{S}_p}\le d_{p,1}\|V_d\chi\|_{L^p(\mathbb{R}^3)},\quad \left\|V_d\frac{\gamma_\chi}{\zeta-H_\chi}\chi\right\|_{\mathfrak{S}_p}\le d_{p,2}\|V_d\chi\|_{L^p(\mathbb{R}^3)}. \tag{4-27}$$

The proof of Lemma 4.5 can be read in Section A4 of the Appendix. Consider $W \in L^q(\mathbb{R}^3)$ for $q = p/(p-1) \in [2, +\infty)$. In view of (4-25), (4-26) and (4-27), by manipulations similar to the ones used in the proof of Lemma 4.5, and Hölder's inequality for Schatten class operators (see for example [Reed and Simon 1975, Proposition 5]), we obtain

$$\begin{aligned}
\|\gamma_{d,1} W\|_{\mathfrak{S}_1} &= \frac{1}{2\pi}\left\| \oint_{\mathfrak{C}} D(\zeta)\,d\zeta\, W \right\|_{\mathfrak{S}_1} \\
&= \left\| \oint_{\mathfrak{C}} \chi \frac{\gamma_{\mathrm{per},L}}{\zeta - H_{\mathrm{per},L}} V_d \frac{1}{\zeta - H_\chi} \chi W + \chi \frac{\gamma_{\mathrm{per},L}^{\perp}}{\zeta - H_{\mathrm{per},L}} V_d \frac{\gamma_\chi}{\zeta - H_\chi} \chi W \, d\zeta \right\|_{\mathfrak{S}_1} \\
&\le \left\| \oint_{\mathfrak{C}} \left(\chi \frac{\gamma_{\mathrm{per},L}}{\zeta - H_{\mathrm{per},L}} V_d \right) \frac{1}{\zeta - H_\chi} (1-\Delta) \left(\frac{1}{1-\Delta} \chi W \right) d\zeta \right\|_{\mathfrak{S}_1} \\
&\qquad + \left\| \oint_{\mathfrak{C}} \left(W \chi \frac{1}{1-\Delta} \right) (1-\Delta) \frac{\gamma_{\mathrm{per},L}^{\perp}}{\zeta - H_{\mathrm{per},L}} \left(V_d \frac{\gamma_\chi}{\zeta - H_\chi} \chi \right) d\zeta \right\|_{\mathfrak{S}_1} \\
&\le C \|V_d \chi\|_{L^p(\mathbb{R}^3)} \left\| \frac{1}{1-\Delta} \chi W \right\|_{\mathfrak{S}_q} \le K_q^1 \|W\|_{L^q(\mathbb{R}^3)},
\end{aligned} \tag{4-28}$$

where we have used the Kato–Seiler–Simon inequality (4-1) as well as the fact that $\|\chi\|_{L^\infty} = 1$. Similar estimates hold for $\gamma_{d,2}$. We therefore can conclude that $\rho_d = \chi^2 \rho_{\mathrm{per},L} + (1-\chi^2)\rho_{\mathrm{per},R} - \rho_\chi$ belongs to $L^p(\mathbb{R}^3)$ for $1 < p \le 2$.

Decay rate in the x-direction. Let us show that the density difference $\chi^2 \rho_{\mathrm{per},L} + (1-\chi^2)\rho_{\mathrm{per},R} - \rho_\chi$ decays exponentially fast in the x-direction. Note that there exists $N_L \in \mathbb{N}$ such that $N_L - 1 < a_L/2 \le N_L$. Setting $\mathbb{D}_{a_L} := [-a_L/2, +\infty) \times \mathbb{R}^2$, we prove the exponential decay when $\mathrm{supp}(w_\alpha) \subset \mathbb{R}^3 \backslash \mathbb{D}_{a_L}$. Let

$$\alpha := (\alpha_x, 0, 0) \in (\mathbb{R}, 0, 0), \qquad \beta = (\beta_x, \beta_y, \beta_z) \in \mathbb{Z}^3, \qquad \beta_x \ge -N_L.$$

We have

$$\mathbb{1}_{\mathbb{D}_{a_L}} \left(\sum_{\beta_x \ge -N_L}^{+\infty} \sum_{\beta_y, \beta_z \in \mathbb{Z}} w_\beta \right) = \mathbb{1}_{\mathbb{D}_{a_L}}, \qquad \mathbb{1}_{\mathbb{D}_{a_L}} V_d = V_d, \qquad \alpha_x < -\frac{a_L}{2} < -N_L + 1 \le \beta_x + 1.$$

The above relations imply, together with (4-27), the Combes–Thomas estimate (see for example [Klopp 1995; Combes and Thomas 1973; Germinet and Klein 2003]) and arguments similar to ones used in (4-28), that there exist positive constants C_1 and t_1 such that, for $1 < p \le 2$ and $q = p/(p-1) \ge 2$,

$$\begin{aligned}
&\|w_\alpha \gamma_d w_\alpha\|_{\mathfrak{S}_1} = \|w_\alpha \gamma_{d,1} w_\alpha\|_{\mathfrak{S}_1} \\
&\quad = \left\| \frac{1}{2\pi \mathrm{i}} \oint_{\mathfrak{C}} \left(w_\alpha \chi \frac{\gamma_{\mathrm{per},L}}{\zeta - H_{\mathrm{per},L}} V_d \frac{1}{\zeta - H_\chi} \chi\, w_\alpha + w_\alpha \chi \frac{\gamma_{\mathrm{per},L}^{\perp}}{\zeta - H_{\mathrm{per},L}} V_d \frac{\gamma_\chi}{\zeta - H_\chi} \chi\, w_\alpha \right) d\zeta \right\|_{\mathfrak{S}_1} \\
&\quad \le \left\| \frac{1}{2\pi \mathrm{i}} \oint_{\mathfrak{C}} \left(w_\alpha \chi \frac{\gamma_{\mathrm{per},L}}{\zeta - H_{\mathrm{per},L}} V_d \right) \left(\mathbb{1}_{\mathbb{D}_{a_L}} \frac{1}{\zeta - H_\chi} \chi\, w_\alpha \right) d\zeta \right\|_{\mathfrak{S}_1} \\
&\qquad\qquad + \left\| \frac{1}{2\pi \mathrm{i}} \oint_{\mathfrak{C}} (w_\alpha \chi \frac{\gamma_{\mathrm{per},L}^{\perp}}{\zeta - H_{\mathrm{per},L}} \mathbb{1}_{\mathbb{D}_{a_L}}) \left(V_d \frac{\gamma_\chi}{\zeta - H_\chi} \chi\, w_\alpha \right) d\zeta \right\|_{\mathfrak{S}_1} \\
&\quad \le K \sum_{\beta_x \ge -N_L}^{+\infty} \sum_{\beta_y, \beta_z \in \mathbb{Z}}^{+\infty} \mathrm{e}^{-t_1(\beta_x - \alpha_x)} \mathrm{e}^{-t_1|\beta_y|} \mathrm{e}^{-t_1|\beta_z|} \le C_1 \mathrm{e}^{-t_1|\alpha_x|}.
\end{aligned}$$

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

4E. *Proof of Lemma 3.3.* From the last item of the Theorem 2.7 we know that $V_{\mathrm{per},L} \in L^p_{\mathrm{per},x}(\Gamma_L)$ (resp. $V_{\mathrm{per},R} \in L^p_{\mathrm{per},x}(\Gamma_R)$) for $1 < p \le +\infty$. Note also that $\partial_x^2(\chi^2)$, $\partial_x(\chi^2)$ are uniformly bounded and have support in $[-a_L/2, a_R/2] \times \mathbb{R}^2$. It therefore suffices to obtain the L^p-estimates on $\partial_x V_{\mathrm{per},L}$ and $\partial_x V_{\mathrm{per},R}$. We treat $\partial_x V_{\mathrm{per},L}$, the L^p-estimates of $\partial_x V_{\mathrm{per},R}$ following similar arguments. First of all in view of the form of the minimizer (4-22), by the Cauchy–Schwarz inequality

$$\begin{aligned}\partial_x \rho_{\mathrm{per},L} &= \partial_x \left(\frac{1}{2\pi} \int_{\Gamma_L^*} \sum_{n\ge1} \mathbb{1}(\lambda_n(\xi) \le \epsilon_L) |e_n(\xi,\cdot)|^2 \, d\xi \right) \\ &\le \frac{1}{\pi} \int_{\Gamma_L^*} \left(\sum_{n\ge1} \mathbb{1}(\lambda_n(\xi) \le \epsilon_L) |\partial_x |e_n|(\xi,\cdot)|^2 \right)^{1/2} \left(\sum_{n\ge1} \mathbb{1}(\lambda_n(\xi) \le \epsilon_L) |e_n(\xi,\cdot)|^2 \right)^{1/2} d\xi \\ &\le \frac{1}{\pi} \sqrt{K_{\xi,L}} \sqrt{\rho_{\mathrm{per},L}},\end{aligned}$$

where $K_{\xi,L}(\boldsymbol{x}) := \int_{\Gamma_L^*} \sum_{n\ge1} \mathbb{1}(\lambda_n(\xi) \le \epsilon_L) |\partial_x e_n(\xi,\boldsymbol{x})\, d\xi|^2$. We also have used the fact that $|\nabla|f|| \le |\nabla f|$ for any complex-valued function f. In view of the potential decomposition (A-5), the term $T(\boldsymbol{r})$ does not contribute to the x-directional derivative; hence

$$|\partial_x V_{\mathrm{per},L}| = |(\partial_x(\rho_{\mathrm{per},L} - \mu_{\mathrm{per},L})) \star \widetilde{G}_{a_L}| \le \left(\frac{1}{2\pi} \sqrt{K_{\xi,L}} \sqrt{\rho_{\mathrm{per},L}} + |\partial_x \mu_{\mathrm{per},L}| \right) \star |\widetilde{G}_{a_L}|.$$

On the other hand, finite kinetic energy condition (2-10) implies that $K_{\xi,L} \in L^1_{\mathrm{per},x}(\Gamma_L)$. Moreover, $\sqrt{\rho_{\mathrm{per},L}}$ belongs to $H^1_{\mathrm{per},x}(\Gamma_L)$ and hence to $L^s_{\mathrm{per},x}(\Gamma_L)$ for $2 \le s \le 6$. Therefore, by Hölder's inequality, for $p, m \ge 1$,

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

with the conditions $pm = 2$ and $2 \le pm/(m-1) \le 6$. This is the case for $\frac{4}{3} \le m \le 2$ and $1 \le p \le \frac{3}{2}$ so that $(K_{\xi,L}\rho_{\mathrm{per},L})^{1/2}$ belongs to $L^p_{\mathrm{per},x}(\Gamma_L)$ for $1 \le p \le \frac{3}{2}$. As $\partial_x \mu_{\mathrm{per},L}$ is in $L^p_{\mathrm{per},x}(\Gamma_L)$ for any $1 \le p \le +\infty$ and $\widetilde{G}_{a_L} \in L^q_{\mathrm{per},x}(\Gamma_L)$ for $1 \le q < 2$ by Lemma 2.3, we obtain by Young's convolution inequality that $\partial_x V_{\mathrm{per},L} \in L^s_{\mathrm{per},x}(\Gamma_L)$ for $1 \le s < 6$. This allows us to conclude the lemma.

4F. *Proof of Theorem 3.6.* We prove this theorem by taking two arbitrary cut-off functions χ_1, χ_2 belonging to $\mathcal{X}$ and proving that $\rho_{\chi_1} + \rho_{Q_{\chi_1}} = \rho_{\chi_2} + \rho_{Q_{\chi_2}}$. For $i = 1, 2$, consider the reference states associated with the Hamiltonian H_{χ_i}. Denote by γ_{χ_i} the spectral projector of H_{χ_i} below ϵ_F and by Q_{χ_i} the solutions of (3-14) associated with χ_i. Consider a test state

$$\widetilde{Q} := \gamma_{\chi_1} + Q_{\chi_1} - \gamma_{\chi_2}. \tag{4-29}$$

We show that $\widetilde{Q}$ is a minimizer of the problem (3-12) associated with the cut-off function χ_2, so that $\rho_{\widetilde{Q}} \equiv \rho_{Q_{\chi_2}}$ by the uniqueness of the density of the minimizer provided by Proposition 3.5. Note that Assumption 2 and Proposition 3.1 guarantee that there is a common spectral gap for H_{χ_i} and $\sigma_{\mathrm{ess}}(H_{\chi_1}) = \sigma_{\mathrm{ess}}(H_{\chi_2})$. We first show that the test state $\widetilde{Q}$ belongs to the convex set

$$\mathcal{K}_{\chi_2} := \{Q \in \mathcal{Q}_{\chi_2} \mid -\gamma_{\chi_2} \le Q \le 1 - \gamma_{\chi_2}\},$$

and hence is an admissible state for the minimization problem (3-12) associated with χ_2. We next show that $\widetilde{Q}$ is a minimizer.

The test state $\widetilde{Q}$ belongs to $\mathcal{K}_{\chi_2}$. We begin by proving that $\widetilde{Q}$ is in $\mathcal{Q}_{\chi_2}$. Let us prove that $\widetilde{Q}$ is γ_{χ_2}-trace class. The following lemma will be useful.

Lemma 4.6. *The difference of the spectral projectors $\gamma_{\chi_1} - \gamma_{\chi_2}$ belongs to $\mathfrak{S}_1^{\gamma_{\chi_2}}$. Moreover,*

$$|\nabla|(\gamma_{\chi_1} - \gamma_{\chi_2}) \in \mathfrak{S}_2, \quad (\gamma_{\chi_1} - \gamma_{\chi_2})|\nabla| \in \mathfrak{S}_2. \tag{4-30}$$

Proof. By Cauchy's resolvent formula and the Kato–Seiler–Simon inequality (4-1),

$$\begin{aligned}\|\gamma_{\chi_1} - \gamma_{\chi_2}\|_{\mathfrak{S}_2} &= \left\| \frac{1}{2i\pi} \oint_{\mathfrak{C}} (\zeta - H_{\chi_1})^{-1} (\chi_1^2 - \chi_2^2)(V_{\mathrm{per},L} - V_{\mathrm{per},R})(\zeta - H_{\chi_2})^{-1}\, d\zeta \right\|_{\mathfrak{S}_2} \\ &\le C \|(1-\Delta)^{-1}(\chi_1^2 - \chi_2^2)(V_{\mathrm{per},L} - V_{\mathrm{per},R})\|_{\mathfrak{S}_2} \\ &\le \frac{C}{2\sqrt{\pi}} \|(\chi_1^2 - \chi_2^2)(V_{\mathrm{per},L} - V_{\mathrm{per},R})\|_{L^2} < +\infty.\end{aligned} \tag{4-31}$$

The results of Lemma 4.4 imply that $|\nabla|(\zeta - H_{\chi_i})^{-1}$ is uniformly bounded with respect to $\zeta \in \mathfrak{C}$. By calculations similar to (4-31),

$$\| |\nabla| (\gamma_{\chi_1} - \gamma_{\chi_2})\|_{\mathfrak{S}_2} \le c_1 \|(\chi_1^2 - \chi_2^2)(V_{\mathrm{per},L} - V_{\mathrm{per},R})(1-\Delta)^{-1}\|_{\mathfrak{S}_2} < +\infty. \tag{4-32}$$

Hence $(\gamma_{\chi_1} - \gamma_{\chi_2})|\nabla|$ also belongs to $\mathfrak{S}_2$ since it is the adjoint of $|\nabla|(\gamma_{\chi_1} - \gamma_{\chi_2})$. On the other hand, as γ_{χ_1} is a bounded operator, in view of (4-31) and by writing $\gamma_{\chi_1} - \gamma_{\chi_2} = \gamma_{\chi_2}^{\perp} - \gamma_{\chi_1}^{\perp}$ and using the fact that $\gamma_{\chi_i} + \gamma_{\chi_i}^{\perp} = 1$,

$$\begin{aligned}\gamma_{\chi_2}^{\perp}(\gamma_{\chi_1} - \gamma_{\chi_2})\gamma_{\chi_2}^{\perp} &= \gamma_{\chi_2}^{\perp}\gamma_{\chi_1}\gamma_{\chi_2}^{\perp} = (\gamma_{\chi_1} - \gamma_{\chi_2})\gamma_{\chi_1}(\gamma_{\chi_1} - \gamma_{\chi_2}) \in \mathfrak{S}_1, \\ \gamma_{\chi_2}(\gamma_{\chi_1} - \gamma_{\chi_2})\gamma_{\chi_2} &= -\gamma_{\chi_2}\gamma_{\chi_1}^{\perp}\gamma_{\chi_2} = -(\gamma_{\chi_2} - \gamma_{\chi_1})\gamma_{\chi_1}^{\perp}(\gamma_{\chi_2} - \gamma_{\chi_1}) \in \mathfrak{S}_1.\end{aligned} \tag{4-33}$$

Together with (4-31) we conclude that $\gamma_{\chi_1} - \gamma_{\chi_2}$ belongs to $\mathfrak{S}_1^{\gamma_{\chi_2}}$. □

The following lemma is a consequence of [Hainzl et al. 2005a, Lemma 1] and the fact that $\gamma_{\chi_1} - \gamma_{\chi_2} \in \mathfrak{S}_2$.

Lemma 4.7. *Any self-adjoint operator A is in $\mathfrak{S}_1^{\gamma_{\chi_1}}$ if and only if A is in $\mathfrak{S}_1^{\gamma_{\chi_2}}$. Moreover* $\mathrm{Tr}_{\gamma_{\chi_1}}(A) = \mathrm{Tr}_{\gamma_{\chi_2}}(A)$.

The fact that $Q_{\chi_1} \in \mathfrak{S}_1^{\gamma_{\chi_1}}$ implies $|\nabla| Q_{\chi_1} \in \mathfrak{S}_2$, and $Q_{\chi_1} \in \mathfrak{S}_1^{\gamma_{\chi_2}}$ by Lemma 4.7. In view of this and Lemma 4.6 we know that $\widetilde{Q} = \gamma_{\chi_1} - \gamma_{\chi_2} + Q_{\chi_1}$ belongs to $\mathfrak{S}_1^{\gamma_{\chi_2}}$. The inequality (4-32) implies $|\nabla|\widetilde{Q} = |\nabla| Q_{\chi_1} + |\nabla|(\gamma_{\chi_1} - \gamma_{\chi_2}) \in \mathfrak{S}_2$. It remains to prove that $|\nabla|\gamma_{\chi_2}^{\perp}\widetilde{Q}\gamma_{\chi_2}^{\perp}|\nabla| \in \mathfrak{S}_1$ and $|\nabla|\gamma_{\chi_2}\widetilde{Q}\gamma_{\chi_2}|\nabla| \in \mathfrak{S}_1$.

In view of (4-29) we have

$$\begin{aligned} |\nabla|\gamma_{\chi_2}^{\perp}\widetilde{Q}\gamma_{\chi_2}^{\perp}|\nabla| &= |\nabla|\gamma_{\chi_2}^{\perp}Q_{\chi_1}\gamma_{\chi_2}^{\perp}|\nabla| + |\nabla|\gamma_{\chi_2}^{\perp}(\gamma_{\chi_1}-\gamma_{\chi_2})\gamma_{\chi_2}^{\perp}|\nabla|, \\ |\nabla|\gamma_{\chi_2}\widetilde{Q}\gamma_{\chi_2}|\nabla| &= |\nabla|\gamma_{\chi_2}Q_{\chi_1}\gamma_{\chi_2}|\nabla| + |\nabla|\gamma_{\chi_2}(\gamma_{\chi_1}-\gamma_{\chi_2})\gamma_{\chi_2}|\nabla|. \end{aligned} \tag{4-34}$$

We estimate (4-34) term by term. By Lemma A.8 we know $\||\nabla|\gamma_{\chi_i}\| \le \||\nabla|(1-\Delta)^{-1}\|\|(1-\Delta)\gamma_{\chi_i}\| < \infty$. Moreover, by writing $\gamma_{\chi_2}^{\perp} = \gamma_{\chi_1}^{\perp} + \gamma_{\chi_1} - \gamma_{\chi_2}$ we obtain

$$\begin{aligned} |\nabla|\gamma_{\chi_2}^{\perp}Q_{\chi_1}\gamma_{\chi_2}^{\perp}|\nabla| &= |\nabla|\gamma_{\chi_1}^{\perp}Q_{\chi_1}\gamma_{\chi_1}^{\perp}|\nabla| + |\nabla|\gamma_{\chi_1}^{\perp}Q_{\chi_1}(\gamma_{\chi_1}-\gamma_{\chi_2})|\nabla| + |\nabla|(\gamma_{\chi_1}-\gamma_{\chi_2})Q_{\chi_1}\gamma_{\chi_2}^{\perp}|\nabla| \\ &= |\nabla|\gamma_{\chi_1}^{\perp}Q_{\chi_1}\gamma_{\chi_1}^{\perp}|\nabla| + |\nabla|Q_{\chi_1}(\gamma_{\chi_1}-\gamma_{\chi_2})|\nabla| - |\nabla|\gamma_{\chi_1}Q_{\chi_1}(\gamma_{\chi_1}-\gamma_{\chi_2})|\nabla| \\ &\quad + |\nabla|(\gamma_{\chi_1}-\gamma_{\chi_2})Q_{\chi_1}|\nabla| - |\nabla|(\gamma_{\chi_1}-\gamma_{\chi_2})Q_{\chi_1}\gamma_{\chi_2}|\nabla|. \end{aligned}$$

In view of (4-32), by the Cauchy–Schwarz inequality for Schatten operators,

$$\begin{aligned} \||\nabla|\gamma_{\chi_2}^{\perp}Q_{\chi_1}\gamma_{\chi_2}^{\perp}|\nabla|\|_{\mathfrak{S}_1} &\le \||\nabla|\gamma_{\chi_1}^{\perp}Q_{\chi_1}\gamma_{\chi_1}^{\perp}|\nabla|\|_{\mathfrak{S}_1} + \||\nabla|Q_{\chi_1}\|_{\mathfrak{S}_2}\|(\gamma_{\chi_1}-\gamma_{\chi_2})|\nabla|\|_{\mathfrak{S}_2} \\ &\quad + \||\nabla|\gamma_{\chi_1}\|\|Q_{\chi_1}\|_{\mathfrak{S}_2}\|(\gamma_{\chi_1}-\gamma_{\chi_2})|\nabla|\|_{\mathfrak{S}_2} + \||\nabla|(\gamma_{\chi_1}-\gamma_{\chi_2})\|_{\mathfrak{S}_2}\|Q_{\chi_1}|\nabla|\|_{\mathfrak{S}_2} \\ &\quad + \||\nabla|(\gamma_{\chi_1}-\gamma_{\chi_2})\|_{\mathfrak{S}_2}\|Q_{\chi_1}\|_{\mathfrak{S}_2}\|\gamma_{\chi_2}|\nabla|\| < \infty, \end{aligned}$$

and similarly by writing $\gamma_{\chi_2} = \gamma_{\chi_1} + \gamma_{\chi_2} - \gamma_{\chi_1}$ the following estimate holds:

$$\begin{aligned} \||\nabla|\gamma_{\chi_2}Q_{\chi_1}\gamma_{\chi_2}|\nabla|\|_{\mathfrak{S}_1} &\le \||\nabla|\gamma_{\chi_1}Q_{\chi_1}\gamma_{\chi_1}|\nabla|\|_{\mathfrak{S}_1} + \||\nabla|\gamma_{\chi_1}\|\|Q_{\chi_1}\|_{\mathfrak{S}_2}\|(\gamma_{\chi_1}-\gamma_{\chi_2})|\nabla|\|_{\mathfrak{S}_2} \\ &\quad + \|\gamma_{\chi_2}|\nabla|\|\|Q_{\chi_1}\|_{\mathfrak{S}_2}\||\nabla|(\gamma_{\chi_1}-\gamma_{\chi_2})\|_{\mathfrak{S}_2} < \infty, \end{aligned}$$

From (4-33) we know that

$$\begin{aligned} \||\nabla|\gamma_{\chi_2}^{\perp}(\gamma_{\chi_1}-\gamma_{\chi_2})\gamma_{\chi_2}^{\perp}|\nabla|\|_{\mathfrak{S}_1} &= \||\nabla|(\gamma_{\chi_1}-\gamma_{\chi_2})\gamma_{\chi_1}(\gamma_{\chi_1}-\gamma_{\chi_2})|\nabla|\|_{\mathfrak{S}_1} \le \||\nabla|(\gamma_{\chi_1}-\gamma_{\chi_2})\|_{\mathfrak{S}_2}^2 < \infty, \\ \||\nabla|\gamma_{\chi_2}(\gamma_{\chi_1}-\gamma_{\chi_2})\gamma_{\chi_2}|\nabla|\|_{\mathfrak{S}_1} &= \||\nabla|(\gamma_{\chi_2}-\gamma_{\chi_1})\gamma_{\chi_1}^{\perp}(\gamma_{\chi_2}-\gamma_{\chi_1})|\nabla|\|_{\mathfrak{S}_1} \le \||\nabla|(\gamma_{\chi_1}-\gamma_{\chi_2})\|_{\mathfrak{S}_2}^2 < \infty. \end{aligned}$$

This shows that $|\nabla|\gamma_{\chi_2}^{\perp}\widetilde{Q}\gamma_{\chi_2}^{\perp}|\nabla| \in \mathfrak{S}_1$ and $|\nabla|\gamma_{\chi_2}\widetilde{Q}\gamma_{\chi_2}|\nabla| \in \mathfrak{S}_1$. In view of (4-34), this allows us to conclude that $\widetilde{Q} \in \mathcal{Q}_{\chi_2}$. On the other hand, it is easy to see that $-\gamma_{\chi_2} \le \widetilde{Q} = \gamma_{\chi_1} + Q_{\chi_1} - \gamma_{\chi_2} \le 1 - \gamma_{\chi_2}$, which shows that $\widetilde{Q}$ belongs to the convex set $\mathcal{K}_{\chi_2}$.

The state $\widetilde{Q}$ is a minimizer. We now prove that $\widetilde{Q}$ is a minimizer of the problem (3-12) associated with the cut-off function χ_2. As $\widetilde{Q} \in \mathcal{K}_{\chi_2}$, the fact that Q_{χ_2} is a minimizer implies

$$\mathcal{E}_{\chi_2}(\widetilde{Q}) - \kappa\,\mathrm{Tr}_{\gamma_{\chi_2}}(\widetilde{Q}) \ge \mathcal{E}_{\chi_2}(Q_{\chi_2}) - \kappa\,\mathrm{Tr}_{\gamma_{\chi_2}}(Q_{\chi_2}). \tag{4-35}$$

Define $\Theta := \widetilde{Q} - Q_{\chi_2} = Q_{\chi_1} - Q_{\chi_2} + \gamma_{\chi_1} - \gamma_{\chi_2}$. The inequality (4-35) can therefore also be written as

$$\mathcal{E}_{\chi_2}(\Theta) - \kappa\,\mathrm{Tr}_{\gamma_{\chi_2}}(\Theta) + D(\rho_\Theta, \rho_{Q_{\chi_2}}) \ge 0. \tag{4-36}$$

It is easy to see that $-1 \le \Theta \le 1$ and Θ belongs to $\mathcal{Q}_{\chi_2}$ (but not necessarily to the convex set $\mathcal{K}_{\chi_2}$), which also implies that the density ρ_Θ of Θ is well-defined and belongs to the Coulomb space $\mathcal{C}$. Therefore (4-36) is well-defined. Introduce another state by exchanging the indices 1 and 2 in the definition of $\widetilde{Q}$:

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

Proceeding as before, it can be shown that $\widetilde{\widetilde{Q}} \in \mathcal{K}_{\chi_1}$. By definition $Q_{\chi_1} = \Theta + \widetilde{\widetilde{Q}}$. Since Q_{χ_1} minimizes the problem (3-12) associated with χ_1 and $\widetilde{\widetilde{Q}} \in \mathcal{K}_{\chi_1}$,

$$\mathcal{E}_{\chi_1}(\widetilde{\widetilde{Q}}) - \kappa \operatorname{Tr}_{\gamma_{\chi_1}}(\widetilde{\widetilde{Q}}) \geq \mathcal{E}_{\chi_1}(\Theta + \widetilde{\widetilde{Q}}) - \kappa \operatorname{Tr}_{\gamma_{\chi_1}}(\Theta + \widetilde{\widetilde{Q}}).$$

The above equation can be simplified as

$$\mathcal{E}_{\chi_1}(\Theta) - \kappa \operatorname{Tr}_{\gamma_{\chi_1}}(\Theta) + D(\rho_\Theta, \rho_{\widetilde{\widetilde{Q}}}) \leq 0. \tag{4-37}$$

Let us show that the left-hand sides of (4-36) and (4-37) are equal. First of all as Θ belongs to $\mathcal{Q}_{\chi_2}$, we know that $\operatorname{Tr}_{\gamma_{\chi_2}}(\Theta) = \operatorname{Tr}_{\gamma_{\chi_1}}(\Theta)$ by Lemma 4.7. Note also that $\rho_{\widetilde{\widetilde{Q}}} = \rho_{\chi_2} - \rho_{\chi_1} + \rho_{Q_{\chi_2}}$. By Lemma 4.7

$$\begin{aligned}
&\mathcal{E}_{\chi_2}(\Theta) - \kappa \operatorname{Tr}_{\gamma_{\chi_2}}(\Theta) + D(\rho_\Theta, \rho_{Q_{\chi_2}}) - (\mathcal{E}_{\chi_1}(\Theta) - \kappa \operatorname{Tr}_{\gamma_{\chi_1}}(\Theta) + D(\rho_\Theta, \rho_{\widetilde{\widetilde{Q}}}))\\
&\quad = \operatorname{Tr}_{\gamma_{\chi_2}}((-\Delta + V_{\chi_2})\Theta) - D(\rho_\Theta, \nu_{\chi_2}) + \tfrac{1}{2} D(\rho_\Theta, \rho_\Theta) - \operatorname{Tr}_{\gamma_{\chi_1}}((-\Delta + V_{\chi_1})\Theta) + D(\rho_\Theta, \nu_{\chi_1})\\
&\qquad\qquad - \tfrac{1}{2} D(\rho_\Theta, \rho_\Theta) - \kappa(\operatorname{Tr}_{\gamma_{\chi_2}}(\Theta) - \operatorname{Tr}_{\gamma_{\chi_1}}(\Theta)) + D(\rho_\Theta, \rho_{Q_{\chi_2}}) - D(\rho_\Theta, \rho_{\widetilde{\widetilde{Q}}})\\
&\quad = \operatorname{Tr}_{\gamma_{\chi_2}}((-\Delta + V_{\chi_2})\Theta) - \operatorname{Tr}_{\gamma_{\chi_1}}((-\Delta + V_{\chi_1})\Theta) + D(\rho_\Theta, \rho_{\chi_1} + \nu_{\chi_1} - \rho_{\chi_2} - \nu_{\chi_2})\\
&\quad = \operatorname{Tr}_{\gamma_{\chi_2}}((V_{\chi_2} - V_{\chi_1})\Theta) + D(\rho_\Theta, \rho_{\chi_1} + \nu_{\chi_1} - \rho_{\chi_2} - \nu_{\chi_2}).
\end{aligned} \tag{4-38}$$

We show that (4-38) is equal to zero by first showing that $(V_{\chi_2} - V_{\chi_1})\Theta \in \mathfrak{S}_1 \subset \mathfrak{S}_1^{\gamma_{\chi_2}}$. Note that $V_{\chi_1} - V_{\chi_2} = (\chi_1^2 - \chi_2^2)(V_{\text{per},L} - V_{\text{per},R}) \in L^\infty(\mathbb{R}^3) \cap L^2(\mathbb{R}^3)$. By the definition of Θ, by the Kato–Seiler–Simon inequality and using calculations similar to (4-31),

$$\begin{aligned}
&\|(V_{\chi_1} - V_{\chi_2})\Theta\|_{\mathfrak{S}_1}\\
&\quad = \|(V_{\chi_1} - V_{\chi_2})(Q_{\chi_1} - Q_{\chi_2} + \gamma_{\chi_1} - \gamma_{\chi_2})\|_{\mathfrak{S}_1}\\
&\quad \leq \|(V_{\chi_1} - V_{\chi_2})(1-\Delta)^{-1}\|_{\mathfrak{S}_2}(\|(1-\Delta)(Q_{\chi_1} - Q_{\chi_2})\|_{\mathfrak{S}_2} + \|(1-\Delta)(\gamma_{\chi_1} - \gamma_{\chi_2})\|_{\mathfrak{S}_2})\\
&\quad \leq \frac{1}{2\sqrt{\pi}} \|V_{\chi_1} - V_{\chi_2}\|_{L^2}(\|(1-\Delta)(Q_{\chi_1} - Q_{\chi_2})\|_{\mathfrak{S}_2} + C\|(\chi_1^2 - \chi_2^2)(V_{\text{per},L} - V_{\text{per},R})(1-\Delta)^{-1}\|_{\mathfrak{S}_2}) < \infty,
\end{aligned}$$

where the fact that $(1-\Delta)Q_{\chi_i} \in \mathfrak{S}_2$ follows arguments similar to the ones used in the proof of [Cancès et al. 2008, Proposition 2]. Hence $(V_{\chi_1} - V_{\chi_2})\Theta$ belongs to $\mathfrak{S}_1$, and

$$\operatorname{Tr}_{\gamma_{\chi_2}}((V_{\chi_2} - V_{\chi_1})\Theta) = \operatorname{Tr}((V_{\chi_2} - V_{\chi_1})\Theta).$$

On the other hand, by the definition of V_{χ_i} in (3-8) and ν_i in (3-10) for $i = 1, 2$, we deduce that

$$\operatorname{Tr}((V_{\chi_2} - V_{\chi_1})\Theta) = D(\rho_\Theta, (\rho_{\chi_2} - \mu_{\chi_2}) - (\rho_{\chi_1} - \mu_{\chi_1})) = D(\rho_\Theta, \rho_{\chi_2} - \rho_{\chi_1} + \nu_{\chi_2} - \nu_{\chi_1}).$$

The above equation implies that the quantity (4-38) is equal to 0. Hence, in view of (4-36) and (4-37),

$$\mathcal{E}_{\chi_2}(\Theta) - \kappa \operatorname{Tr}_{\gamma_{\chi_2}}(\Theta) + D(\rho_\Theta, \rho_{Q_{\chi_2}}) = \mathcal{E}_{\chi_1}(\Theta) - \kappa \operatorname{Tr}_{\gamma_{\chi_1}}(\Theta) + D(\rho_\Theta, \rho_{\widetilde{\widetilde{Q}}}) \equiv 0.$$

We conclude with (4-35) that

$$\mathcal{E}_{\chi_2}(\widetilde{Q}) - \kappa \operatorname{Tr}_{\gamma_{\chi_2}}(\widetilde{Q}) \equiv \mathcal{E}_{\chi_2}(Q_{\chi_2}) - \kappa \operatorname{Tr}_{\gamma_{\chi_2}}(Q_{\chi_2}).$$

Therefore $\widetilde{Q}$ is a minimizer of the problem (3-12) associated with the cut-off function χ_2. From Proposition 3.5 we know that $\rho_{\widetilde{Q}} \equiv \rho_{Q_{\chi_2}}$, which is equivalent to $\rho_{Q_{\chi_2}} + \rho_{\chi_2} = \rho_{\chi_1} + \rho_{Q_{\chi_1}}$. By the arbitrariness of the choice of χ_1, χ_2 we deduce that $\rho_\chi + \rho_{Q_\chi}$ is independent of the cut-off function $\chi \in \mathcal{X}$.

Appendix

A1. *Proof of Lemma 2.3.* For $n \in \mathbb{Z}$, let us consider the 2-dimensional equation

$$-\Delta_{\boldsymbol{r}} G_n + 4\pi^2 n^2 G_n = 2\pi \delta_{\boldsymbol{r}=0} \quad \text{in } \mathscr{S}'(\mathbb{R}^2).$$

It is well known (see for example [Lieb and Loss 2001; Lahbabi 2014]) that the solution of the above equation is

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

where $K_0(\alpha) := \int_0^{+\infty} \mathrm{e}^{-\alpha \cosh(t)}\, dt$ is the modified Bessel function of the second kind. Therefore the Green's function $G(x, \boldsymbol{r})$ defined in (2-7) can be rewritten as

$$G(x, \boldsymbol{r}) = 2 \sum_{n \in \mathbb{Z}} \mathrm{e}^{2i\pi n x} G_n(\boldsymbol{r}) \in \mathscr{S}'_{\mathrm{per},x}(\Gamma). \tag{A-1}$$

This implies

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

Taking the Fourier transform $\mathscr{F}$ on both sides of (A-1) we obtain (2-8). Let us now give some estimates on $\widetilde{G}$ defined in (2-7). Recall that there exist two positive constants C_0 and C_1 such that [Duffin 1971]

$$0 \leq K_0(\alpha) \leq \begin{cases} C_0|\log(\alpha)|, & \text{when } \alpha \leq 2\pi, \\ C_1 \mathrm{e}^{-\alpha}(\pi/2\alpha)^{1/2}, & \text{when } \alpha > 2\pi. \end{cases}$$

For $|\boldsymbol{r}| > 1$, it holds that

$$|\widetilde{G}(x, \boldsymbol{r})| \leq 2C_1 \sum_{n=1}^{+\infty} \frac{\mathrm{e}^{-2\pi n|\boldsymbol{r}|}}{\sqrt{n|\boldsymbol{r}|}} \leq \frac{2C_1}{1 - \mathrm{e}^{-2\pi}} \frac{\mathrm{e}^{-2\pi|\boldsymbol{r}|}}{\sqrt{|\boldsymbol{r}|}}. \tag{A-2}$$

For $|\boldsymbol{r}| \leq 1$ fixed, there exists $N \geq 1$ such that $N \leq 1/|\boldsymbol{r}| < N + 1$. In particular, for $n > N + 1$ we have $2\pi n|\boldsymbol{r}| > 2\pi$. There exists therefore a positive constant C such that

$$|\widetilde{G}(x, \boldsymbol{r})| \leq 4C_0 \left| \sum_{n=1}^{N} \log(2\pi n|\boldsymbol{r}|) \right| + 2C_1 \sum_{n=N+1}^{\infty} \frac{\mathrm{e}^{-2\pi n|\boldsymbol{r}|}}{\sqrt{n|\boldsymbol{r}|}} \leq \frac{C}{|\boldsymbol{r}|}. \tag{A-3}$$

Together with (A-2) we deduce that $\widetilde{G}(x, \boldsymbol{r}) \in L^p_{\mathrm{per},x}(\Gamma)$ for $1 \leq p < 2$. Note that for all $\boldsymbol{r} \in \mathbb{R}^2 \backslash \{0\}$, it holds $\int_{-1/2}^{1/2} \overline{G}(x, \boldsymbol{r})\, dx \equiv 0$. Consider, for $\boldsymbol{r} \neq 0$,

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

From [Blanc and Le Bris 2000, equation (1.8)],

$$-\Delta(\overline{G}(x,\boldsymbol{r}) - 2\log(|\boldsymbol{r}|)) = 4\pi \sum_{k\in\mathbb{Z}} \delta_{(x,\boldsymbol{r})=(k,0)} \in \mathscr{S}'(\mathbb{R}^3),$$

with $\overline{G}(x,\boldsymbol{r}) = \mathcal{O}(1/|\boldsymbol{r}|)$ when $|\boldsymbol{r}| \to \infty$ by [Blanc and Le Bris 2000, Lemma 2.2]. Setting $u(x,\boldsymbol{r}) = \widetilde{G}(x,\boldsymbol{r}) - \overline{G}(x,\boldsymbol{r})$ we therefore obtain that $-\Delta u(x,\boldsymbol{r}) \equiv 0$. As $u(x,\boldsymbol{r})$ belongs to $L^1_{\mathrm{loc}}(\mathbb{R}^3)$, by Weyl's lemma for the Laplace equation we obtain that $u(x,\boldsymbol{r})$ is $C^\infty(\mathbb{R}^3)$. On the other hand, by the decay properties of $\widetilde{G}$ and $\overline{G}$, we deduce that $|u(\,\cdot\,,\boldsymbol{r})| \to 0$ when $|\boldsymbol{r}| \to \infty$ uniformly in x, hence by the maximum modulus principle for harmonic functions we can conclude that $u \equiv 0$; hence $\widetilde{G}(x,\boldsymbol{r}) = \overline{G}(x,\boldsymbol{r})$.

A2. ***Proof of Lemma 2.10.*** Assume that (2-23) holds, that is $\mu_{\mathrm{per}}(x,\boldsymbol{r}) \equiv \mu_{\mathrm{per}}(x,|\boldsymbol{r}|)$ has radial symmetry in the $\boldsymbol{r}$-direction. It is clear that the results of Theorem 2.7 hold. We employ the same notation as in Theorem 2.7 in the sequel. By the uniqueness of density, $\rho_{\gamma_{\mathrm{per}}}$ enjoys the same radial symmetry in the $\boldsymbol{r}$-direction. Recall that $q_{\mathrm{per}} = \rho_{\gamma_{\mathrm{per}}} - \mu_{\mathrm{per}}$. Together with the facts that $\int_\Gamma |\boldsymbol{r}|\rho_{\gamma_{\mathrm{per}}}(x,\boldsymbol{r})\,dx\,d\boldsymbol{r} < +\infty$ and that μ_{per} has compact support in the $\boldsymbol{r}$-direction, the radial symmetry in the $\boldsymbol{r}$-direction implies

$$\int_\Gamma \boldsymbol{r}\cdot q_{\mathrm{per}}(x,\boldsymbol{r})\,dx\,d\boldsymbol{r} \equiv 0. \tag{A-4}$$

Note also that the exponential decay of density implies

$$\int_\Gamma |\boldsymbol{r}|^2 |q_{\mathrm{per}}(x,\boldsymbol{r})|\,dx\,d\boldsymbol{r} < +\infty.$$

Following calculations similar to the those in (4-9), (4-10) and (4-12), it is easy to deduce that

$$\partial_{\boldsymbol{k}} \mathscr{F} q_{\mathrm{per}}(0,\boldsymbol{k}) \equiv 0$$

and $\partial^2_{\boldsymbol{k}} \mathscr{F} q_{\mathrm{per}}(0,\boldsymbol{k})$ is continuous and bounded, so that $\mathscr{F} V_{\mathrm{per}}(0,\cdot\,)$ belongs to $L^2(\mathbb{R}^2)$, and V_{per} also belongs to $L^2_{\mathrm{per},x}(\Gamma)$. Let us prove that $V_{\mathrm{per}} \in L^p_{\mathrm{per},x}(\Gamma)$ for $1 < p < 2$ (for which we can conclude that V_{per} belongs to $L^p_{\mathrm{per},x}(\Gamma)$ for $1 < p \le +\infty$). Let us rewrite V_{per} as

$$V_{\mathrm{per}}(x,\boldsymbol{r}) = (q_{\mathrm{per}} \star_\Gamma G)(x,\boldsymbol{r}) = (q_{\mathrm{per}} \star_\Gamma \widetilde{G})(x,\boldsymbol{r}) + T(\boldsymbol{r}), \tag{A-5}$$

where

$$T(\boldsymbol{r}) = -2\int_{\mathbb{R}^2} \bar{q}_{\mathrm{per}}(\boldsymbol{r}')\log(|\boldsymbol{r}-\boldsymbol{r}'|)\,d\boldsymbol{r}', \quad \bar{q}_{\mathrm{per}}(\boldsymbol{r}) := \int_{-1/2}^{1/2} q_{\mathrm{per}}(x,\boldsymbol{r})\,dx.$$

Recall that μ_{per} has compact support in the $\boldsymbol{r}$-direction; hence there exist positive constants C_q, α_q such that,

$$\text{for all } (x,\boldsymbol{r}) \in \mathbb{R}^3, \quad |q_{\mathrm{per}}(\,\cdot\,,\boldsymbol{r})| \le C_q \mathrm{e}^{-\alpha_q|\boldsymbol{r}|}, \quad |\bar{q}_{\mathrm{per}}(\boldsymbol{r})| \le C_q \mathrm{e}^{-\alpha_q|\boldsymbol{r}|}.$$

As $\widetilde{G}$ belongs to $L^p_{\mathrm{per},x}(\Gamma)$ for $1 \le p < 2$, by Young's convolution inequality we deduce that $q_{\mathrm{per}} \star_\Gamma \widetilde{G}$ belongs to $L^t_{\mathrm{per},x}(\Gamma)$ for $1 \le t \le +\infty$.

It remains to prove that $T(\boldsymbol{r})$ belongs to $L^p(\mathbb{R}^2)$ for $1 < p < 2$. Let us use the partition $\mathbb{R}^2 = \{|\boldsymbol{r}| \le 2R\} \cup \{|\boldsymbol{r}| > 2R\}$ for the integration domain of $T(\boldsymbol{r})$. Note first that $\log(|\boldsymbol{r}|)$ is $L^t_{\mathrm{loc}}(\mathbb{R}^2)$ for

$1 \le t < +\infty$. Therefore, by a Cauchy–Schwarz inequality, there exists a positive constant $C_{R,1}$ such that, for $p' = p/(p-1) \in (2, +\infty)$,

$$\begin{aligned}\Big(\int_{|\boldsymbol{r}|\le 2R} |T(\boldsymbol{r})|^p \, d\boldsymbol{r}\Big)^{1/p} &= 2\Big(\int_{|\boldsymbol{r}|\le 2R}\Big|\int_{\mathbb{R}^2} \bar{q}_{\mathrm{per}}(\boldsymbol{r}')\log(|\boldsymbol{r}-\boldsymbol{r}'|)\,d\boldsymbol{r}'\Big|^p\,d\boldsymbol{r}\Big)^{1/p}\\ &\le 2\Big(\int_{|\boldsymbol{r}|\le 2R}\Big|\int_{|\boldsymbol{r}'|\le 3R} \bar{q}_{\mathrm{per}}(\boldsymbol{r}')\log(|\boldsymbol{r}-\boldsymbol{r}'|)\,d\boldsymbol{r}'\Big|^p\,d\boldsymbol{r}\Big)^{1/p}\\ &\qquad + 2C_q\Big(\int_{|\boldsymbol{r}|\le 2R}\Big|\int_{|\boldsymbol{r}'|> 3R} \mathrm{e}^{-\alpha_q|\boldsymbol{r}'|}|\log(|\boldsymbol{r}-\boldsymbol{r}'|)|\,d\boldsymbol{r}'\Big|^p\,d\boldsymbol{r}\Big)^{1/p}\\ &\le 2\Big(\int_{|\boldsymbol{r}'|\le 3R}|\bar{q}_{\mathrm{per}}|^p\Big)^{1/p}\Big(\int_{|\boldsymbol{r}|\le 2R}\Big(\int_{|\boldsymbol{r}'|\le 3R}|\log(|\boldsymbol{r}-\boldsymbol{r}'|)|^{p'}\,d\boldsymbol{r}'\Big)^{p/p'}\,d\boldsymbol{r}\Big)^{1/p}\\ &\qquad + 2C_q\Big(\int_{|\boldsymbol{r}|\le 2R}\Big|\int_{|\boldsymbol{r}'|> 3R} \mathrm{e}^{-\alpha_q|\boldsymbol{r}'|}\big|\log(|(R,R)-\boldsymbol{r}'|)\big|\,d\boldsymbol{r}'\Big|^p\,d\boldsymbol{r}\Big)^{1/p}\\ &\le C_{R,1}.\end{aligned} \tag{A-6}$$

Let us look at the integration domain $\{|\boldsymbol{r}| > 2R\}$. Note that by the charge neutrality condition and the radial symmetry condition (A-4), it holds, for any $\boldsymbol{r} \neq 0$,

$$\int_{\mathbb{R}^2} \bar{q}_{\mathrm{per}}(\boldsymbol{r}')\log(|\boldsymbol{r}|)\,d\boldsymbol{r}' \equiv 0, \qquad \int_{\mathbb{R}^2} \bar{q}_{\mathrm{per}}(\boldsymbol{r}')\frac{\boldsymbol{r}'\boldsymbol{r}}{|\boldsymbol{r}|^2}\,d\boldsymbol{r}' \equiv 0.$$

Denote by

$$Q(\boldsymbol{r},\boldsymbol{r}') := \log(|\boldsymbol{r}-\boldsymbol{r}'|) - \log(|\boldsymbol{r}|) - \frac{\boldsymbol{r}'\boldsymbol{r}}{|\boldsymbol{r}|^2} = \frac{1}{2}\log\Big(1 - \frac{2\boldsymbol{r}\boldsymbol{r}'}{|\boldsymbol{r}|^2} + \frac{|\boldsymbol{r}'|^2}{|\boldsymbol{r}|^2}\Big) - \frac{\boldsymbol{r}'\boldsymbol{r}}{|\boldsymbol{r}|^2}.$$

Then

$$T(\boldsymbol{r}) = -2\int_{\mathbb{R}^2} \bar{q}_{\mathrm{per}}(\boldsymbol{r}')Q(\boldsymbol{r},\boldsymbol{r}')\,d\boldsymbol{r}'.$$

Note that when $|\boldsymbol{r}| > 2R$ and $|\boldsymbol{r}'|/|\boldsymbol{r}| \le \epsilon_R$ for $\epsilon_R > 0$ fixed. A Taylor expansion shows that there exists a positive constant C such that $|Q(\boldsymbol{r},\boldsymbol{r}')| \le C|\boldsymbol{r}'|^2/|\boldsymbol{r}|^2$. This motivates the following partition of $\mathbb{R}^2$ given $|\boldsymbol{r}| > 2R$:

$$\mathbb{R}^2 = \mathbb{B}_{\epsilon_R} \cup \mathbb{B}_{\epsilon_R}^{\complement}, \quad \mathbb{B}_{\epsilon_R} := \Big\{\boldsymbol{r}' \in \mathbb{R}^2 \;\Big|\; \frac{|\boldsymbol{r}'|}{|\boldsymbol{r}|} \le \epsilon_R\Big\}.$$

Hence

$$T(\boldsymbol{r}) = T_{\mathrm{int}}(\boldsymbol{r}) + T_{\mathrm{ext}}(\boldsymbol{r}), \quad T_{\mathrm{int}}(\boldsymbol{r}) := \int_{\mathbb{B}_{\epsilon_R}} \bar{q}_{\mathrm{per}}(\boldsymbol{r}')Q(\boldsymbol{r},\boldsymbol{r}')\,d\boldsymbol{r}', \quad T_{\mathrm{ext}}(\boldsymbol{r}) := \int_{\mathbb{B}_{\epsilon_R}^{\complement}} \bar{q}_{\mathrm{per}}(\boldsymbol{r}')Q(\boldsymbol{r},\boldsymbol{r}')\,d\boldsymbol{r}'.$$

Therefore, for $1 < p < 2$,

$$\begin{aligned}\int_{|\boldsymbol{r}|>2R} |T_{\mathrm{int}}(\boldsymbol{r})|^p\,d\boldsymbol{r} &\le 2C^p\int_{|\boldsymbol{r}|>2R}\Big|\int_{\mathbb{B}_{\epsilon_R}} \bar{q}_{\mathrm{per}}(\boldsymbol{r}')\frac{|\boldsymbol{r}'|^2}{|\boldsymbol{r}|^2}\,d\boldsymbol{r}'\Big|^p\,d\boldsymbol{r}\\ &\le 2C'\int_{|\boldsymbol{r}|>2R}\Big|\int_{|\boldsymbol{r}'|\le\epsilon_R|\boldsymbol{r}|} \mathrm{e}^{-\alpha_q|\boldsymbol{r}'|}|\boldsymbol{r}'|^2\,d\boldsymbol{r}'\Big|^p|\boldsymbol{r}|^{-2p}\,d\boldsymbol{r} < +\infty.\end{aligned} \tag{A-7}$$

Similarly,

$$\int_{|\boldsymbol{r}|>2R} |T_{\text{ext}}(\boldsymbol{r})|^p \, d\boldsymbol{r} \le C_1 \int_{|\boldsymbol{r}|>2R} \left| \int_{|\boldsymbol{r}'|>\epsilon_R|\boldsymbol{r}|} \mathrm{e}^{-\alpha_q|\boldsymbol{r}'|} |Q(\boldsymbol{r},\boldsymbol{r}')| \, d\boldsymbol{r}' \right|^p d\boldsymbol{r}$$
$$\le C_1 \int_{|\boldsymbol{r}|>2R} \left| \int_{|\boldsymbol{r}'|>\epsilon_R|\boldsymbol{r}|} \mathrm{e}^{-\alpha_q\epsilon_R|\boldsymbol{r}|/2} \mathrm{e}^{-\alpha_q|\boldsymbol{r}'|/2} |Q(\boldsymbol{r},\boldsymbol{r}')| \, d\boldsymbol{r}' \right|^p d\boldsymbol{r} < +\infty. \tag{A-8}$$

In view of (A-6), (A-7) and (A-8) we conclude that $T(\boldsymbol{r})$ belongs to $L^p(\mathbb{R}^2)$ for $1 < p < 2$. This leads to the conclusion that V_{per} belongs to $L^p_{\text{per},x}(\Gamma)$ for $1 < p \le +\infty$.

A3. ***Proof of Proposition 3.1.*** Let us emphasize that the function χ being translation-invariant in the $\boldsymbol{r}$-direction makes it difficult to control the compactness in the $\boldsymbol{r}$-direction across the junction surface. Our geometry is very different from the cylindrical geometry considered in [Hempel et al. 2015] for instance which automatically provides compactness in the $\boldsymbol{r}$-direction.

The proof is organized as follows: we first prove that any $\lambda \in \sigma_{\text{ess}}(H_{\text{per},L}) \cup \sigma_{\text{ess}}(H_{\text{per},R})$ also belongs to $\sigma_{\text{ess}}(H_\chi)$. We then prove that $\sigma_{\text{ess}}(H_\chi)$ is included in $\sigma_{\text{ess}}(H_{\text{per},L}) \cup \sigma_{\text{ess}}(H_{\text{per},R})$ based on the IMS formula [Ismagilov 1961; Morgan 1979; Morgan and Simon 1980; Simon 1983].

The union of $\sigma_{\text{ess}}(H_{\text{per},L}) \cup \sigma_{\text{ess}}(H_{\text{per},R})$ is included in $\sigma_{\text{ess}}(H_\chi)$. Without loss of generality we prove that λ_L belonging to $\sigma_{\text{ess}}(H_{\text{per},L})$ also belongs to $\sigma_{\text{ess}}(H_\chi)$. Consider a Weyl sequence $\{w_n\}_{n\in\mathbb{N}^*}$ for $H_{\text{per},L}$ associated with λ_L. Let us construct a Weyl sequence for H_χ from $\{w_n\}_{n\in\mathbb{N}^*}$. Fix $n \in \mathbb{N}^*$. There exists a sequence $\{v_{k,n}\}_{k\in\mathbb{N}^*}$ belonging to $C_c^\infty(\mathbb{R}^3)$ such that, for all $\epsilon > 0$, there exists a $K_n \in \mathbb{N}^*$ such that, for any $k \ge K_n$,

$$\|v_{k,n} - w_n\|_{H^2(\mathbb{R}^3)} \le \epsilon. \tag{A-9}$$

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 w_n converges weakly to 0. As $v_{K_n,n}$ has compact support, for any fixed $n \in \mathbb{N}^*$ and for $m \in \mathbb{N}^*$ large enough,

$$\operatorname{supp}(\tau^x_{a_L m} v_{K_n,n}) \cap \left(([-a_L/2, +\infty) \times \mathbb{R}^2) \bigcup \mathfrak{B}_n \right) = \varnothing, \tag{A-10}$$

where $\mathfrak{B}_n$ denotes the ball of radius n centered at 0 in $\mathbb{R}^3$. Note that the above equality also ensures that $\tau^x_{a_L m} v_{K_n,n}$ tends weakly to 0 in $L^2(\mathbb{R}^3)$ when $m \to +\infty$ for n fixed. In view of (A-9) and (A-10), we introduce $\tilde{w}_n := \tau^x_{a_L m_n} v_{K_n,n}$ for $n \in \mathbb{N}^*$ so that (A-10) is satisfied. This implies that $\tilde{w}_n$ tends weakly to 0 in $L^2(\mathbb{R}^3)$ when $n \to +\infty$. Moreover, in view of (A-9) and by the definition of the Weyl sequence

$$\|(H_\chi - \lambda_L)\tilde{w}_n\|_{L^2} = \|(H_\chi - \lambda_L)\tau^x_{a_L m_n} v_{K_n,n}\|_{L^2} = \|(H_{\text{per},L} - \lambda_L)\tau^x_{a_L m_n} v_{K_n,n}\|_{L^2}$$
$$\le \|\tau^x_{a_L m_n}(H_{\text{per},L} - \lambda_L)(v_{K_n,n} - w_n)\|_{L^2} + \|\tau^x_{a_L m_n}(H_{\text{per},L} - \lambda_L)w_n\|_{L^2}$$
$$\le (1 + \|V_{\text{per},L}\|_{L^\infty} + |\lambda_L|)\|v_{K_n,n} - w_n\|_{H^2} + \|(H_{\text{per},L} - \lambda_L)w_n\|_{L^2} \xrightarrow[n\to\infty]{} 0.$$

Therefore the sequence $\tilde{w}_n/\|\tilde{w}_n\|_{L^2}$ is a Weyl sequence of H_χ associated with λ_L. This leads to the conclusion that

$$\sigma_{\text{ess}}(H_{\text{per},L}) \cup \sigma_{\text{ess}}(H_{\text{per},R}) \subseteq \sigma_{\text{ess}}(H_\chi). \tag{A-11}$$

The essential spectrum $\sigma_{\text{ess}}(H_\chi)$ in included in $\sigma_{\text{ess}}(H_{\text{per},L}) \cup \sigma_{\text{ess}}(H_{\text{per},R})$. We prove that $\lambda \in \sigma_{\text{ess}}(H_\chi)$ also belongs to $\sigma_{\text{ess}}(H_{\text{per},L}) \cup \sigma_{\text{ess}}(H_{\text{per},R})$. We prove this statement by the IMS localization formula (see for example [Simon 1983, Lemma 3.1]), which states that for any smooth partition of unity $\{J_a\}_{a=0}^k$ (k does not need to be finite) such that $\sum_{a=0}^k J_a^2 = 1$, the following algebraic decomposition holds (on the proper form domain) for an operator H:

$$H = \sum_{a=0}^{k} \bigl(J_a H J_a + \tfrac{1}{2}[J_a, [J_a, H]]\bigr). \tag{A-12}$$

The proof of the above statement is based on the following algebraic relation:

$$\text{for all } 0 \le a \le k, \quad J_a^2 H + H J_a^2 - 2 J_a H J_a \equiv [J_a, [J_a, H]].$$

Consider a partition of unity $\sum_{i=1}^3 f_i^2 = 1$ such that

$$\begin{aligned} f_1 &\equiv 1 \quad \text{on } (-\infty, -a_L) \times \mathbb{R}^2, & f_2 &\equiv 1 \quad \text{on } (a_R, +\infty) \times \mathbb{R}^2, \\ f_1 &\equiv 0 \quad \text{on } (-a_L/2, +\infty) \times \mathbb{R}^2, & f_2 &\equiv 0 \quad \text{on } (-\infty, a_R/2) \times \mathbb{R}^2. \end{aligned}$$

This implies that f_3 has support in $[-a_L, a_R] \times \mathbb{R}^2$.

Consider a Weyl sequence $(\phi_n)_{n \in \mathbb{N}^*} \in H^2(\mathbb{R}^3)$ of H_χ associated with $\lambda \in \sigma_{\text{ess}}(H_\chi)$. For $R \in \mathbb{R}^+$ large enough, by applying (A-12) to the operator $(H_\chi - \lambda)^2$ it holds that

$$\begin{aligned} (H_\chi - \lambda)^2 = f_1(x/R, \cdot)(H_{\text{per},L} - \lambda)^2 f_1(x/R, \cdot) + f_2(x/R, \cdot)(H_{\text{per},R} - \lambda)^2 f_2(x/R, \cdot) \\ + f_3(x/R, \cdot)(H_\chi - \lambda)^2 f_3(x/R, \cdot) + \frac{1}{2} \sum_{i=1}^{3} [f_i(x/R, \cdot), [f_i(x/R, \cdot), (H_\chi - \lambda)^2]]. \end{aligned}$$

In view of the above formula, for any ϕ_n,

$$\begin{aligned} \|(H_\chi - \lambda)\phi_n\|_{L^2}^2 = \|(H_{\text{per},L} - \lambda) f_1(x/R, \cdot)\phi_n\|_{L^2}^2 + \|(H_{\text{per},R} - \lambda) f_2(x/R, \cdot)\phi_n\|_{L^2}^2 \\ + \bigl\|\bigl(-\tfrac{1}{2}\Delta - \lambda\bigr) f_3(x/R, \cdot)\phi_n\bigr\|_{L^2}^2 \\ + \|V_\chi f_3(x/R, \cdot)\phi_n\|_{L^2}^2 + 2\Re\langle V_\chi f_3(x/R, \cdot)\phi_n, \bigl(-\tfrac{1}{2}\Delta - \lambda\bigr) f_3(x/R, \cdot)\phi_n\rangle_{L^2} \\ + \frac{1}{2} \sum_{i=1}^{3} \langle \phi_n, [f_i(x/R, \cdot), [f_i(x/R, \cdot), (H_\chi - \lambda)^2]]\phi_n\rangle_{L^2}. \end{aligned} \tag{A-13}$$

Let us show that we can find a sequence of $R_n \to +\infty$ such that the last two terms of (A-13) tends to 0. First of all, remark that $\bigl[f_i(x/R, \cdot), \bigl[f_i(x/R, \cdot), -\frac{1}{2}\Delta\bigr]\bigr] = -|\nabla f_i(x/R, \cdot)|^2$. Hence, for $i = 1, 2, 3$,

$$\begin{aligned} &[f_i(x/R, \cdot), [f_i(x/R, \cdot), (H_\chi - \lambda)^2]] \\ &\quad = 2[H_\chi - \lambda, f_i(x/R, \cdot)]^2 + (H_\chi - \lambda)[f_i(x/R, \cdot), [f_i(x/R, \cdot), H_\chi - \lambda]] \\ &\qquad\qquad + [f_i(x/R, \cdot), [f_i(x/R, \cdot), H_\chi - \lambda]](H_\chi - \lambda) \\ &\quad = \tfrac{1}{2}\bigl(\Delta f_i(x/R, \cdot) + 2(\nabla f_i(x/R, \cdot)) \cdot \nabla\bigr)^2 - (H_\chi - \lambda)|\nabla f_i(x/R, \cdot)|^2 - |\nabla f_i(x/R, \cdot)|^2(H_\chi - \lambda). \end{aligned}$$

Note also that there exists $C \in \mathbb{R}^+$ such that $|\nabla f_i(x/R)| \le C/R$, and $|\Delta f_i(x/R)| \le C/R^2$. Therefore there exists a positive constant C_r such that, for all $n \in \mathbb{N}^*$,

$$\left| \frac{1}{2} \sum_{i=1}^{3} \langle \phi_n, [f_i(x/R, \cdot), [f_i(x/R, \cdot), (H_\chi - \lambda)^2]]\phi_n \rangle \right| \le C_r \frac{\|\phi_n\|^2_{H^2(\mathbb{R}^3)}}{R}. \tag{A-14}$$

On the other hand, note that $f_3(x/R, \cdot)V_\chi$ tends to 0 in all directions. Hence, for every fixed $R \in \mathbb{R}^+$,

$$\begin{aligned}\Big| \|V_\chi f_3(x/R, \cdot)\phi_n\|^2_{L^2} + 2\Re\big\langle V_\chi f_3(x/R, \cdot)\phi_n, \big(-\tfrac{1}{2}\Delta - \lambda\big) f_3(x/R, \cdot)\phi_n \big\rangle_{L^2} \Big| \\ \le \|V_\chi f_3(x/R, \cdot)\phi_n\|^2_{L^2} + 2(1+|\lambda|)\|V_\chi f_3(x/R, \cdot)\phi_n\|_{L^2}\|\phi_n\|_{H^2(\mathbb{R}^3)} \xrightarrow[n\to\infty]{} 0.\end{aligned}$$

In view of the above formula as well as (A-14), there exists a sequence $R_n \to +\infty$ such that the last two terms of (A-13) tends to 0. In particular, this implies

$$\|(H_{\mathrm{per},L} - \lambda) f_1(x/R_n, \cdot)\phi_n\|^2_{L^2} + \|(H_{\mathrm{per},R} - \lambda) f_2(x/R_n, \cdot)\phi_n\|^2_{L^2} + \big\|\big(-\tfrac{1}{2}\Delta - \lambda\big) f_3(x/R_n, \cdot)\phi_n\big\|^2_{L^2} \xrightarrow[n\to\infty]{} 0.$$

On the other hand,

$$\text{for all } n \in \mathbb{N}^*, \quad \|f_1(x/R_n, \cdot)\phi_n\|^2_{L^2} + \|f_2(x/R_n, \cdot)\phi_n\|^2_{L^2} + \|f_3(x/R_n, \cdot)\phi_n\|^2_{L^2} \equiv 1.$$

Therefore one of them cannot vanish in the limit; hence λ is in the spectrum of $H_{\mathrm{per},L}$, $H_{\mathrm{per},R}$ or $-\frac{1}{2}\Delta$. This allows us to conclude that

$$\sigma_{\mathrm{ess}}(H_\chi) \subseteq \sigma_{\mathrm{ess}}(H_{\mathrm{per},L}) \cup \sigma_{\mathrm{ess}}(H_{\mathrm{per},R}). \tag{A-15}$$

By gathering (A-11) and (A-15) we conclude that $\sigma_{\mathrm{ess}}(H_\chi) \equiv \sigma_{\mathrm{ess}}(H_{\mathrm{per},L}) \cup \sigma_{\mathrm{ess}}(H_{\mathrm{per},R})$. In particular, $\sigma_{\mathrm{ess}}(H_\chi)$ is independent of the function $\chi \in \mathcal{X}$.

A4. *Proof of Lemma 4.5.* First of all the following lemma will be useful.

Lemma A.8. *Consider a self-adjoint operator $H = -\Delta + V$ defined on $L^2(\mathbb{R}^3)$ with domain $H^2(\mathbb{R}^2)$ and $V \in L^\infty(\mathbb{R}^3)$. For $E \in \mathbb{R}\backslash\sigma(H)$ denote by $\gamma = \mathbb{1}_{(-\infty,E]}(H)$. Then for any $a, b \in \mathbb{R}$, the operator $(1-\Delta)^a\gamma(1-\Delta)^b$ is bounded. Moreover, if $\gamma \in \mathfrak{S}_k$ for some $k \ge 1$, then $(1-\Delta)^a\gamma(1-\Delta)^b \in \mathfrak{S}_k$.*

Proof. Much as in Lemma 4.4 it can be shown that for any $\zeta \in \mathbb{R}\backslash\sigma(H)$ the operator $(\zeta - H)^{-a}(1-\Delta)^a$ and its inverse are bounded. Fix $\delta > 0$ and define $\lambda_0 := -\|V\|_{L^\infty} - \delta$. Then $\lambda_0 \notin \sigma(H)$. By writing $\gamma = \gamma^2$, there exists a positive constant C such that

$$\|(1-\Delta)^a\gamma(1-\Delta)^b\|_{\mathfrak{S}_k} \le C\|(\lambda_0 - H)^a\gamma(\lambda_0 - H)^b\|_{\mathfrak{S}_k} = C\|\gamma^2(\lambda_0 - H)^{a+b}\|_{\mathfrak{S}_k} < +\infty,$$

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

Let us prove the statement for $\chi\gamma_{\mathrm{per},L}(\zeta - H_{\mathrm{per},L})^{-1}V_d$, the proof of the bound of $V_d\gamma_\chi(\zeta - H_\chi)^{-1}\chi$ follows similar arguments. Fix $R > 0$. Recall that $\mathfrak{B}_R$ is the ball in $\mathbb{R}^3$ centered at 0 with radius R. Denote by φ_R the characteristic function of $\mathfrak{B}_R$. For any $R > 0$, by the Kato–Seiler–Simon inequality (4-1) and the boundedness of $(1-\Delta)(\zeta-H_{\mathrm{per},L})^{-1}$ it is easy to see that $\varphi_R\chi(\zeta-H_{\mathrm{per},L})^{-1}$ and $(\zeta-H_{\mathrm{per},L})^{-1}V_d\varphi_R$ belong to $\mathfrak{S}_2$. The operator $\gamma_{\mathrm{per},L}(\zeta-H_{\mathrm{per},L})^m$ is bounded for any $m\in\mathbb{R}$ in view of Lemma 4.5. Therefore

$$\varphi_R\left(\chi\frac{\gamma_{\mathrm{per},L}}{\zeta-H_{\mathrm{per},L}}V_d\right)\varphi_R=\left(\varphi_R\chi\frac{1}{\zeta-H_{\mathrm{per},L}}\right)\gamma_{\mathrm{per},L}(\zeta-H_{\mathrm{per},L})\left(\frac{1}{\zeta-H_{\mathrm{per},L}}V_d\varphi_R\right)\in\mathfrak{S}_1.$$

Let us first prove that for any $1\le p\le 2$, there exists a positive constant $d_{p,1}$ only depending on p such that, for any $R>0$,

$$\left\|\varphi_R\chi\frac{\gamma_{\mathrm{per},L}}{\zeta-H_{\mathrm{per},L}}V_d\varphi_R\right\|_{\mathfrak{S}_p}\le d_{p,1}\|V_d\varphi_R^2\chi\|_{L^p(\mathbb{R}^3)}. \tag{A-16}$$

We first prove (A-16) for $p=1$ and $p=2$, and conclude by an interpolation argument for $1\le p\le 2$. Consider $p=1$. By the cyclicity of the trace and the Kato–Seiler–Simon inequality (4-1),

$$\begin{aligned}\left\|\varphi_R\chi\frac{\gamma_{\mathrm{per},L}}{\zeta-H_{\mathrm{per},L}}V_d\varphi_R\right\|_{\mathfrak{S}_1}&=\left\|\varphi_R\chi\frac{1}{\zeta-H_{\mathrm{per},L}}\gamma_{\mathrm{per},L}(\zeta-H_{\mathrm{per},L})\frac{1}{\zeta-H_{\mathrm{per},L}}V_d\varphi_R\right\|_{\mathfrak{S}_1}\\&=\left\|\gamma_{\mathrm{per},L}(\zeta-H_{\mathrm{per},L})\frac{1}{\zeta-H_{\mathrm{per},L}}V_d\varphi_R^2\chi\frac{1}{\zeta-H_{\mathrm{per},L}}\right\|_{\mathfrak{S}_1}\\&\le c\left\|\frac{1}{|1-\Delta|}|V_d\varphi_R^2\chi|\frac{1}{|1-\Delta|}\right\|_{\mathfrak{S}_1}=c\left\|\frac{1}{|1-\Delta|}|V_d\varphi_R^2\chi|^{1/2}\right\|_{\mathfrak{S}_2}^2\le d_{1,1}\|V_d\varphi_R^2\chi\|_{L^1}.\end{aligned}$$

Let us next prove (A-16) for $p=2$. Use again the cyclicity of the trace and the Kato–Seiler–Simon inequality (4-1),

$$\begin{aligned}\left\|\varphi_R\chi\frac{\gamma_{\mathrm{per},L}}{\zeta-H_{\mathrm{per},L}}V_d\varphi_R\right\|_{\mathfrak{S}_2}^2&=\left\|V_d\varphi_R\frac{\gamma_{\mathrm{per},L}}{\bar\zeta-H_{\mathrm{per},L}}\varphi_R^2\chi^2\frac{\gamma_{\mathrm{per},L}}{\zeta-H_{\mathrm{per},L}}V_d\varphi_R\right\|_{\mathfrak{S}_1}\\&=\left\|\frac{\gamma_{\mathrm{per},L}}{\bar\zeta-H_{\mathrm{per},L}}\varphi_R^2\chi^2\frac{\gamma_{\mathrm{per},L}}{\zeta-H_{\mathrm{per},L}}V_d^2\varphi_R^2\right\|_{\mathfrak{S}_1}\\&\le c'\left\|\varphi_R^2\chi^2\frac{1}{\zeta-H_{\mathrm{per},L}}\gamma_{\mathrm{per},L}(\zeta-H_{\mathrm{per},L})\frac{1}{\zeta-H_{\mathrm{per},L}}V_d^2\varphi_R^2\right\|_{\mathfrak{S}_1}\\&=c'\left\|\gamma_{\mathrm{per},L}(\zeta-H_{\mathrm{per},L})\frac{1}{\zeta-H_{\mathrm{per},L}}V_d^2\varphi_R^4\chi^2\frac{1}{\zeta-H_{\mathrm{per},L}}\right\|_{\mathfrak{S}_1}\\&\le c''\left\|\frac{1}{\zeta-H_{\mathrm{per},L}}V_d^2\varphi_R^4\chi^2\frac{1}{\zeta-H_{\mathrm{per},L}}\right\|_{\mathfrak{S}_1}\\&=c''\left\||V_d\varphi_R^2\chi|\frac{1}{\zeta-H_{\mathrm{per},L}}\right\|_{\mathfrak{S}_2}^2\le d_{2,1}^2\|V_d\varphi_R^2\chi\|_{L^2}^2.\end{aligned}$$

By the interpolation arguments we can conclude (A-16) for $1\le p\le 2$. Note that for $1<p\le 2$ the following uniform bound holds:

$$\left\|\varphi_R\chi\frac{\gamma_{\mathrm{per},L}}{\zeta-H_{\mathrm{per},L}}V_d\varphi_R\right\|_{\mathfrak{S}_p}\le d_{p,1}\|V_d\varphi_R^2\chi\|_{L^p(\mathbb{R}^3)}\le d_{p,1}\|V_d\chi\|_{L^p(\mathbb{R}^3)}.$$

By passing the limit $R\to+\infty$ we can conclude the proof.

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