Removing a slab from the Fermi sea: the reduced Hartree-Fock model

Éric Cancès, Ling-Ling Cao, Gabriel Stoltz
Université Paris-Est, CERMICS (ENPC), INRIA, F-77455 Marne-la-Vallée

July 19, 2018

Abstract

Studying the electronic structure of defects in materials is an important subject in condensed matter physics. From a mathematical point of view, nonlinear mean-field models of localized defects in insulators are well understood. We present here a mean-field model to study a particular instance of extended defects in metals. These extended defects typically correspond to taking out a slab of finite width in the three-dimensional homogeneous electron gas. We work in the framework of the reduced Hartree-Fock model with either Yukawa or Coulomb interactions. Using techniques developed in [12] to study local perturbations of the free-electron gas, we show that our model admits minimizers, and that Yukawa ground state energies and density matrices converge to ground state Coulomb energies and density matrices as the Yukawa parameter tends to zero. We moreover present numerical simulations where we observe Friedel oscillations in the total electronic density.

1 Introduction

The study of the electronic structure of defects in materials is an important topic in condensed matter physics (see e.g. [13, 21, 22, 26, 31] and references therein). The case of linear one-body Hamiltonians describing independent electrons has been thoroughly investigated, in particular to study the effect of disorder on transport properties (see e.g. [1, 20] and references therein). Nonlinear mean-field models such as Hartree-Fock or Kohn-Sham type models are much more difficult to handle, mainly because of the long-range of Coulomb interactions. For insulators, a reduced Hartree-Fock model [30] with Coulomb interactions has been proposed in [4] to study a local defect in an insulating (or semiconducting) crystal, based on the ideas and techniques from [16, 17, 18, 19]. This model is variational and consists in minimizing some renormalized energy formally obtained by taking the difference between the (infinite) energies of the crystal with the defect, and of the perfect crystal. This approach can be mathematically justified by a thermodynamic limit argument. The zero-frequency dielectric polarizability properties of insulating crystals can be inferred from this model by a homogenization procedure [7]. Extensions to the time-dependent setting are discussed in [8]. The numerical analysis of the steady case is dealt with in [15] (see also [5]).

The above mentioned works are only valid for insulators and semiconductors, and crucially rely on the existence of a spectral gap in the spectrum of the mean-field Hamiltonian of the corresponding perfect crystal. Mean-field model for defects in metals are much more difficult to analyze since small perturbations can cause electrons to escape at infinity. On the other hand, many interesting physical problems, such as electronic transport, occur in metals. In [12], the authors have considered local perturbations of the Fermi sea of the free-electron gas. The well-posedness of the dynamics of time-dependent setting is proved in [24]. These works are important milestones in the construction of mathematical sound mean-field models for local defects in real (nonuniform) metals.

Let us also mention the works [6, 23] in which crystals with stationary random distributions of local defects have been studied.
In this work, we study a particular instance of extended defects in metals within the reduced Hartree-Fock model. More precisely, we consider 2D-translational invariant defects in a 3D homogeneous electron gas. A typical situation is the case when a slab of finite width of the jellium modeling the uniform nuclear distribution is taken out. This gives rise to a model describing the uncharged state of a capacitor composed of two semi-infinite leads separated by some dielectric medium or vacuum. This could be a first step toward the construction of a mean-field model for electronic transport. Our mathematical analysis heavily relies on the translation invariance in the directions parallel to the slab. Technically, this allows us to reduce the study of a three-dimensional model to the one of a family of one-dimensional problems labeled by a two-dimensional quasimomentum.

This article is organized as follows. In Section 2, we introduce a reduced Hartree-Fock model amenable to describe an extended two-dimensional defect in the three-dimensional Fermi sea, under the assumption that the defect is translation invariant in the (x, y)-directions. After introducing the functional setting in Section 2.1, we define renormalized free kinetic and potential energy functionals for an (x, y)-translation invariant defect in Section 2.2. In Section 2.3, we use these elementary bricks to define reduced Hartree-Fock (rHF) energy functionals for (x, y)-translation invariant defects, both for Coulomb and Yukawa interactions, and prove the existence of a ground state. We also show that the Yukawa ground states converge to the Coulomb ground states when the characteristic length of the Yukawa interaction goes to infinity. The proof of the results presented in Section 2 can be read in Section 3. Finally, results of numerical simulations are reported in Section 4 for a model capacitor.

2 Construction of the model

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 \( r = (r, z) \), where \( r = (x, y) \in \mathbb{R}^2 \) and \( z \in \mathbb{R} \). We denote respectively by \( \mathcal{S}(\mathbb{R}^d) \) the Schwartz space of rapidly decreasing functions on \( \mathbb{R}^d \), and by \( \mathcal{S}'(\mathbb{R}^d) \) the space of tempered distributions on \( \mathbb{R}^d \).

Let \( \mathcal{H} \) be a separable Hilbert space. We denote by \( \mathcal{L}(\mathcal{H}) \) the space of bounded (linear) operators on \( \mathcal{H} \), by \( \mathcal{S}(\mathcal{H}) \) the space of bounded self-adjoint operators on \( \mathcal{H} \), and by \( \mathcal{K}(\mathcal{H}) \) the space of compact operators on \( \mathcal{H} \). We denote by \( \mathcal{S}_p(\mathcal{H}) \) the \( p \)-Schatten class on \( \mathcal{H} \), for \( 1 \leq p < \infty \): \( A \in \mathcal{K}(\mathcal{H}) \) if and only if \( \|A\|_{\mathcal{S}_p} = (\text{Tr}(|A|^p))^{1/p} < \infty \). Recall that operators in \( \mathcal{S}_1(\mathcal{H}) \) and \( \mathcal{S}_2(\mathcal{H}) \) are respectively called trace-class and Hilbert-Schmidt.

If \( A \in \mathcal{S}_1(L^2(\mathbb{R}^d)) \), there exists a unique function \( \rho_A \in L^1(\mathbb{R}^d) \) such that

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

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

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

\[
\forall W \in C_0^\infty(\mathbb{R}^d), \quad \text{Tr}(AW) = \int_{\mathbb{R}^d} \rho_A \, W.
\]

We denote respectively by \( \hat{u} \) and \( \hat{u}^{-1} \) the Fourier transform and the inverse Fourier transform of a tempered distribution \( u \in \mathcal{S}'(\mathbb{R}^d) \). We use the normalization convention for which

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

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

In Section 2.1.1, we introduce a natural decomposition of \((x, y)\)-translation invariant operators based on partial Fourier transform. In Section 2.1.2, we apply it to the special case of \((x, y)\)-translation invariant one-body density matrices.

2.1.1 Decomposition of \((x, y)\)-translation invariant operators

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

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

An operator \(A\) on \(L^2(\mathbb{R}^3)\) is called \((x, y)\)-translation invariant if it commutes with \(\tau_r\) for all \(r \in \mathbb{R}^2\). In order to decompose \((x, y)\)-translation invariant operators on \(L^2(\mathbb{R}^3)\), we introduce the constant fiber direct integral [27, Section XIII.16]

\[
L^2(\mathbb{R}^2; L^2(\mathbb{R})) \equiv \int_{\mathbb{R}^2} L^2(\mathbb{R}) \, dq
\]

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

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

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

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

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

\[
A = \left( \int_{\mathbb{R}^2} A_q \, dq \right) U.
\]

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

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

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

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

Likewise, if \(A\) is a (not necessarily bounded) self-adjoint operator such that \(\tau_r (A + i)^{-1} = (A + i)^{-1} \tau_r\) for all \(r \in \mathbb{R}^2\), then \(A\) is decomposed by \(U\) (see [27, Theorem XIII.84 and XIII.85]). In particular, the kinetic energy operator \(T = -\frac{1}{2} \Delta\) on \(L^2(\mathbb{R}^3)\) is decomposed by \(U\) as follows:

\[
T = U^{-1} \left( \int_{\mathbb{R}^2} T_q \, dq \right) U \quad \text{with} \quad T_q := -\frac{1}{2} \frac{d^2}{dz^2} + \frac{|q|^2}{2}.
\] (2.2)
2.1.2 One-body density matrices

In Hartree-Fock and Kohn-Sham models, electronic states are described by one-body density matrices (see e.g. [11, 4, 12]). Recall that for a finite system with $N$ electrons, a density matrix is a trace-class self-adjoint operator $\gamma \in \mathcal{S}(L^2(\mathbb{R}^3)) \cap \mathcal{S}_1(L^2(\mathbb{R}^3))$ satisfying the Pauli principle $0 \leq \gamma \leq 1$ and the normalization condition $\text{Tr}(\gamma) = \int_{\mathbb{R}^3} \rho_\gamma = N$. The kinetic energy of $\gamma$ is given by $\text{Tr}(\frac{i}{2} \Delta \gamma) := \frac{1}{2} \text{Tr}(|\nabla|\gamma|\nabla|)$ (see [10, 4]).

Let us from now on focus on the reduced Hartree-Fock (rHF) model, i.e. the Hartree-Fock model without exchange terms. In this case, the ground state density matrix of a homogeneous electron gas with density $\rho_0$ can be uniquely defined by a thermodynamic limit argument (relying on the strict convexity of the rHF model with respect to the density). It is given by

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

with the Fermi level

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

which is the chemical potential of the electrons. Although $\gamma_0$ is not trace-class, it is locally trace-class and its density is $\rho_0$ by construction. The operator $\gamma_0$ can be seen as the rHF ground-state density matrix of an infinite, locally neutral system, whose nuclear distribution is a jellium of uniform density $\rho_{\text{nuc}}^0 = \rho_0$.

Since $T$ is decomposed by $\mathcal{U}$, so is $\gamma_0$, and we have

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

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

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

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

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

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

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

2.2 Renormalized free energy functionals

Defects that are $(x,y)$-translation invariant are extended (non-local) defects, and therefore, do not fall into the frameworks of [12, 24] (nor a fortiori of [4] since the homogeneous electron gas is a metal). However, the approach consisting in characterizing the ground states as the minimizers of some renormalized free energy functional can still be used.

In Section 2.2.1, we define a renormalized kinetic free energy per unit area adapted to $(x,y)$-translation invariant perturbations of the homogeneous electron gas. In Section 2.2.2, we focus on the potential energy contributions, and define renormalized energies per unit area for $(x,y)$-translation invariant systems, both for Yukawa and Coulomb interactions.
2.2.1 Renormalized kinetic free energy functional

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

$$t_{\gamma_0}(r) := \rho_{T^{1/2}Q_{T^{1/2}}}(r),$$
$$t_{\gamma}(r) := \rho_{T^{1/2}\gamma T^{1/2}}(r) = t_{\gamma_0}(r) + t_Q(r) \quad \text{with} \quad t_Q(r) := \rho_{T^{1/2}Q_{T^{1/2}}}(r).$$

By $(x,y)$-translation invariance, the functions $t_{\gamma_0}$, $t_{\gamma}$, and $t_Q$ are in fact functions of the transverse variable $z$ only. Fixing the Fermi level $\epsilon_F > 0$, we can therefore define a renormalized kinetic free energy per unit area as

$$T_{\text{ren}}(Q) := \left( \int_{\mathbb{R}} t_{\gamma}(z) \, dz - \epsilon_F \int_{\mathbb{R}} \rho_{\gamma}(z) \, dz \right) - \left( \int_{\mathbb{R}} t_{\gamma_0}(z) \, dz - \epsilon_F \int_{\mathbb{R}} \rho_{\gamma_0}(z) \, dz \right) = \int_{\mathbb{R}} (t_Q(z) - \epsilon_F \rho_Q(z)) \, dz.$$

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

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

we obtain

$$T_{\text{ren}}(Q) = \int_{\mathbb{R}} \left( \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} \left( \rho_{T_q^{1/2}Q_{T_q^{1/2}}}(z) - \epsilon_F \rho_Q(z) \right) \, dz \right) \, dq$$

$$= \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} \left\{ \text{Tr}(T_q^{1/2}Q_{T_q^{1/2}}) - \epsilon_F \parallel Q \parallel_{S} \right\} \, dq$$

$$= \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} \left\{ \text{Tr}((T_q - \epsilon_F)Q_q) \right\} \, dq$$

$$= \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} \left\{ \text{Tr}[(T_q - \epsilon_F)(\gamma_{0,q} + (1 - \gamma_{0,q}))Q_q] \right\} \, dq$$

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

where

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

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

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

so that

$$\int_{\mathbb{R}^2} \left\{ |T_q - \epsilon_F|^{1/2} Q_q \right\}^2_{\mathfrak{S}_2(L^2(\mathbb{R}))} \, dq \leq \int_{\mathbb{R}^2} \left\{ |T_q - \epsilon_F|^{1/2} (Q_q^{++} + Q_q^{-}) |T_q - \epsilon_F|^{1/2} \right\} \, dq.$$

Reasoning as in [12, 24], the above formal manipulations lead us to introduce

- the functional space

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

which, equipped with the norm

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

is a Banach space;
the convex set $\mathcal{K}_q := \left\{ Q_q \in \mathcal{K}_q \mid -\gamma_{0,q} \leq Q_q \leq 1 - \gamma_{0,q} \right\};$

- the linear form

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

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

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

$$\gamma = \gamma_0 + Q$$

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

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

It is not obvious *a priori* that operators in $\mathcal{K}$, which are not trace-class, nor even compact, have densities. However, it is in fact possible to define the density $\rho_Q$ of any state $Q \in \mathcal{K}$, which will be useful to define renormalized rHF free energy functionals involving Yukawa or Coulomb interactions (see Section 2.3).

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

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

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

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

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

The proof of this result is based on Lieb–Thirring type inequalities and can be read in Section 3.1.

### 2.2.2 Coulomb and Yukawa energy functionals

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

$$\rho := \rho_{0} + Q - (\rho_{0uc} + \nu) = \rho_Q - \nu$$

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

$$\int_{\mathbb{R}} \rho(z) v_p(0)(z) \, dz = \int_{\mathbb{R}} |k|^2 \hat{\nu}_{p,0}(k) = 2 \int_{\mathbb{R}} |\hat{\rho}(k)|^2 |k|^2 \, dk.$$  \hfill (2.10)

This motivates the following definition of the 1D Coulomb space

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

which, endowed with the inner product

$$\langle \rho_1, \rho_2 \rangle := 2 \int_{\mathbb{R}} \frac{\hat{\rho}_1(k) \hat{\rho}_2(k)}{|k|^2} \, dk,$$  \hfill (2.10)

is a Hilbert space. The quantity $\frac{1}{2} \mathcal{D}(\rho, \rho) \in [0, +\infty]$ represents the Coulomb energy per unit area of the $(x,y)$-translation invariant renormalized charge density $\rho$.  \hfill (2.11)
Remark 2.3. Note that charge densities in $\mathcal{C}$ are neutral in some weak sense. In particular, if $\rho \in \mathcal{C} \cap L^1(\mathbb{R})$, then $\int_\mathbb{R} \rho = (2\pi)^{1/2} \hat{\rho}(0) = 0$ since the function $k \mapsto \frac{\lvert \hat{\rho}(k) \rvert^2}{\lvert k \rvert^2}$ has to be integrable in the vicinity of 0.

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

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

This leads us to introduce the Yukawa space of parameter $m$

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

endowed with the inner product

$$
D_m(\rho_1, \rho_2) := 2 \int_\mathbb{R} \frac{\hat{\rho}_1(k) \hat{\rho}_2(k)}{\sqrt{\lvert k \rvert^2 + m^2}} \, dk.
$$

We will use in the sequel the consistent notation $D_0 := D$ for Coulomb interactions.

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

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

### 2.3 Formulation and mathematical properties of the model

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

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

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

Based on the content of Section 2.2, we can define the renormalized free energy per unit area associated with a trial density matrix $\gamma = \gamma_0 + Q$ by

$$
\mathcal{E}_{\nu, m}(Q) = \text{Tr} ((T - \epsilon F) Q) + \frac{1}{2} D_m(\rho_Q - \nu, \rho_Q - \nu),
$$

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

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

We can then state the following result.

Theorem 2.6 (Existence of minimizers).
(1) Yukawa interaction: for any $\nu \in H^{-1}(\mathbb{R})$, the minimization problem
\[ I_{\nu,m} = \inf \{ E_{\nu,m}(Q), Q \in \mathcal{K} \} \tag{2.14} \]
has a minimizer $Q_{\nu,m}$ and all the minimizers share the same density $\rho_{\nu,m}$.

(2) Coulomb interaction: for any $\nu \in L^1(\mathbb{R})$ such that $|\cdot| \nu(\cdot) \in L^1(\mathbb{R})$, the set $\mathcal{F}_\nu$ is non-empty, the minimization problem
\[ I_{\nu,0} = \inf \{ E_{\nu,0}(Q), Q \in \mathcal{F}_\nu \} \tag{2.15} \]
has a minimizer $Q_{\nu,0}$, and all the minimizers share the same density $\rho_{\nu,0}$.

(3) For any $\nu \in H^{-1}(\mathbb{R})$, the function $(0, +\infty) \ni m \mapsto I_{\nu,m} \in \mathbb{R}_+$ is continuous, non-increasing,
\[ \lim_{m \to 0} I_{\nu,m} = I_{\nu,0} \quad \text{and} \quad \lim_{m \to +\infty} I_{\nu,m} = 0, \]
with the convention that $I_{\nu,0} = +\infty$ if $\mathcal{F}_\nu$ is empty. When $\nu \in L^1(\mathbb{R})$ and $|\cdot| \nu(\cdot) \in L^1(\mathbb{R})$,
\[ \lim_{m \to 0} I_{\nu,m} = I_{\nu,0}. \]
Moreover, if $\nu \in L^1(\mathbb{R})$ and $|\cdot| \nu(\cdot) \in L^1(\mathbb{R})$, there exists a sequence $(m_k)_{k \in \mathbb{N}}$ of positive real numbers decreasing to zero, and a sequence $(Q_{\nu,m_k})_{k \in \mathbb{N}}$ of elements of $\mathcal{K}$ such that, for each $k \in \mathbb{N}$, $Q_{\nu,m_k}$ is a minimizer of (2.14) for $m = m_k$, converging to a minimizer $Q_{\nu,0}$ of (2.15) in the following sense:
\[ UQ_{\nu,m_k}U^{-1} \xrightarrow{k \to \infty} UQ_{\nu,0}U^{-1} \quad \text{for the weak-* topology of } L^\infty(\mathbb{R}^2; \mathcal{S}(L^2(\mathbb{R}))); \tag{2.16} \]
\[ U|T - \epsilon_F|^{1/2}Q_{\nu,m_k}U^{-1} \xrightarrow{k \to \infty} U|T - \epsilon_F|^{1/2}Q_{\nu,0}U^{-1} \quad \text{weakly in } L^2(\mathbb{R}^2; \mathcal{S}_2(L^2(\mathbb{R}))); \tag{2.17} \]

The proof of Theorem 2.6 can be read in Section 3.2.

3 Proof of the results

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

3.1 Proof of Proposition 2.2

The proof of Proposition 2.2 is based on the following technical results, which show that the decomposed kinetic energy of defects actually satisfies Lieb–Thirring-like inequalities [25]. The density associated with the state of the defect can therefore be controlled by the kinetic energy of the defect.

For $q \in \mathfrak{S}_\epsilon F$, Lemma 3.1 (resp. 3.2) provides a lower bound of the densities of diagonal blocks (resp. off-diagonal blocks) of operators in $\mathcal{K}_q$. The proof of these results, obtained by the same techniques as in [12], can be read in Section 3.1.1 (resp. Section 3.1.2).

**Lemma 3.1**. There exist positive constants $C_{1,\text{diag}}, C_{2,\text{diag}}$ such that, for all $q \in \mathfrak{S}_\epsilon F$ and $Q_q \in \mathcal{K}_q$,
\[ \pm \text{Tr}_{L^2(\mathbb{R})} \left( |T_q - \epsilon_F|^{1/2}Q_q^{\pm} |T_q - \epsilon_F|^{1/2} \right) \geq C_{1,\text{diag}} \int_\mathbb{R} |\rho_{Q_q^\pm}(z)|^3 dz + C_{2,\text{diag}} \sqrt{2 \epsilon_F - |q|^2} \int_\mathbb{R} |\rho_{Q_q^\pm}(z)| dz. \tag{3.1} \]

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

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Lemma 3.2. There exist $C_{+-} \in \mathbb{R}_+$ such that, for all $q \in \mathbb{B}_{\epsilon} \cap K_q$, 

\[
\text{Tr}_{L^2(\mathbb{R})} \left( |T_q - \epsilon_F|^{|1/2} (Q_q^{++} - Q_q^{-}) |T_q - \epsilon_F|^{|1/2} \right) \geq C_{+-} (2\epsilon_F - |q|^2)^{1/4} \int_{\mathbb{R}} \left| \hat{\rho}_{Q_q^{+}}(k) \right|^2 \left| k - 2\sqrt{2\epsilon_F - |q|^2} \right|^{1/2} dk.
\]  

(3.2)

For $q \in \mathbb{R}^2 \setminus \mathbb{B}_{\epsilon} \cap K_q$, it holds $\gamma_0, q \equiv 0$ and $0 \leq Q_q^{-} \leq 1$, so that $Q_q^{++} \equiv Q_q$ and $Q_q^{-} \equiv 0$. In particular, $\rho_Q q \geq 0$. The following estimate therefore follows from the one dimensional Lie–Thirring inequality [25].

Lemma 3.3. There exists a positive constant $C$ such that, for all $q \in \mathbb{R}^2 \setminus \mathbb{B}_{\epsilon} \cap K_q$, 

\[
\text{Tr}_{L^2(\mathbb{R})} \left( |T_q - \epsilon_F|^{|1/2} (Q_q^{++} - Q_q^{-}) |T_q - \epsilon_F|^{|1/2} \right) \geq C \int_{\mathbb{R}} \rho_Q q(z) dz + \left( \frac{|q|^2}{2} - \epsilon_F \right) \int_{\mathbb{R}} \rho_Q q(z) dz.
\]  

(3.3)

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

\[
f(q) := \left| q \right|^2 - 2\epsilon_F = \begin{cases} |q|^2 - 2\epsilon_F > 0 & \text{if } q \in \mathbb{R}^2 \setminus \mathbb{B}_{\epsilon} \cap K_q, \\ 2\epsilon_F - |q|^2 & \text{if } q \in \mathbb{B}_{\epsilon} \cap K_q, \end{cases}
\]  

(3.4)

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

\[
\int_A \left( \int_A |\rho_Q q(z)| \, dq \right)^{\beta} \, dz \leq \int_A \left( \int_A |\rho_Q q(z)|^\alpha \, dq \right)^{\alpha \beta} \left( \int_A f_{-\alpha \beta/(\beta - 1)}(q) \, dq \right)^{-1/(\beta - 1)} \, dz.
\]

(3.5)

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

Estimates for the total density on $\mathbb{R}^2 \setminus \mathbb{B}_{\epsilon} \cap K_q$. Lemma 3.3 shows that

\[
\int_{\mathbb{R}^2 \setminus \mathbb{B}_{\epsilon}} \left( \int_{\mathbb{R}} \rho_Q q(z) \, dz + \left( \frac{|q|^2}{2} - \epsilon_F \right) \int_{\mathbb{R}} \rho_Q q(z) \, dz \right) \, dq 
\leq \int_{\mathbb{R}^2 \setminus \mathbb{B}_{\epsilon}} \text{Tr}_{L^2(\mathbb{R})} \left( |T_q - \epsilon_F|^{|1/2} (Q_q^{++} - Q_q^{-}) |T_q - \epsilon_F|^{|1/2} \right) \, dq \leq \text{Tr}((T - \epsilon_F)Q) < +\infty.
\]

The above inequality implies that

\[
\int_{\mathbb{R}^2 \setminus \mathbb{B}_{\epsilon}} \int_{\mathbb{R}} \rho_Q q(z) \, dz \, dq \leq \frac{1}{C} \text{Tr}((T - \epsilon_F)Q), \quad \int_{\mathbb{R}^2 \setminus \mathbb{B}_{\epsilon}} \int_{\mathbb{R}} f(q) \rho_Q q(z) \, dz \, dq \leq 2\text{Tr}((T - \epsilon_F)Q).
\]

(3.6)

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

We first set $A = \mathbb{R}^2 \setminus \mathbb{B}_{\epsilon+c}$ in (3.5). The last integral in this inequality reads

\[
\int_A f_{-\alpha \beta/(\beta - 1)}(q) \, dq = \int_{\mathbb{R}^2 \setminus \mathbb{B}_{\epsilon+c}} \left( |q|^2 - 2\epsilon_F \right)^{-\alpha \beta/(\beta - 1)} \, dq = 2\pi \int_{\sqrt{2(\epsilon_F + c)}}^{+\infty} r \left( r^2 - 2\epsilon_F \right)^{-\alpha \beta/(\beta - 1)} \, dr.
\]

The latter integral is finite if and only if $\alpha \beta/(\beta - 1) > 1$. Moreover, a Hölder inequality combined with (3.6) implies that the following integral is finite for $a > 1$:

\[
\int_{\mathbb{R}^2 \setminus \mathbb{B}_{\epsilon+c}} \int_{\mathbb{R}} \frac{3 - \frac{2}{a}}{a} f^{1/a}(q) \, dq \, dz 
\leq \left( \int_{\mathbb{R}^2 \setminus \mathbb{B}_{\epsilon+c}} \int_{\mathbb{R}} f(q) \rho_Q q(z) \, dz \, dq \right)^{1/a} \left( \int_{\mathbb{R}^2 \setminus \mathbb{B}_{\epsilon+c}} \int_{\mathbb{R}} \rho_Q q(z) \, dz \, dq \right)^{(a-1)/a}
\leq \max \left( 2, \frac{1}{C} \right) \text{Tr}((T - \epsilon_F)Q).
\]
In view of (3.5), this suggests taking $\alpha \beta = 1/a$ and $\beta = 3 - 2/a$. The condition $\alpha \beta / (\beta - 1) > 1$ can be rephrased as $1/(2a - 2) > 1$. The latter inequality is satisfied for $1 < a < 3/2$, which is equivalent to $1 < \beta < 5/3$. For the latter choice, inequality (3.5) combined with (3.6) then shows that there exists $K_{\beta, R^2} : \mathbb{R}_{x, \epsilon} \in R_+$ such that

$$
\int_{R} \left( \int_{\mathbb{R}_{x, \epsilon}^2} \rho_{q}(z) \, dq \right)^{\beta} \, dz \leq K_{\beta, R^2} \mathbb{E}_{x, \epsilon} \, \text{Tr}((T - \epsilon)Q). \tag{3.7}
$$

We next set $A = \mathbb{R}_{x, \epsilon}^2 \setminus \mathbb{R}_{x, \epsilon}$ in (3.5) and follow the same strategy as in the previous case. We still take $\alpha \beta = 1/a$ and $\beta = 3 - 2/a$, but need now that $\alpha \beta / (\beta - 1) < 1$ in order to ensure that the last integral in (3.5) is finite. This condition is equivalent to $a \geq 3/2$, i.e. $5/3 < \beta < 3$. We therefore consider $\beta = 2$. The inequality (3.5) combined with (3.6) then shows that there exists $K_{\beta, R^2} : \mathbb{R}_{x, \epsilon} \in R_+$ such that

$$
\int_{R} \left( \int_{\mathbb{R}_{x, \epsilon}^2 \setminus \mathbb{R}_{x, \epsilon}} \rho_{q}(z) \, dq \right)^{2} \, dz \leq K_{\beta, R^2} \mathbb{E}_{x, \epsilon} \, \text{Tr}((T - \epsilon)Q). \tag{3.8}
$$

**Estimates for $q \in \mathbb{R}_{x, \epsilon}$, diagonal blocks.** We write the estimates for $\rho_{q^{++}}$ only, the bounds for $\rho_{q^{--}}$ being similar. Lemma 3.1 shows that

$$
\int_{\mathbb{R}_{x, \epsilon}^2} \int_{R} \rho_{q^{++}}^{3/2}(z) \, dz \, dq \leq \frac{1}{C_{1, \text{diag}}} \mathbb{E}_{x, \epsilon} \mathbb{E}_{x, \epsilon} \, \text{Tr}((T - \epsilon)Q),
$$

$$
\int_{\mathbb{R}_{x, \epsilon}^2} \int_{R} f^{1/2}(q) \rho_{q^{++}}^{1/2}(z) \, dz \, dq \leq \frac{1}{C_{2, \text{diag}}} \mathbb{E}_{x, \epsilon} \mathbb{E}_{x, \epsilon} \, \text{Tr}((T - \epsilon)Q),
$$

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

$$
\int_{\mathbb{R}_{x, \epsilon}^2} \int_{R} \rho_{q^{++}}^{(3-1/a)}(z) f^{1/(2a)}(q) \, dz \, dq \leq \left( \int_{\mathbb{R}_{x, \epsilon}^2} \int_{R} f^{1/2}(q) \rho_{q^{++}}^{2}(z) \, dz \, dq \right)^{1/a} \left( \int_{\mathbb{R}_{x, \epsilon}^2} \int_{R} \rho_{q^{++}}^{3}(z) \, dz \, dq \right)^{(a-1)/a}
$$

$$
\leq C_{1, \text{diag}}^{1-1/a} C_{2, \text{diag}}^{1/a} \mathbb{E}_{x, \epsilon} \mathbb{E}_{x, \epsilon} \, \text{Tr}((T - \epsilon)Q) < +\infty. \tag{3.10}
$$

We now consider (3.5) with $A = \mathbb{R}_{x, \epsilon}$ and $\rho_{q}$ replaced by $\rho_{q^{++}}$. The previous inequality suggests choosing $eta = 3 - 1/a$ and $\alpha \beta = 1/(2a)$. The last integral in (3.5) is finite if and only if $\alpha \beta / (\beta - 1) < 1$, which is equivalent to $1/(4a - 2) < 1$, i.e. $a > 3/4$ and $5/3 < \beta < 3$. We therefore choose $\beta = 2$. The inequality (3.5) combined with (3.6) then shows that there exists $K_{\beta, R^2} : \mathbb{R}_{x, \epsilon} \in R_+$ such that

$$
\int_{R} \left( \int_{\mathbb{R}_{x, \epsilon}^2} \rho_{q^{++}}(z) \, dq \right)^{2} \, dz \leq K_{\beta, R^2} \mathbb{E}_{x, \epsilon} \, \text{Tr}((T - \epsilon)Q). \tag{3.11}
$$

**Estimates for $q \in \mathbb{R}_{x, \epsilon}$, off-diagonal blocks.** Define, for $k \in R$ and $q \in \mathbb{R}_{x, \epsilon}$,

$$
g(k, q) = \left| k \right| - 2\sqrt{2\epsilon \rho - |q|^2} \left( 2\epsilon \rho - |q|^2 \right)^{1/4}. \tag{3.12}
$$

In view of Lemma 3.2 and the inequality $\left| \rho_{q^{--}}^{1/2}(k) + \rho_{q^{--}}^{1/2}(k) \right| \leq 2 \left| \rho_{q^{--}}^{1/2}(k) \right|$, it holds

$$
\int_{\mathbb{R}_{x, \epsilon}^2} \int_{R} \left| \rho_{q^{--}}^{1/2}(k) + \rho_{q^{--}}^{1/2}(k) \right|^{2} g(k, q) \, dk \, dq \leq \frac{4}{C_{1}^{+}} \mathbb{E}_{x, \epsilon} \mathbb{E}_{x, \epsilon} \, \text{Tr}((T - \epsilon)Q). \tag{3.12}
$$
Note that, by the change of variables $t = |q|/\sqrt{2\epsilon_F}$ and $w = \sqrt{1 - t^2}$,

\[ G(k) := \int_{\mathbb{R} \setminus F} g(k, q)^{-1} dq = 2\pi \int_0^1 \frac{\sqrt{2\epsilon_F} t}{|2\epsilon_F|^{-1/2}|k| - 2\sqrt{1 - t^2}|1/2} \frac{dt}{(1 - t^2)^{1/4}} = 2\pi \int_0^1 \frac{\sqrt{2\epsilon_F} \sqrt{w}}{|2\epsilon_F|^{-1/2}|k| - 2w^{1/2}} dw, \]

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

\[ \rho_{Q_{\text{off-diag}}}(z) := \frac{1}{(2\pi)^2} \int_{\mathbb{R} \setminus F} \left( \rho_{Q_{\downarrow}}(z) + \rho_{Q_{\uparrow}}(z) \right) dq. \]

Using the isometry property of the Fourier transform, the Cauchy–Schwarz inequality and (3.12), we obtain the following bound on the $L^2$ norm of $\rho_{Q_{\text{off-diag}}}$:

\[
\| \rho_{Q_{\text{off-diag}}} \|_{L^2(\mathbb{R})}^2 = \int_{\mathbb{R}} \| \rho_{Q_{\text{off-diag}}}(k) \|^2 dk = \frac{1}{(2\pi)^4} \int_\mathbb{R} \left[ \int_{\mathbb{R} \setminus F} \left( \rho_{Q_{\downarrow}}(k) + \rho_{Q_{\uparrow}}(k) \right) dq \right]^2 dk \\
\leq \frac{1}{(2\pi)^4} \int_{\mathbb{R}} \left[ \int_{\mathbb{R} \setminus F} \left| \rho_{Q_{\downarrow}}(k) + \rho_{Q_{\uparrow}}(k) \right|^2 g(k, q) dq \right] G(k) dk \\
\leq \frac{1}{(2\pi)^4} \|G\|_{L^\infty(\mathbb{R})} \int_{\mathbb{R} \setminus F} \int_{\mathbb{R} \setminus F} \left| \rho_{Q_{\downarrow}}(k) + \rho_{Q_{\uparrow}}(k) \right|^2 g(k, q) dq dk \\
\leq \frac{1}{4\pi^4 C_+} \|G\|_{L^\infty(\mathbb{R})} \text{Tr}((T - \epsilon_F)Q). \quad (3.13)
\]

**Conclusion of the proof.** The estimate (2.8) finally follows from (3.7), (3.8), (3.11) and (3.13).

### 3.1.1 Proof of Lemma 3.1

Let us first state a useful technical result showing that finite–rank operators are dense in $\mathcal{X}_q$ and $\mathcal{K}_q$. It is a direct adaptation of [12, Lemma 3.2].

**Lemma 3.4.** Fix $q \in \mathbb{R}^2$ and consider $Q_q \in \mathcal{X}_q$. There exists a sequence $(Q_{n,q})_{n \geq 1} \subset \mathcal{X}_q$ of finite–rank operators such that $T_q Q_{n,q} \in \mathcal{L}(L^2(\mathbb{R}))$, and

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

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

We now can provide the proof of Lemma 3.1, which follows the proof of [12, Lemma 3.3] and uses in particular ideas from [28]. Let $0 \leq \gamma \leq 1$ be a smooth enough self-adjoint finite–rank operator on $L^2(\mathbb{R})$ (with density $\rho_\gamma$). For $q \in \mathcal{O}_\epsilon F$, $T_q - \epsilon_F = -\frac{1}{2} \frac{d^2}{dz^2}$ and (3.1) boils down to the one-dimensional Lieb–Thirring inequality [25]. For $q \in \mathcal{O}_\epsilon F$, denote by $\rho_{e,q}$ the density of the finite-rank operator $P_{e,q} \gamma P_{e,q}$ where $P_{e,q} := 1_{[e, +\infty)} (T_q - \epsilon_F)$. Then, by the same manipulations as in [12],

\[
\text{Tr}_{L^2(\mathbb{R})} \left( |T_q - \epsilon_F|^{1/2} \right| T_q - \epsilon_F |^{1/2}) = \int_0^{+\infty} \left( \int_{\mathbb{R}} \rho_{e,q}(z) dz \right) de \geq \int_{\mathbb{R}} R_q(\rho_\gamma(z)) dz, \\
\text{with} \quad R_q(t) = \int_0^{f_q^{-1}(t)} \left( \sqrt{t} - \sqrt{f_q(e)} \right)^2 de,
\]
where (introducing $a_+ = \max(0, a)$) the nonnegative function

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

is increasing, hence invertible.

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

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

and

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

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

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

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

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

from which we deduce that

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

The final result is obtained by a continuity argument and the density result of Lemma 3.4.

### 3.1.2 Proof of Lemma 3.2

We follow the proofs of [12, Theorem 2.1 and Lemma 3.4]. Inequality (3.2) is trivial for $q \in \partial \mathbb{B}_{\epsilon_F}$. Fix $q \in \mathbb{B}_{\epsilon_F}$ and $Q_q \in \mathbb{K}_q$. Since $Q_q^+ = (Q_q^+)^*$, it holds $\rho_{Q_q^+} + \rho_{Q_q^-} = 2\rho_{Q_q^+}$. It suffices therefore to obtain estimates for $\rho_{Q_q^+}$. We rely on a duality argument. Consider to this end $V \in L^2(\mathbb{R})$. By proceeding as in [12],

$$\left| \int_{\mathbb{R}} V \rho_{Q_q^+} \right| \leq \frac{1 - \gamma_{0,q}}{|T_q - \epsilon_F|^{1/4}} V \frac{\gamma_{0,q}}{|T_q - \epsilon_F|^{1/4}} \sqrt{\text{tr} L^2(\mathbb{R}) \left( |T_q - \epsilon_F|^{1/2} (Q_q^{++} - Q_q^{-}) |T_q - \epsilon_F|^{1/2} \right)} (3.14)$$

Now,

$$\left| \frac{1 - \gamma_{0,q}}{|T_q - \epsilon_F|^{1/4}} V \frac{\gamma_{0,q}}{|T_q - \epsilon_F|^{1/4}} \right|^2 = \frac{1}{2\pi} \int_{\mathbb{R}} |\hat{V}(k)|^2 \Phi_q(k) \, dk,$$

with

$$\Phi_q(k) := \frac{1}{2\pi} \int_{|q|/2 \leq \epsilon_F} \frac{ds}{\sqrt{\left( \frac{|q|^2}{2} + \frac{(s-k)^2}{2} - \epsilon_F \right) \left( \epsilon_F - \frac{|q|^2}{2} - \frac{s^2}{2} \right)}}.$$ 

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

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

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The bounds (3.14) and (3.15) then lead to
\[
\left| \int E \rho Q_{q^+}^{-1} \right|^2 \leq 2 \int (k) \Phi_q(k) d k \right) \right) \phi_{q^+}^{-1} \right)^2 \left( |T_q - \epsilon_F|^{1/2} (Q_q^+ - Q_q^-) |T_q - \epsilon_F|^{1/2} \right).
\]
From the estimates on $\psi$ provided by \cite[Lemma 3.4]{12} (namely $\psi$ of the densities relies on a technical result whose proof is postponed to Section 3.2.3. Finally, we show in Section 3.2.2 the existence of minimizers for Yukawa and Coulomb interactions. The uniqueness shows that 0 implies that 0 of the charges per unit area of the defect:
\[
\begin{align*}
\forall 0 < w_q \leq \sqrt{2\epsilon_F}, \forall k \in \mathbb{R}, \quad 0 \leq \Phi_q(k) \leq \frac{R}{||k|| - 2\omega_q^{1/2} \sqrt{\omega_q}}, \quad (3.16)
\end{align*}
\]
which implies
\[
\frac{2\pi}{R} \sqrt{\omega_q} \int E | \rho Q_{q^+}^{-1}(k) |^2 ||k|| - 2\omega_q^{1/2} d k \leq 2\pi \int \frac{| \rho Q_{q^+}^{-1}(k) |^2}{\Phi_q(k)} d k \leq \text{Tr}_{L^2(\mathbb{R})} \left( |T_q - \epsilon_F|^{1/2} (Q_q^+ - Q_q^-) |T_q - \epsilon_F|^{1/2} \right).
\]
This gives the claimed result.

3.2 Proof of Theorem 2.6

We first show in Section 3.2.1 that the minimization set $F_{\nu}$ for Coulomb interactions is not empty. We then prove in Section 3.2.2 the existence of minimizers for Yukawa and Coulomb interactions. The uniqueness of the densities relies on a technical result whose proof is postponed to Section 3.2.3. Finally, we show in Section 3.2.4 that the Yukawa ground state converges to the Coulomb ground state when $m \to 0$.

3.2.1 The set $F_{\nu}$ is not empty

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

Non-negative total charge per unit area. Consider first the case when $\kappa \geq 0$. We introduce an even cut-off function $\chi \in C_{\infty}^\infty(\mathbb{R})$ such that
\[
0 \leq \chi \leq 1, \quad \int \chi^2 = 1.
\]
For a parameter $\mu \in (\epsilon_F, +\infty)$ to be specified and almost all $q \in \mathbb{R}^2$, we then define the self-adjoint operator
\[
Q_{\mu,q} := U \left( \int_{\mathbb{R}^2} Q_{\mu,q} dq \right)^{-1} \right), \quad Q_{\mu,q} := 1_{(\epsilon_F, \mu]}(T_q) \chi^2 1_{(\epsilon_F, \mu]}(T_q).
\]
Note first that $Q_{\mu,q} = 0$ when $|q|^2 > 2\mu$. The operator inequality $0 \leq 1_{(\epsilon_F, \mu]}(T_q) \leq 1_{(\epsilon_F, +\infty)}(T_q) = 1 - \gamma_{0,q}$ also implies that $0 \leq Q_{\mu,q} = Q_{\mu,q}^+$ from $\gamma_{0,q}$. Therefore, $q \mapsto Q_{\mu,q} \in L^\infty(\mathbb{R}^2; S(L^2(\mathbb{R})))$. Moreover, the Kato–Seiler–Simon inequality \cite[Theorem 4.1]{20}
\[
\forall p \geq 2, \quad \|f(-i\nabla)g\|_{L_p} \leq (2\pi)^{-1/p} \|g\|_{L_p} \|f\|_{L_p},
\]
shows that
\[
|T_q - \epsilon_F|^{1/2} Q_{\mu,q} T_q - \epsilon_F |^{1/2} = \left( |T_q - \epsilon_F|^{1/2} 1_{(\epsilon_F, \mu]}(T_q) \right) \left( \chi^2 1_{(\epsilon_F, \mu]}(T_q) T_q - \epsilon_F |^{1/2} \right) \in \mathcal{S}_1
\]
as the product of two Hilbert–Schmidt operators. We have therefore proven at this stage that $Q_{\mu,q} \in \mathcal{K}_q$ for all $q \in \mathbb{R}^2$.

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

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

we obtain

$$\text{Tr} \left( (T - \epsilon F)Q_\mu \right) = \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} \text{Tr}_{L^2(\mathbb{R})} \left( |T_q - \epsilon F|^{1/2}Q_{\mu,q}|T_q - \epsilon F|^{1/2} \right) \, dq = \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} \left( \int_{\mathbb{R}} \chi^2 \right) \left( \int_{\mathbb{R}} |g_q|^2 \right) \, dq$$

$$= \frac{1}{(2\pi)^3} \int_{\mathbb{R}^2} \int_{\epsilon F < \frac{|q|^2}{2} + \frac{k^2}{2} \leq \mu} \left( k^2 + |q|^2 \right) \frac{dk \, dq}{2 - \epsilon F} < \infty,$$

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

It remains to prove that $\rho_{Q_\mu} - \nu \in \mathcal{C}$. First, it easily follows from (3.17) that $\rho_{Q_\mu}$ is smooth and compactly supported. By computations similar to the ones used to establish (3.20), and noting that $Q_{\mu,q} \in \mathcal{G}_1$ by a decomposition similar to (3.19),

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

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

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

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

It is easy to see that $-\gamma_{0,q} \leq Q_{\alpha,q} = Q_{\alpha,q}^{-1} \leq 0$ and that $Q_{\alpha,q} = 0$ when $|q|^2 > 2\epsilon F$, so that $q \mapsto Q_{\alpha,q} \in L^\infty(\mathbb{R}^2; \mathcal{S}(L^2(\mathbb{R})))$. Moreover, $|T_q - \epsilon F|^{1/2}Q_{\alpha,q} \in \mathcal{G}_2$ by the Kato–Seiler–Simon inequality (3.18), so that $|T_q - \epsilon F|^{1/2}Q_{\alpha,q}T_q - \epsilon F|^{1/2} \in \mathcal{G}_1$. This shows that $Q_{\alpha,q} \in \mathcal{K}_q$ for all $q \in \mathbb{R}^2$. In addition, by computations similar to the ones performed for the case $\kappa \geq 0$,

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

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

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

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

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

### 3.2.2 Existence of ground state for Yukawa (resp. Coulomb) interactions

We write a detailed proof for Coulomb interactions, the result for Yukawa interactions following the same lines. We first construct a candidate minimizer $\overline{Q}$ by as the limit of some minimizing sequence for (2.14) and next show that $\overline{Q}$ is an admissible state (i.e. $\overline{Q} \in \mathcal{K}$). We finally prove that $Q_{\kappa}$ is a minimizer and that all minimizers share the same density.
Construction of a candidate minimizer. It is easy to see that the functional \( \mathcal{E}_{\nu,0}(Q) \) is well defined on the non-empty set \( \mathcal{F}_\nu \). Consider a minimizing sequence \( \{Q_n\}_{n \geq 1} \subset \mathcal{F}_\nu \). There exists \( C \in \mathbb{R}_+ \) such that
\[
\forall n \geq 1, \quad \text{Tr}((T - \varepsilon_F)Q_n) \leq C, \quad \text{D}(\rho_{Q_n} - \nu, \rho_{Q_n} - \nu) \leq C. \tag{3.21}
\]
Consider any exponent \( 1 < p < 5/3 \). Inequality (2.8) shows that the sequence of densities \( \{\rho_{Q_n}\}_{n \geq 1} \) is uniformly bounded in \( L^2(\mathbb{R}) + L^p(\mathbb{R}) \). Up to extraction, there exist
\[
\begin{align*}
\mathcal{Q} & := U^{-1} \left( \int_{\mathbb{R}^2} \mathcal{Q}_q \, dq \right) U, \quad \forall \mathcal{Q} \in L^2(\mathbb{R}) + L^p(\mathbb{R}), \quad \tilde{\rho}_Q - \nu \in \mathbb{C} \\
\end{align*}
\]
such that \( \rho_{Q_n} \rightharpoonup \mathcal{Q} \) weakly in \( L^2(\mathbb{R}) + L^p(\mathbb{R}) \) and \( \rho_{Q_n} - \nu \rightharpoonup \tilde{\rho}_Q - \nu \) weakly in \( \mathbb{C} \), while \( -\gamma_0 \leq \mathcal{Q} \leq 1 - \gamma_0 \) and \( Q_n \rightharpoonup Q \) in the following sense:
\begin{itemize}
\item for any operator-valued function \( q \mapsto U_q \in L^1(\mathbb{R}^2; \mathcal{S}_1) \),
\[
\int_{\mathbb{R}^2} \text{Tr}_{L^2(\mathbb{R})}(U_q Q_{n,q}) \, dq \rightarrow \int_{\mathbb{R}^2} \text{Tr}_{L^2(\mathbb{R})}(U_q \mathcal{Q}) \, dq; \tag{3.22}
\]
\item for any operator-valued function \( q \mapsto M_q \in L^2(\mathbb{R}^2; \mathcal{S}_2) \),
\[
\int_{\mathbb{R}^2} \text{Tr}_{L^2(\mathbb{R})}(|T_q - \varepsilon_F|^{1/2} Q_{n,q} M_q) \, dq \rightarrow \int_{\mathbb{R}^2} \text{Tr}_{L^2(\mathbb{R})}(|T_q - \varepsilon_F|^{1/2} \mathcal{Q} M_q) \, dq; \tag{3.23}
\]
\[
\int_{\mathbb{R}^2} \text{Tr}_{L^2(\mathbb{R})}(M_q |T_q - \varepsilon_F|^{1/2} Q_{n,q}) \, dq \rightarrow \int_{\mathbb{R}^2} \text{Tr}_{L^2(\mathbb{R})}(M_q |T_q - \varepsilon_F|^{1/2} \mathcal{Q}) \, dq; \tag{3.24}
\]
\[
\int_{\mathbb{R}^2} \text{Tr}_{L^2(\mathbb{R})}(M_q Q_{n,q} |T_q - \varepsilon_F|^{1/2}) \, dq \rightarrow \int_{\mathbb{R}^2} \text{Tr}_{L^2(\mathbb{R})}(M_q \mathcal{Q} |T_q - \varepsilon_F|^{1/2}) \, dq. \tag{3.25}
\]
\end{itemize}
The weak-\( * \) convergence (3.22) is a consequence of the fact that the sequence \( \{Q_n\}_{n \geq 1} \) is uniformly bounded in \( L^\infty(\mathbb{R}^2; \mathcal{L}(L^2(\mathbb{R}))) \), whose pre-dual is \( L^1(\mathbb{R}^2; \mathcal{S}_1) \). The weak convergences (3.23) to (3.25) are a consequence of the inequality
\[
\int_{\mathbb{R}^2} \left\| |T_q - \varepsilon_F|^{1/2} Q_{n,q} \right\|^2_{\mathcal{S}_2} \, dq \leq \int_{\mathbb{R}^2} \text{Tr}_{L^2(\mathbb{R})}(|T_q - \varepsilon_F|^{1/2}(Q_{n,q}^+ - Q_{n,q}^-)|T_q - \varepsilon_F|^{1/2}) \, dq \leq C, \tag{3.26}
\]
which shows that the sequence of operator-valued functions \( q \mapsto |T_q - \varepsilon_F|^{1/2} Q_{n,q} \) and \( q \mapsto Q_{n,q} |T_q - \varepsilon_F|^{1/2} \) are uniformly bounded in the Hilbert space \( L^2(\mathbb{R}^2; \mathcal{S}_2) \).

The state \( \mathcal{Q} \) belongs to \( \mathcal{K} \). Note first that the weak convergence of \( \{q \mapsto |T_q - \varepsilon_F|^{1/2} Q_{n,q}\}_{n \geq 1} \) to \( q \mapsto |T_q - \varepsilon_F|^{1/2} Q \) in \( L^2(\mathbb{R}^2; \mathcal{S}_2) \) implies
\[
\int_{\mathbb{R}^2} \left\| |T_q - \varepsilon_F|^{1/2} \mathcal{Q} \right\|^2_{\mathcal{S}_2} \, dq \leq \liminf_{n \to \infty} \int_{\mathbb{R}^2} \left\| |T_q - \varepsilon_F|^{1/2} Q_{n,q} \right\|^2_{\mathcal{S}_2} \, dq.
\]
It is therefore sufficient to show that \( \text{Tr}((T - \varepsilon_F) \mathcal{Q}) < \infty \) in order to conclude that \( \mathcal{Q} \in \mathcal{K} \). Consider to this end an orthonormal basis \( \{\phi_i\}_{i \in \mathbb{N}} \subset H^1(\mathbb{R}) \) of \( L^2(\mathbb{R}) \), and define, for \( N \geq 1 \) and \( R > 0 \), the family of operators
\[
M_{q,R}^N := |T_q - \varepsilon_F|^{1/2} \left( \sum_{i=1}^N \phi_i \langle \phi_i \rangle \right) g_R(q),
\]
where
\[
g_R(q) := \begin{cases} 
1 \quad \text{if } |q|^2 < R \\
\frac{1}{(1 + |q|^2)^2} \quad \text{if } |q|^2 \geq R.
\end{cases}
\]
A simple computation shows that \( q \rightarrow M_{q,R}^N \) is in \( L^2(\mathbb{R}^2; \mathcal{G}_2) \). Using (3.23) with \( q \rightarrow (1 - \gamma_{0,q})M_{q,R}^N(1 - \gamma_{0,q}) \),

\[
0 \leq \int_{\mathbb{R}^2} \text{Tr}_{L^2(\mathbb{R})} \left( |T_q - \epsilon F|^{1/2} T_q \right) dq
\]

\[
= \int_{\mathbb{R}^2} \text{Tr}_{L^2(\mathbb{R})} \left( |T_q - \epsilon F|^{1/2} \mathcal{Q}_q^+ \right) \left( |T_q - \epsilon F|^{1/2} \sum_{i=1}^N |\phi_i \rangle \langle \phi_i| \right) g_R(q) dq
\]

\[
= \lim_{n \to \infty} \int_{\mathbb{R}^2} \sum_{i=1}^N \langle \phi_i \left| T_q - \epsilon F \right|^{1/2} Q_{n,q}^+ \left| T_q - \epsilon F \right|^{1/2} \langle \phi_i \rangle g_R(q) dq
\]

\[
\leq \liminf_{n \to \infty} \int_{\mathbb{R}^2} \text{Tr}_{L^2(\mathbb{R})} \left( |T_q - \epsilon F|^{1/2} Q_{n,q}^+ \right) \left| T_q - \epsilon F \right|^{1/2} dq \leq C,
\]

where the last inequality is a consequence of the uniform bound (3.21). We can then pass to the limits \( R \to +\infty \) and \( N \to +\infty \) with Fatou’s Lemma and get

\[
0 \leq \int_{\mathbb{R}^2} \text{Tr}_{L^2(\mathbb{R})} \left( |T_q - \epsilon F|^{1/4} Q_q^+ \right) \left( |T_q - \epsilon F|^{1/4} \right) dq \leq \liminf_{n \to +\infty} \int_{\mathbb{R}^2} \text{Tr}_{L^2(\mathbb{R})} \left( |T_q - \epsilon F|^{1/2} Q_{n,q}^+ \right) \left( |T_q - \epsilon F|^{1/2} \right) dq.
\]

A similar reasoning shows that

\[
0 \leq -\int_{\mathbb{R}^2} \text{Tr}_{L^2(\mathbb{R})} \left( |T_q - \epsilon F|^{1/2} Q_q^- \right) \left( |T_q - \epsilon F|^{1/2} \right) dq \leq -\liminf_{n \to +\infty} \int_{\mathbb{R}^2} \text{Tr}_{L^2(\mathbb{R})} \left( |T_q - \epsilon F|^{1/2} Q_{n,q}^- \right) \left( |T_q - \epsilon F|^{1/2} \right) dq.
\]

The combination of the last two inequalities shows that

\[
0 \leq \text{Tr} \left( (T - \epsilon F) \mathcal{Q} \right) \leq \liminf_{n \to +\infty} \text{Tr} \left( (T - \epsilon F) Q_n \right) \leq C,
\]

(3.27)

so that \( \mathcal{Q} \in \mathcal{K} \).

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

**Lemma 3.5.** (Consistency of densities) It holds \( \rho_{\mathcal{Q}} - \nu = \tilde{\rho}_Q - \nu = \bar{\rho}_Q - \nu \) in \( D'(\mathbb{R}) \). In particular, \( \rho_{\mathcal{Q}} = \tilde{\rho}_Q \) as elements of \( L^2(\mathbb{R}) + L^p(\mathbb{R}) \), and \( \rho_{\mathcal{Q}} - \nu = \bar{\rho}_Q - \nu \) as elements of \( \mathcal{C} \).

We postpone the proof of this result to Section 3.2.3. We use it to obtain that, since \( D(\cdot,\cdot) \) defines an inner product on \( \mathcal{C} \),

\[
D(\rho_{\mathcal{Q}} - \nu, \rho_{\mathcal{Q}} - \nu) \leq \liminf_{n \to +\infty} D(\rho_{Q_n} - \nu, \rho_{Q_n} - \nu).
\]

(3.28)

This shows in particular that \( \mathcal{Q} \) is an admissible state (i.e. \( \mathcal{Q} \in \mathcal{F}_\nu \)). Moreover, (3.27) and (3.28) imply that the minimizing sequence \( \{Q_n\}_{n \geq 1} \) is such that

\[
E_{\nu,0}(\mathcal{Q}) \leq \liminf_{n \to +\infty} E_{\nu,0}(Q_n),
\]

(3.29)

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

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

\[
E_{\nu,0} \left( \frac{\mathcal{Q}_1 + \mathcal{Q}_2}{2} \right) = \frac{1}{2} E_{\nu,0} (\mathcal{Q}_1) + \frac{1}{2} E_{\nu,0} (\mathcal{Q}_2) - \frac{1}{4} D \left( \rho_{\mathcal{Q}_1} - \rho_{\mathcal{Q}_2}, \rho_{\mathcal{Q}_1} - \rho_{\mathcal{Q}_2} \right),
\]

which shows that \( D \left( \rho_{\mathcal{Q}_1} - \rho_{\mathcal{Q}_2}, \rho_{\mathcal{Q}_1} - \rho_{\mathcal{Q}_2} \right) = 0 \). This implies that all minimizers share the same density.
3.2.3 Proof of Lemma 3.5

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

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

\[
\langle \rho_{Q_n} - \nu, w \rangle \xrightarrow{n \to \infty} \langle \tilde{\rho}_Q - \nu, w \rangle.
\]

Note next that

\[
\langle \rho_{Q_n} - \nu, w \rangle = \int_\mathbb{R} (\rho_{Q_n} - \nu) w = \int_\mathbb{R} \left( \hat{\rho}_{Q_n} - \hat{\nu} \right)(k) \hat{w}(k) \, dk = 2 \int_\mathbb{R} \frac{\left| \hat{\rho}_{Q_n} - \hat{\nu} \right| \hat{f}(k) \hat{f}(k)}{|k|^2} \, dk = \mathcal{D} \left( \rho_{Q_n} - \nu, f \right),
\]

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

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

\[
\langle \rho_{Q_n}, w \rangle \xrightarrow{n \to \infty} \langle \bar{\rho}_Q, w \rangle.
\]

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

\[
\frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} \text{Tr}_L^2(\mathbb{R}) \left( wQ_{n,q} \right) \, dq = \text{Tr} (wQ_{n,q}) = \langle \rho_{Q_n}, w \rangle \xrightarrow{n \to \infty} \langle \rho_{\mathcal{Q}}, w \rangle = \text{Tr} (w\mathcal{Q}) \equiv \langle \rho_{\mathcal{Q}}, w \rangle. \tag{3.30}
\]

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

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

\[
\forall q \in \mathbb{R}^2 \backslash \mathfrak{B}_R, \quad \|T_q - \epsilon_F|^{-1/2} w |T_q - \epsilon_F|^{-1/2} \| \leq \|w\|_{L^\infty} \|R - \epsilon_F\|^{-1}.
\]

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

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

Integrating over \( q \in \mathbb{R}^2 \backslash \mathfrak{B}_R \) and relying on the uniform bound (3.21), we finally obtain

\[
\left| \int_{\mathbb{R}^2 \backslash \mathfrak{B}_R} \text{Tr}_L^2(\mathbb{R}) \left( wQ_{n,q} \right) \, dq \right| \leq C \|w\|_{L^\infty} \|R - \epsilon_F\|^{-1}. \tag{3.31}
\]

This term therefore vanishes as \( R \to +\infty \). Note that a similar inequality holds if \( Q_{n,q} \) is replaced by \( \bar{Q}_{n,q} \).
Consider next the case when \( q \in \mathfrak{B}_{R,1} (\mathbb{R}) \). The Kato–Seiler–Simon inequality (3.18) shows that \( w |T_q - \epsilon_F|^{-1/2} \) is Hilbert Schmidt, and \( q \mapsto w |T_q - \epsilon_F|^{-1/2} \) is in \( L^2 (\mathfrak{B}_{R,1}, \mathfrak{S}_2) \). The convergence (3.24) then shows that

\[
\int_{\mathfrak{B}_{R,1}} \text{Tr}_{L^2(\mathbb{R})} \left( wQ_n,q \right) dq = \int_{\mathfrak{B}_{R,1}} \text{Tr}_{L^2(\mathbb{R})} \left( w |T_q - \epsilon_F|^{-1/2} |T_q - \epsilon_F|^{1/2} Q_n,q \right) dq.
\]

(3.32)

Consider finally the case when \( q \in \mathfrak{B}_{e^F} \). Define \( \Pi_{1,q} := 1_{(-\infty,2\epsilon_F]} (T_q) \) and \( \Pi_{2,q} := 1 - \Pi_{1,q} \). We decompose the operator \( wQ_n,q \) as \( w\Pi_{2,q} Q_n,q + \Pi_{1,q} w\Pi_{1,q} Q_n,q + \Pi_{2,q} w\Pi_{1,q} Q_{n,q} \). We show successively that these three operators are trace-class, and characterize their limits as \( n \to +\infty \). Note first that \( w\Pi_{2,q} Q_{n,q} = w\Pi_{2,q} |T_q - \epsilon_F|^{-1/2} |T_q - \epsilon_F|^{1/2} Q_{n,q} \) is the product of two Hilbert–Schmidt operators. In fact, a simple computation based on the Kato–Seiler–Simon inequality (3.18) shows that \( q \mapsto w\Pi_{2,q} |T_q - \epsilon_F|^{-1/2} \in L^2 (\mathfrak{B}_{e^F}; \mathfrak{S}_2) \). Therefore, by (3.24),

\[
\int_{\mathfrak{B}_{e^F}} \text{Tr}_{L^2(\mathbb{R})} \left( w\Pi_{2,q} Q_n,q \right) dq \quad \longrightarrow \quad \int_{\mathfrak{B}_{e^F}} \text{Tr}_{L^2(\mathbb{R})} \left( w\Pi_{2,q} \bar{Q}_q \right) dq.
\]

(3.33)

For the second operator, we denote by \( w_+ \) (resp. \( w_- \)) the positive (resp. negative) part of \( w \), so that \( w = w_+ - w_- \). Since \( \Pi_{1,q} w \sqrt{w} \in \mathfrak{S}_2 \), it follows that \( \Pi_{1,q} w \sqrt{w} \Pi_{1,q} \in \mathfrak{S}_1 \). A simple computation shows that \( q \mapsto \Pi_{1,q} w \sqrt{w} \Pi_{1,q} \in L^1 (\mathfrak{B}_{e^F}; \mathfrak{S}_1) \), so that \( q \mapsto \Pi_{1,q} w \Pi_{1,q} \in L^1 (\mathfrak{B}_{e^F}; \mathfrak{S}_1) \). Therefore, in view of (3.22),

\[
\int_{\mathfrak{B}_{e^F}} \text{Tr}_{L^2(\mathbb{R})} \left( \Pi_{1,q} w \Pi_{1,q} Q_n,q \right) dq \quad \longrightarrow \quad \int_{\mathfrak{B}_{e^F}} \text{Tr}_{L^2(\mathbb{R})} \left( \Pi_{1,q} w \Pi_{1,q} \bar{Q}_q \right) dq.
\]

(3.34)

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

**Lemma 3.6.** The operator-valued function \( q \mapsto \Pi_{2,q} w \Pi_{1,q} \) belongs to \( L^\infty (\mathfrak{B}_{e^F}; \mathfrak{S}_1) \).

In particular, \( q \mapsto \Pi_{2,q} w \Pi_{1,q} \) belongs to \( L^1 (\mathfrak{B}_{e^F}; \mathfrak{S}_1) \), so that, by (3.22),

\[
\int_{\mathfrak{B}_{e^F}} \text{Tr}_{L^2(\mathbb{R})} \left( \Pi_{2,q} w \Pi_{1,q} Q_n,q \right) dq \quad \longrightarrow \quad \int_{\mathfrak{B}_{e^F}} \text{Tr}_{L^2(\mathbb{R})} \left( \Pi_{2,q} w \Pi_{1,q} \bar{Q}_q \right) dq.
\]

(3.35)

We finally obtain, by summing (3.33), (3.35) and (3.34), that

\[
\int_{\mathfrak{B}_{e^F}} \text{Tr}_{L^2(\mathbb{R})} \left( wQ_n,q \right) dq \quad \longrightarrow \quad \int_{\mathfrak{B}_{e^F}} \text{Tr}_{L^2(\mathbb{R})} \left( w \bar{Q}_q \right) dq.
\]

(3.36)

The combination of (3.31), (3.32) and (3.36) shows that (3.30) holds, which allows to conclude the proof of the equality \( \rho_{\bar{Q}_q} - \nu = \bar{\mathfrak{B}}_Q - \nu \) in the sense of distributions.

Let us conclude this section by providing the proof of Lemma 3.6.

**Proof of Lemma 3.6.** Consider \( q \in \mathfrak{B}_{e^F} \). We decompose the operator \( \Pi_{2,q} w \Pi_{1,q} \) as follows:

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

By the Kato–Seiler–Simon inequality (3.18), \( q \mapsto \Pi_{2,q} (T_q - \epsilon_F)^{-1} \sqrt{w} \) and \( q \mapsto \sqrt{w} (T_q - \epsilon_F) \Pi_{1,q} \) both belong to \( L^\infty (\mathfrak{B}_{e^F}; \mathfrak{S}_2) \), so that \( q \mapsto \Pi_{2,q} (T_q - \epsilon_F)^{-1} w (T_q - \epsilon_F) \Pi_{1,q} \) is in \( L^\infty (\mathfrak{B}_{e^F}; \mathfrak{S}_1) \). Moreover,

\[
\Pi_{2,q} (T_q - \epsilon_F)^{-1} \left[ \frac{d^2}{dz^2}, w \right] \Pi_{1,q} = 2 \Pi_{2,q} (T_q - \epsilon_F)^{-1} w' \frac{d}{dz} \Pi_{1,q} + \Pi_{2,q} (T_q - \epsilon_F)^{-1} w'' \Pi_{1,q}.
\]
The decomposition
\[
\Pi_{2,q}(T_q - \epsilon_F)^{-1}w' \frac{d}{dz} \Pi_{1,q} = \left[ \Pi_{2,q}(T_q - \epsilon_F)^{-1}\sqrt{(w')} \right] \left[ \sqrt{(w')} - \frac{d}{dz} \Pi_{1,q} \right]
\]
shows that \( q \mapsto \Pi_{2,q}(T_q - \epsilon_F)^{-1}w' \frac{d}{dz} \Pi_{1,q} \) belongs to \( L^\infty(\mathcal{B}_{\epsilon_F+c}, \mathcal{G}_1) \) as the sum of products of operator-valued functions in \( L^\infty(\mathcal{B}_{\epsilon_F+c}, \mathcal{G}_2) \). It can also similarly be shown that \( q \mapsto \Pi_{2,q}(T_q - \epsilon_F)^{-1}w'' \Pi_{1,q} \) is in \( L^\infty(\mathcal{B}_{\epsilon_F+c}, \mathcal{G}_1) \), which proves the statement of the lemma. 

\[\square\]

3.2.4 Convergence of Yukawa to Coulomb

Monotonicity of the ground state. Fix \( \nu \in H^{-1}(\mathbb{R}) \) and \( m_1 \geq m_2 > 0 \). Note first that, for any \( f \in H^{-1}(\mathbb{R}) \),
\[
D_{m_1}(f, f) \leq D_{m_2}(f, f) \leq D(f, f), \tag{3.37}
\]
with the convention that \( D(f, f) := +\infty \) if \( f \notin \mathcal{C} \). Since \( \rho_Q - \nu \in \mathcal{C}_m \) for any \( m > 0 \) when \( Q \in \mathcal{K} \) (see Proposition 2.2), it holds \( 0 \leq \mathcal{E}_{\nu, m_1}(Q) \leq \mathcal{E}_{\nu, m_2}(Q) \leq \mathcal{E}_{\nu, 0}(Q) \) for any \( Q \in \mathcal{K} \). This immediately implies that
\[
\forall m \geq m_2 > 0, \quad 0 \leq I_{\nu, m_1} \leq I_{\nu, m_2} \leq I_{\nu, 0}, \tag{3.38}
\]
which proves that \( m \mapsto I_{\nu, m} \) is non-increasing on \( (0, +\infty) \).

Continuity of the ground state. Fix \( m > 0 \) and \( \delta m > 0 \). Denote by \( \overline{Q}_m \) (resp. \( \overline{Q}_{m+\delta m} \)) one of the minimizers of the energy functional \( \mathcal{E}_{\nu, m} \) (resp. \( \mathcal{E}_{\nu, m+\delta m} \)) on \( \mathcal{K} \). Then, in view of the monotonicity property (3.38),
\[
0 \leq I_{\nu, m} - I_{\nu, m+\delta m} = \mathcal{E}_{\nu, m}(\overline{Q}_m) - \mathcal{E}_{\nu, m+\delta m}(\overline{Q}_{m+\delta m}) \\
\leq \mathcal{E}_{\nu, m}(\overline{Q}_{m+\delta m}) - \mathcal{E}_{\nu, m+\delta m}(\overline{Q}_{m+\delta m}) \\
= \frac{1}{2} D_m \left( \rho_{\overline{Q}_{m+\delta m}} - \nu, \rho_{\overline{Q}_{m+\delta m}} - \nu \right) - D_{m+\delta m} \left( \rho_{\overline{Q}_{m+\delta m}} - \nu, \rho_{\overline{Q}_{m+\delta m}} - \nu \right) \\
= \int_{\mathbb{R}} \frac{(m + \delta m)^2 - m^2}{k^2 + m^2} \frac{|\hat{\rho}_{\overline{Q}_{m+\delta m}}(k) - \hat{\rho}(k)|^2}{|k|^2 + (m + \delta m)^2} \, dk \\
\leq \frac{1}{2} \left( 1 + \frac{\delta m}{m} \right)^2 - 1 \frac{1}{D_{m+\delta m}} \left( \rho_{\overline{Q}_{m+\delta m}} - \nu, \rho_{\overline{Q}_{m+\delta m}} - \nu \right) \\
\leq \left[ \left( 1 + \frac{\delta m}{m} \right)^2 - 1 \right] I_{\nu, m+\delta m} \leq \left[ \left( 1 + \frac{\delta m}{m} \right)^2 - 1 \right] I_{\nu, m}.
\]
A similar inequality can be obtained for \( \delta m < 0 \) sufficiently small. This allows to conclude that \( m \mapsto I_{\nu, m} \) is continuous on \( (0, +\infty) \).

Limit as \( m \to +\infty \). Fix \( \nu \in H^{-1}(\mathbb{R}) \). Note that \( 0 \in \mathcal{K} \), so that
\[
0 \leq I_{\nu, m} \leq \mathcal{E}_{\nu, m}(0) = D_m(\nu, \nu) = 2 \int_{\mathbb{R}} \frac{|\hat{\rho}(k)|^2}{k^2 + m^2} \, dk.
\]
The latter integral converges to 0 as \( m \to +\infty \) by dominated convergence. This shows that \( I_{\nu, m} \to 0 \) as \( m \to +\infty \).
Limit as \( m \to 0 \). Note first that (3.38) implies that \( \lim_{m \to 0} I_{\nu,m} \leq I_{\nu,0} \) for any \( \nu \in H^{-1}(\mathbb{R}) \). Let us now prove the converse inequality under the conditions \( \nu \in L^1(\mathbb{R}) \) and \( | \cdot | \nu(\cdot) \in L^1(\mathbb{R}) \). Denote one of the minimizers of (2.14) by \( Q_{\nu,m} \). By (3.38),

\[
\forall m > 0, \quad I_{\nu,m} = \text{Tr} \left( (T - \epsilon F) Q_{\nu,m} \right) + \frac{1}{2} D_m(\rho_{Q_{\nu,m}} - \nu, \rho_{Q_{\nu,m}} - \nu) \leq I_{\nu,0}.
\]

In particular, \( \text{Tr} \left( (T - \epsilon F) Q_{\nu,m} \right) \) is uniformly bounded. By arguments similar to the ones used to establish (3.27) and Lemma 3.5, there exists \( Q_{\nu,0} \in \mathcal{K} \) and a subsequence \( (Q_{\nu,m_k})_{k \in \mathbb{N}} \) with \( m_k \to 0 \) such that (2.16) and (2.17) hold true, \( \rho_{Q_{\nu,m_k}} \to \rho_{Q_{\nu,0}} \) weakly in \( L^2(\mathbb{R}) + L^p(\mathbb{R}) \) (for a fixed \( 1 < p < 5/3 \) and

\[
\text{Tr} \left( (T - \epsilon F) Q_{\nu,0} \right) \leq \lim_{k \to \infty} \text{Tr} \left( (T - \epsilon F) Q_{\nu,m_k} \right). \tag{3.39}
\]

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

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

\[
\langle \rho_{Q_{\nu,m_k}} - \nu, \Phi \rangle = \left( \frac{\hat{\rho}_{Q_{\nu,m_k}} - \hat{\nu}}{\sqrt{1 + m_k^2}}, f_{m_k} \right)_{L^2(\mathbb{R})} \overset{k \to \infty}{\longrightarrow} \left( \hat{\omega}, f \right)_{L^2(\mathbb{R})} = \left( \hat{\omega}, |f| \Phi \right)_{L^2(\mathbb{R})}. \tag{3.40}
\]

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

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

The weak convergence \( \rho_{Q_{\nu,m_k}} \to \rho_{Q_{\nu,0}} \) in \( L^2(\mathbb{R}) + L^p(\mathbb{R}) \) (for a fixed \( 1 < p < 5/3 \)) then allows to identify \( \rho_{Q_{\nu,0}} - \nu \) and \( \mathcal{F}^{-1}( | \cdot | \hat{\omega} ) \) in the sense of distributions. This shows that \( \rho_{Q_{\nu,0}} - \nu \in \mathcal{C} \), which together with (3.39) implies that \( Q_{\nu,0} \in \mathcal{F}_{\nu} \). Moreover, by the properties of weak limits in Hilbert spaces,

\[
D(\rho_{Q_{\nu,0}} - \nu, \rho_{Q_{\nu,0}} - \nu) = 2 \| \hat{\omega} \|_{L^2}^2 \leq 2 \liminf_{k \to +\infty} \left\| \frac{\hat{\rho}_{Q_{\nu,m_k}} - \hat{\nu}}{\sqrt{1 + m_k^2}} \right\|_{L^2}.
\]

This inequality combined with (3.39) shows that \( I_{\nu,0} \leq \mathcal{E}_{\nu,0}(Q_{\nu,0}) \leq \liminf_{m \to 0} I_{\nu,m} \). We can finally conclude that \( Q_{\nu,0} \) is a minimizer of (2.15), and that \( \lim_{m \to 0} I_{\nu,m} = I_{\nu,0} \) when \( \nu \in L^1(\mathbb{R}) \) and \( | \cdot | \nu(\cdot) \in L^1(\mathbb{R}) \).

4 Numerical simulation of slab-like defects

We present in this section some numerical simulations where we compute an approximation of the minimal energy states for (2.14). The approximation first consists in restricting the physical space to a supercell with periodic boundary conditions in the \( z \) direction, the problem being still invariant by translation in the \( (x,y) \)-directions. As made precise in Section 4.1, it is then possible to formulate the counterpart of the minimization problem (2.14) in this setting, see (4.2) below. In particular, solutions of the supercell minimization problem are characterized by a nonlinear Euler–Lagrange equation. We discuss in Section 4.2 how to numerically solve the latter equation. We finally present some results of numerical simulations for defects corresponding to sharp trenches in Section 4.3. In particular, we observe Friedel oscillations. These results are obtained for Yukawa interactions only since the convergence of our numerical method is poor for Coulomb interactions, and most likely would deserve a dedicated mathematical analysis.
4.1 Supercell model

Supercell models consider states periodic in the z-direction, and invariant by translation in the (x, y)-directions. We first make precise the set of admissible states in Section 4.1.1, then present the reduced Hartree–Fock model in this setting in Section 4.1.2, and finally write the Euler–Lagrange equations characterizing the ground state in this framework (see Section 4.1.3).

4.1.1 Admissible states for supercell models

Supercell models are obtained by restricting the z-variable to the unit cell $\Lambda_L = [-L/2, L/2)$ of the physical space $\mathbb{R}$. This unit cell is seen as a periodic domain of spatial periodicity $L > 0$. More precisely, denoting by $\mathcal{R}_L := L\mathbb{Z}$, we consider all operators to be defined on the functional space

$$L^2_{\text{per},z}(\mathbb{R}^2 \times \Lambda_L) = \left\{ u \in L^2_{\text{loc}}(\mathbb{R}^3) \mid u(r, \cdot) \text{ is } \mathcal{R}_L\text{-periodic for a.e. } r \in \mathbb{R}, \int_{\mathbb{R}^2} \int_{\Lambda_L} |u(r, z)|^2 dr dz < +\infty \right\}.$$ 

It is possible to introduce a supercell unitary transform $\mathcal{U}_L$ which is the counterpart of (2.1): for $q, r \in \mathbb{R}^2$ and $z \in \mathbb{R}$, we can first define, for functions $\Phi \in L^2_{\text{per},z}(\mathbb{R}^2 \times \Lambda_L)$ which are smooth and with compact support in $\mathbb{R}^2 \times \Lambda_L$,

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

and extend this formula as an isometric isomorphism from $L^2_{\text{per},z}(\mathbb{R}^2 \times \Lambda_L)$ to $L^2(\mathbb{R}^2, L^2_{\text{per}}(\Lambda_L))$, where $L^2_{\text{per}}(\Lambda_L) = \{ \phi \in L^2_{\text{loc}}(\mathbb{R}) \mid \phi \text{ is } \mathcal{R}_L\text{-periodic} \}$. The inverse of the unitary transform $\mathcal{U}_L^{-1}$ reads, for $\Psi = (\Psi_q)_{q \in \mathbb{R}^2} \in L^2(\mathbb{R}^2, L^2_{\text{per}}(\Lambda_L))$,

$$(\mathcal{U}_L^{-1} \Psi_q)(r, z) := \frac{1}{2\pi} \int_{\mathbb{R}^2} e^{iq \cdot r} \Psi_q(z) \, dq.$$ 

In order to introduce the set of admissible states, we define the kinetic energy operator on $L^2_{\text{per},z}(\mathbb{R}^2 \times \Lambda_L)$ as

$$T_L = \mathcal{U}_L^{-1} \left( \int_{\mathbb{R}^2} T_{q,L} \, dq \right) \mathcal{U}_L, \quad T_{q,L} = T_{\text{per},z,L} + \frac{|q|^2}{2},$$

where $T_{\text{per},z,L} = -\frac{1}{2} \frac{d^2}{dz^2}$ is considered as an operator on $L^2_{\text{per}}(\Lambda_L)$. The corresponding supercell free Fermi state operator reads

$$\gamma_0^L = \mathcal{U}_L^{-1} \left( \int_{\mathbb{R}^2} \gamma^L_{0,q} \, dq \right) \mathcal{U}_L,$$

where $\{ \gamma^L_{0,q} \}_{q \in \mathbb{R}^2}$ is the following family of orthogonal projectors acting on $L^2_{\text{per}}(\Lambda_L)$:

$$\gamma^L_{0,q} := \begin{cases} 1_{(-\infty, \epsilon_F]}(T_{q,L}) & \text{if } q \in \mathfrak{B}_{\epsilon_F}, \\ 0 & \text{if } q \in \mathbb{R}^2 \backslash \mathfrak{B}_{\epsilon_F}. \end{cases}$$

We can finally define admissible defect states for the supercell model by mimicking the construction in Section 2.2.1: for any $q \in \mathbb{R}^2$, we introduce

$$\mathcal{X}^L_q := \left\{ Q^L_q \in S(L^2_{\text{per}}(\Lambda_L)) \mid \left| T_{q,L} - \epsilon_F \right|^{1/2} Q^L_q \in \mathfrak{S}_2(L^2_{\text{per}}(\Lambda_L)), \right\} \left| T_{q,L} - \epsilon_F \right|^{1/2} Q^L_q, \epsilon_F \in \mathfrak{S}_1(L^2_{\text{per}}(\Lambda_L)) \right\},$$

equipped with the norm

$$\| Q^L_q \|_{\mathcal{X}^L_q} := \| Q^L_q \|_{\mathcal{X}(L^2_{\text{per}}(\Lambda_L))} + \left\| T_{q,L} - \epsilon_F \right|^{1/2} \left\| Q^L_q \right\|_{\mathfrak{S}_2(L^2_{\text{per}}(\Lambda_L))} + \sum_{\alpha \in {+,-}} \left\| T_{q,L} - \epsilon_F \right|^{1/2} \left\| Q^L_{\alpha,q} \right\|_{\mathfrak{S}_1(L^2_{\text{per}}(\Lambda_L))},$$

where $\mathfrak{S}_i(L^2_{\text{per}}(\Lambda_L))$ is the Hilbert space of all square-integrable functions on $\mathbb{R}^2 \times \Lambda_L$ that are $\mathcal{R}_L$-periodic in the first variable.
as well as the convex set $\mathcal{K}_{q}^{L} := \{ Q_{q}^{L} \in \mathcal{X}_{q}^{L} | -\gamma_{q}^{L} \leq Q_{q}^{L} \leq 1 - \gamma_{q}^{L} \}$, Admissible states $Q^{L}$ with finite renormalized kinetic free energy per unit area in the supercell model are elements of

$$\mathcal{K}_{q}^{L} := \left\{ Q^{L} = \mathcal{U}_{L}^{-1} \left( \int_{\mathbb{R}^{2}} Q_{q}^{L} \, dq \right) \mathcal{U}_{L} \mid q \mapsto Q_{q}^{L} \in L^{2} \left( \mathbb{R}^{2} ; S(L_{2}^{2}(\Lambda_{L})) \right), Q_{q}^{L} \in \mathcal{K}_{q}^{L} \text{ a.e.}, \right\} \text{ Tr}_{L} \left( (T_{L} - \epsilon_{F}) Q^{L} \right) < \infty,$$

where

$$\text{Tr}_{L} \left( (T_{L} - \epsilon_{F}) Q^{L} \right) := \frac{1}{(2\pi)^{2}} \int_{\mathbb{R}^{2}} \text{Tr}_{L_{2}^{2}(\Lambda_{L})} \left( |T_{q,L} - \epsilon_{F}|^{1/2} (Q_{q}^{L,++} - Q_{q}^{L,--}) |T_{q,L} - \epsilon_{F}|^{1/2} \right) \, dq.$$

### 4.1.2 Reduced Hartree–Fock model for supercells

Before we construct the reduced Hartree–Fock energy functional, we need to define Yukawa interactions for models periodic in the $z$-variable. We rely to this end on a Fourier series decomposition (instead of a Fourier transform as in Section 2.2.2), obtained with the orthonormal basis $\{ e_{k} \}_{k \in \mathbb{Z}}$ of $L_{2}^{2}(\Lambda_{L})$ composed of the Fourier modes $e_{k}(z) := \frac{1}{\sqrt{L}} e^{i2\pi k z / L}$. Any function $u \in L_{2}^{2}(\Lambda_{L})$ can be decomposed as

$$u = \sum_{k \in \mathbb{Z}} c_{k}(u) e_{k}, \quad c_{k}(u) := (e_{k}, u)_{L_{2}^{2}(\Lambda_{L})}.$$

The Yukawa space for the supercell model is then defined as the following subset of periodic distributions:

$$\mathcal{C}_{m,L} := \left\{ \rho = \sum_{k \in \mathbb{Z}} c_{k}(\rho) e_{k} \left| \sum_{k \in \mathbb{Z}} \frac{|c_{k}(\rho)|^{2}}{m^{2} + \frac{2\pi k}{L}} < \infty \right. \right\},$$

and for $\rho_{1}, \rho_{2} \in \mathcal{C}_{m,L}$, the supercell Yukawa interaction is given by

$$D_{m,L}(\rho_{1}, \rho_{2}) := 2 \sum_{k \in \mathbb{Z}} \frac{c_{k}(\rho_{1}) c_{k}(\rho_{2})}{m^{2} + \frac{2\pi k}{L}}.$$

Consider now a periodized defect obtain from the reference perturbation $\nu$:

$$\nu_{\text{per},L} := \sum_{n \in \mathbb{Z}} (1_{\Lambda_{L}} \nu)(\cdot - nL).$$

The density $\nu_{\text{per},L}$ belongs to $\mathcal{C}_{m,L}$ when

$$\sum_{k \in \mathbb{Z}} \frac{1}{m^{2} + \frac{2\pi k}{L}} \left| \int_{\Lambda_{L}} \nu(z) c_{k}(z) \, dz \right|^{2} < \infty,$$

which we assume in the sequel. The supercell energy functional is then defined as

$$\mathcal{E}_{m,L}(Q^{L}) = \text{Tr}_{L} \left( (T_{L} - \epsilon_{F}) Q^{L} \right) + \frac{1}{2} D_{m,L}(\rho_{Q^{L}} - \nu_{\text{per},L}, \rho_{Q^{L}} - \nu_{\text{per},L}),$$

on the admissible set $\mathcal{F}_{m,L} := \{ Q^{L} \in \mathcal{K}_{q}^{L} | \rho_{Q^{L}} - \nu_{\text{per}} \in \mathcal{C}_{m,L} \}$. The counterpart of the minimization problem (2.14) in the supercell framework finally is:

$$I_{m,L} = \inf \{ \mathcal{E}_{m,L}(Q^{L}), Q^{L} \in \mathcal{F}_{m,L} \}.$$  (4.2)
4.1.3 Euler–Langrange equations

Since the energy functional $\mathcal{E}_{m,\Lambda_L}$ is convex, standard techniques from calculus of variation can be used to prove that (4.2) admits minimizers. Moreover, using the compactness of the domain $\Lambda_L$ (and hence the fact that $T_{q,L}$ has compact resolvent for any $q \in \mathbb{R}^2$), minimizers are characterized by the following Euler-Lagrange equations (where for clarity we do not indicate the dependence on $L$ in all quantities):

\[
\begin{aligned}
&T_{q,L} + V) \phi^q_1 = \varepsilon^q_1 \phi^q_1, \quad \forall q \in \mathbb{R}^2, \quad \phi^q_1 \in L^2_{\text{per}}(\Lambda_L), \quad (\phi^q_i, \phi^q_j)_{L^2_{\text{per}}} = 1, \quad \varepsilon^q_1 \leq \varepsilon^q_2 \leq \cdots \\
&- V'' + m^2 V = 2 \left( \rho_T - \nu_{\text{per},L} \right), \\
&\rho_Q = \rho - \rho_0, \\
&\gamma := \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} \mathbb{1}_{(-\infty,\varepsilon_F)}(T_{q,L} + V) \, dq = \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} \left( \sum_{i=1}^{+\infty} \mathbb{1}_{(-\infty,\varepsilon_F)}(\varepsilon^q_i) \right) \left| \phi^q_1 \right|^2 \, dq,
\end{aligned}
\]

(4.3) with $\rho_0 = (2\varepsilon_F)^3/(6\pi^2)$ and

\[
\rho_\varepsilon(z) = \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} \left( \sum_{i=1}^{+\infty} \mathbb{1}_{(-\infty,\varepsilon_F)}(\varepsilon^q_i) \left| \phi^q_i(z) \right|^2 \right) \, dq.
\]

In fact, solving the family of eigenproblems in the first line of (4.3) requires only solving a single eigenvalue problem for $q = 0$ since $T_{q,L} = T_{\text{per},z,L} + |q|^2/2$. More precisely, (4.3) can be rewritten as

\[
\begin{aligned}
&T_{\text{per},z,L} + V \phi_i = \varepsilon_i \phi_i, \quad \phi_i \in L^2_{\text{per}}(\Lambda_L), \quad (\phi_i, \phi_j)_{L^2_{\text{per}}} = \delta_{i,j}, \quad \varepsilon_1 \leq \varepsilon_2 \leq \cdots \\
&- V'' + m^2 V = 2 \left( \rho - (\rho_0 + \nu_{\text{per}}) \right), \\
&\rho_\varepsilon(z) = \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} \left( \sum_{i=1}^{+\infty} \mathbb{1}_{(-\infty,\varepsilon_F)}(\varepsilon_i) \left| \phi_i(z) \right|^2 \right) \, dq = \frac{1}{2\pi} \sum_{i=1}^{+\infty} \max(0, \varepsilon_F - \varepsilon_i) \left| \phi_i(z) \right|^2.
\end{aligned}
\]

(4.4)

Therefore, in order to solve (4.2), we look for a solution to (4.4). We discuss in the next section how to do this in practice.

4.2 Discretization of the supercell model

We explain in this section how to solve (4.4). The method is based on two ingredients: discretizing the variational formula associated with the first equation in (4.4) using a spectral Galerkin basis of Fourier modes, as studied in [3]; and relying on a fixed-point strategy (with appropriate mixing) in order to find a solution to the nonlinear problem (4.4). We only briefly describe the numerical strategy, and refer to [9] for a complete presentation.

4.2.1 Discretization of the variational formulation of the Euler–Lagrange equations

We assume in this section that the potential $V$ is fixed, and discuss how to construct a density from a given potential. We consider to this end the following finite-dimensional subspace of $H^1_{\text{per}}(\Lambda_L)$ (for $N \geq 1$)

\[
X_N(\Lambda_L) := \text{Span} \{ e_k \mid k \in \mathbb{Z}, |k| \leq N \},
\]

(4.5)

and the variational problem: find $\phi_{0,N}, \phi_{1,N}, \cdots \in X_N(\Lambda_L)$ and $\varepsilon_{0,N} \leq \varepsilon_{1,N} \leq \cdots$ such that

\[
\begin{aligned}
&\forall \varphi_N \in X_N(\Lambda_L), \quad \frac{1}{2} \int_{\Lambda_L} \phi_{i,N}(z) \varphi'(N)(z) \, dz + \int_{\Lambda_L} \Pi_N(V \phi_{i,N})(z) \varphi_N(z) \, dz = \varepsilon_{i,N} \int_{\Lambda_L} \phi_{i,N}(z) \varphi_N(z) \, dz, \\
&\int_{\Lambda_L} \phi_{j,N}(z) \phi_{i,N}(z) \, dz = \delta_{i,j},
\end{aligned}
\]

(4.6)
where $\Pi_N$ is the projection onto $X_N(\Lambda_L)$. The latter problem can be recast as some matrix eigenvalue problem. Once the wavefunctions $\phi_{i,N}$ are obtained, the density follows from the last equation in (4.4) as

$$
\rho_{\gamma,N}(z) = \frac{1}{2\pi} \sum_{i=1}^{2N+1} \max(0, \epsilon_F - \epsilon_i) |\phi_{i,N}(z)|^2.
$$

Note that the density is represented in $X_{2N}(\Lambda_L)$ since it involves squares of functions in $X_N(\Lambda_L)$. Finally, it is possible to associate a potential $V_N \in X_{2N}(\Lambda_L)$ to $\rho_{\gamma,N} \in X_{2N}(\Lambda_L)$ with the second equation in (4.4). The Fourier coefficients of $V_N$ read

$$
c_k(\tilde{V}_N) = 2\frac{c_k(\rho_{\gamma,N}) - \sqrt{L} \rho_0 \delta_{k,0} - c_k(\nu_{\text{per},L})}{m^2 + |2\pi k/L|^2}, \quad (4.7)
$$

where $\delta_{k,\ell}$ is the Kronecker symbol.

### 4.2.2 Iterative resolution of the problem

We rely on an iterative procedure to solve the nonlinear fixed-point problem (4.4). The integer $N$ is related to the dimension of the Galerkin space (4.5), while the integer $n$ indexes the iterations in the fixed-point loop. Starting from the potential $V_N^0 = 0$, the procedure is the following: For $n \geq 0$,

1. Compute the wavefunctions $\{\phi_{i,N}\}_{i \geq 1}$ and eigenvalues $\{\epsilon_{i,N}\}_{i \geq 1}$ obtained from (4.6) with $V$ replaced by $V_N^0$, and construct the corresponding density matrix as

$$
\tilde{\gamma}_N^{n+1} = \frac{1}{2\pi} \sum_{i=1}^{2N+1} \max(0, \epsilon_F - \epsilon_{i,N}) |\phi_{i,N}^n|^2 |\phi_{i,N}^n|;
$$

2. Use the optimal damping algorithm (ODA) to obtain the new density matrix $\gamma_N^{n+1}$ from $\tilde{\gamma}_N^{n+1}$ and $\tilde{\gamma}_N^{n+1}$ (see below);

3. Construct the potential $V_N^{n+1}$ from the new density $\rho_N^{n+1}(z) = \gamma_N^{n+1}(z, z)$ using (4.7);

4. check whether some termination criterion is met (e.g. $\|\rho_N^{n+1} - \rho_N^0\|_{L^p_{\text{per}}(\Lambda_L)} \leq \eta \|\rho_N^0\|_{L^p_{\text{per}}(\Lambda_L)}$ for some small tolerance $\eta$); otherwise increment $n$ and go back to (1).

Let us now make precise how Step (2) is performed. The idea of ODA [2] is to write $\gamma_N^{n+1}$ as a convex combination of $\gamma_N^n$ and $\gamma_N^{n+1}$, and optimize upon the parameter determining the combination in order to minimize the energy. More precisely, we introduce a mixing parameter $\alpha \in [0, 1]$ and the objective function

$$
f_N^{n+1}(\alpha) := \mathcal{E}_{m,\Lambda_L} \left( (1 - \alpha)\gamma_N^n + \alpha \gamma_N^{n+1} \right).
$$

Denoting by $\alpha_{\text{opt}} = \arg \min \{f_N^{n+1}(\alpha), \alpha \in [0, 1] \}$ the optimal mixing parameter, the new density matrix is then defined as $(1 - \alpha_{\text{opt}})\gamma_N^n + \alpha_{\text{opt}} \gamma_N^{n+1}$. For the rHF model, determining this parameter amounts to finding the roots of a second order polynomial.

### 4.3 Numerical results

We finally present results of numerical simulations to illustrate the behavior of the perturbation of the electronic density induced by sharp trenches modeling a capacitor. More precisely, we consider $\nu(z) = -\rho_0 1_{|z| \leq w}$ for $w > 0$. The physical parameters are chosen as $\epsilon_F = 2.0$, $w = 4$, while the computational parameters are set to $L = 300$, $N = 1500$ and $\eta = 10^{-8}$.

We plot in Figures 1 and 2 the total electronic density $\rho_0 + \nu + \rho_{\nu,m}$ for two values of the Yukawa parameter $m > 0$. We can observe Friedel oscillations [14] in the densities, which can be fitted away from the defect as

$$
\rho_{\nu,m}(z) = \rho_0 + a \frac{\cos(2 \epsilon z + \delta)}{|z|^3};
$$

see the values of $a, \delta, \epsilon$ obtained by our fit in the captions of the figures. Remark that the fitted value of $\epsilon$ is close to the Fermi level, as predicted by [14].
Figure 1: Electronic density $\rho_{\nu,m}$ for $m = 4$.

Figure 2: Electronic density $\rho_{\nu,m}$ for $m = 2$.

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