THE KOHN-SHAM EQUATION FOR DEFORMED CRYSTALS

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Abstract. The solution to the Kohn-Sham equation in the density functional theory of the quantum many-body problem is studied in the context of the electronic structure of smoothly deformed macroscopic crystals. An analog of the classical Cauchy-Born rule for crystal lattices is established for the electronic structure of the deformed crystal under the following physical conditions: (1) the band structure of the undeformed crystal has a gap, i.e. the crystal is an insulator, (2) the charge density waves are stable, and (3) the macroscopic dielectric tensor is positive definite. The effective equation governing the piezoelectric effect of a material is rigorously derived. Along the way, we also establish a number of fundamental properties of the Kohn-Sham map.

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1. Introduction

The Kohn-Sham density functional theory [7, 15, 16, 18, 19] provides the most popular class of approximate models for the quantum many-body problem in material science. Yet except for some existence results for the Kohn-Sham equation [2, 17, 21], we know very little about the mathematical nature of the problem, such as the uniqueness of solutions; compactness of the various operators associated with the Kohn-Sham equation; whether these operators behave more like differential operators of some order, or like integral operators; how the physical nature of the underlying material, for example, whether it is a metal or an insulator, is reflected at the mathematical level. From a practical viewpoint, one most interesting question is how to connect the Kohn-Sham density functional theory, which describes materials at the level of their electronic structure, to the more conventional macroscopic continuum models, such as the models of nonlinear elasticity and the Landau-Lifshitz theory of magnetic materials.

It is not a surprise that we know so little about the mathematical properties of the Kohn-Sham equation. After all, this is a rather unconventional set of nonlocal and nonlinear system for a large collection of coupled one-particle wave functions, the number of wave functions is equal to the number of electrons in the material. Consequently, in the continuum limit, the number of unknown wave functions goes to infinity. In addition, the Fermionic nature of the electrons poses further mathematical challenges.

The present paper is the third of a series of papers that are devoted to the study of the electronic structure of smoothly deformed crystals or crystals in an external field, by analyzing various quantum mechanics models at different levels of complexity, including the Kohn-Sham density functional theory, Thomas-Fermi type of models and tight-binding models. Our overall objective is to establish the microscopic foundation of the continuum theories of solids, such as the nonlinear elasticity theory and the theory of magnetic materials, in terms of quantum mechanics and to examine the boundary where the continuum theories break down. In this regard, our objective is a lot like the one in [11, 12], except that [11] and [12] considered only classical models of atoms in a crystal, and in this series we consider quantum mechanics models and focus on the behavior of the electrons and spins. In particular, in analogy with the stability condition for phonons and elastic waves established in [11, 12], we will establish stability conditions for charge density waves and spin waves.

In [10], we considered a non-interacting quantum mechanical model for multi-electrons and we examined the structure of the subspace spanned by the wave functions. In particular, we extended the construction of Wannier functions for perfect crystals to smoothly deformed crystals. We also established for this construction an extension of the classical Cauchy-Born rule which historically was developed in the
context of crystal lattices [13], to the realm of electronic structure. Roughly speaking, this extended Cauchy-Born rule asserts that locally, the electronic structure of a smoothly deformed crystal is well approximated by the electronic structure of a homogeneously deformed crystal with the same deformation gradient. This is a linearization principle, or more generally, a locality principle: It states that the electronic structure depends only on the local behavior of the deformation.

In [9], we studied the continuum limit for the nonlinear tight-binding model for the electronic structure of insulating crystalline solids. Under sharp stability conditions, we established the extended Cauchy-Born rule for this class of models.

In the current paper, we continue this study for the Kohn-Sham density functional theory. This is a rather popular class of models in quantum many-body theory and has become a basic tool in material science and chemistry. As in the previous work, our reference point is the electronic structure of a perfect crystal, i.e. the equilibrium crystal lattice. The solution of the Kohn-Sham equation we are interested in is a continuation of the solution for the perfect crystal. This works as long as certain stability conditions are satisfied. One main objective is to identify these stability conditions. The overall strategy is quite simple and similar to the one in the previous paper [9]. However, a substantial amount of machinery has to be developed in order to carry out this program in the setting of Kohn-Sham density functional theory, especially to deal with the long-range Coulomb interaction present in the Kohn-Sham model, as well as the continuous character of the model.

Another related work that we should mention is [3] where the Thomas-Fermi-von Weizsäcker model was studied for smoothly deformed crystals. It was shown that in the continuum limit, the total energy of the system converges to a limiting value given by the extended Cauchy-Born construction. The Thomas-Fermi-von Weizsäcker model is one of the simplest versions of density functional theory in which the electronic structure is represented solely by the electron density instead of the wave functions as in the Kohn-Sham theory. There, the stability condition is automatically satisfied since the model is convex. [8] extended this kind of results to the tight-binding models. The strategy in the current series of papers is quite different from those in [3] or [8]. Here our interest is to study the behavior of the wave functions of a many-electron system, with emphasis on the stability conditions.

For a system with \(N\) electrons, given a set of orthonormal functions \(\{\psi_i\}, i = 1, \ldots, N\), the Kohn-Sham energy functional [7, 18, 19] is given by

\[
I_{KS}(\{\psi_i\}) = \sum_{i=1}^{N} \int_{\mathbb{R}^3} |\nabla \psi_i|^2 \, dx + \frac{1}{2} \int_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{(\rho - m)(x)(\rho - m)(y)}{|x - y|} \, dx \, dy + \int_{\mathbb{R}^3} \epsilon_{xc}(\rho) \, dx,
\]
where the density $\rho$ is defined to be
\begin{equation}
\rho(x) = \sum_{i=1}^{N} |\psi_i(x)|^2,
\end{equation}
and $m$ is the background charge contributed by the atoms. Here for simplicity, we have ignored the spin degeneracy and we have adopted the local density approximation (LDA) for the exchange-correlation functional, which amounts to assuming that integrand in the last term of (1.1) is a local function of $\rho$.

To determine the electronic structure of a system, one minimizes (1.1) under the orthonormality constraints on $\psi_i$. The latter plays the role of the Pauli exclusion principle here. The Euler-Lagrange equations for (1.1) are
\begin{equation}
(-\Delta + V)\psi_i = \sum_{j=1}^{N} \psi_j \lambda_{ji},
\end{equation}
with $V$ given by
\begin{equation}
V = \int_{\mathbb{R}^3} \frac{(\rho - m)(y)}{|x - y|} \, dy + \eta(\rho).
\end{equation}
Here $\eta(\rho) = \epsilon'_xc(\rho)$ and the $\{\lambda_{ij}\}$s are the Lagrange multipliers corresponding to the orthonormality constraints. $\eta$ is called the exchange-correlation potential (in local density approximation). Specific forms of $\eta$ used in applications can be found in [18]. We will simply assume that $\eta$ is smooth: $\eta \in C^\infty(0, \infty)$.

Since the functional (1.1) is invariant under unitary transformations, (1.3) can be reduced to
\begin{equation}
(-\Delta + V)\psi_i = \epsilon_i \psi_i,
\end{equation}
so that $\{\lambda_{ij}\}$ becomes a diagonal matrix. Indeed, consider a set of solutions of (1.3) $\{\psi_i\}$ with Lagrange multipliers $\{\lambda_{ij}\}$. The matrix $\Lambda = (\lambda_{ij})$ is Hermitian, since
\begin{equation}
\lambda_{ij} = \langle \psi_j | (-\Delta + V) | \psi_i \rangle = \langle \psi_i | (-\Delta + V) | \psi_j \rangle^* = \lambda_{ji}^*.
\end{equation}
Hence, $\Lambda$ can be diagonalized by a unitary matrix $U$:
\begin{equation}
U^* \Lambda U = E, \quad E = \text{diag}(\epsilon_1, \ldots, \epsilon_N).
\end{equation}

Letting $\tilde{\psi}_i = \sum_j \psi_j U_{ji}$ and substituting into (1.3), we get
\begin{equation}
\sum_j (-\Delta + V) \tilde{\psi}_j (U^*)_{ji} = \sum_{jk} \tilde{\psi}_k (U^*)_{kj} \lambda_{ji}.
\end{equation}
Multiplying both sides by $U_{il}$ and summing over $i$, we arrive at
\begin{equation}
(-\Delta + V) \tilde{\psi}_l = \epsilon_l \tilde{\psi}_l.
\end{equation}
Since $\{\tilde{\psi}_l\}$ gives the same energy as $\{\psi_i\}$, we just need to solve (1.5).

Observe that (1.5) is a set of eigen-equations for the operator $\mathcal{H} = -\Delta + V$, which is a one-body Hamiltonian. The potential $V$ depends on the density $\rho$ which in turn depends on the eigenfunctions $\{\psi_i\}$. This set of nonlinear, nonlocal equations is
called the *Kohn-Sham equation*. The Hamiltonian operator $H$ can be extended to be a self-adjoint operator with domain $H^1(\mathbb{R}^3)$. Therefore the eigenvalues are real. If exists, the minimizer of (1.1) (or rather, an equivalent set of minimizers under unitary transformation) satisfies (1.5), the functions $\{\psi_i\}$ are eigenfunctions of the Hamiltonian given by $\rho$.

Using spectral theory, assuming that the $N$-th eigenvalue of $\mathcal{H}$ is strictly smaller than the $(N+1)$-th eigenvalue, the density matrix i.e., the projection operator to the lowest $N$ eigenfunctions, is given by

$$
\mathcal{P} = \phi_{\text{FD}}^0 (\mathcal{H} - \mu) = \frac{1}{2\pi i} \int_{\mathcal{C}} (\lambda - \mathcal{H})^{-1} \text{d}\lambda,
$$

where $\phi_{\text{FD}}^0$ is the zero-temperature Fermi-Dirac function, which is simply a step function

$$
\phi_{\text{FD}}^0 (x) = \begin{cases} 
1, & x \leq 0, \\
0, & x > 0. 
\end{cases}
$$

$\mu \in (\epsilon_N, \epsilon_{N+1})$ is the chemical potential, and $\mathcal{C}$ is a contour in the complex plane around the eigenvalues $\epsilon_1, \ldots, \epsilon_N$, intersecting with the real axis at $\mu$ and some value below $\epsilon_1$. We note that in terms of wave functions, the kernel of the projection operator is given by

$$
\mathcal{P}(x, y) = \sum_i \psi_i(x) \psi_i(y)^*.
$$

Using the spectral representation, the Kohn-Sham equation can be written in a more compact form as

$$
\rho(x) = \frac{1}{2\pi i} \int_{\mathcal{C}} (\lambda - \mathcal{H})^{-1} \text{d}\lambda(x, x),
$$

where the right hand side is the diagonal of the kernel associated to the projection operator $\mathcal{P}$, which is well defined since $\mathcal{P}$ is in trace class [23]. Note that $\mathcal{H}$ depends on $\rho$ through the potential. This form of the Kohn-Sham equation is a nonlinear, nonlocal equation for the density $\rho$ directly. We will focus on this form of the Kohn-Sham equation since it is much easier than handling the large number of wave functions $\{\psi_i\}$.

Throughout this paper, we use the notation $\lesssim$ for inequalities up to an absolute constant: $f \lesssim g$ if $f \leq Cg$ where $C$ is an absolute constant. Sometimes, it is more convenient to explicitly use $C$ to denote the constant, which might change from line to line. When it is necessary to specify the dependence of the constant on parameters, we will use the notation $C(a, b)$ to indicate that the constant depends on parameters $a$ and $b$.

We will use standard notations for function spaces like $L^2$, $H^1$ and $W^{m,p}$ so on for functions on $\mathbb{R}^3$, or $L^2(\mathbb{R}^3)$ if we want to emphasize the domain of the functions. We also need function spaces for periodic functions. Let $L \subset \mathbb{R}^3$ be a lattice with
unit cell \( \Gamma \). Denote the reciprocal lattice as \( L^* \) and its unit cell (the first Brillouin zone) as \( \Gamma^* \). For a given \( n \), define
\[
L^p_n(\mathbb{R}^3) = \{ f \in \mathcal{S}'(\mathbb{R}^3) \mid \tau_R f = f, \forall R \in n\mathbb{L}; \int_{n\Gamma} |f|^p \, dx < \infty \}, \quad 1 \leq p < \infty,
\]
with the norm
\[
\|f\|_{L^p_n(\mathbb{R}^3)} = \left( \int_{n\Gamma} |f|^p \, dx \right)^{1/p},
\]
and similarly for \( L^\infty_n(\mathbb{R}^3) \). Here \( \tau_R \) is the translational operator with translation vector \( R \), \( (\tau_R f)(x) = f(x - R) \). It is easy to see that the space \( L^p_n(\mathbb{R}^3) \) is equivalent with the space \( L^p(n\Gamma) \). The periodic Sobolev space is defined similarly
\[
W^{m,p}_n(\mathbb{R}^3) = \{ f \in \mathcal{S}'(\mathbb{R}^3) \mid \tau_R f = f, \forall R \in n\mathbb{L}; f \in W^{m,p}(n\Gamma) \}, \quad m \in \mathbb{Z}_+
\]
with its natural norm
\[
\|f\|_{W^{m,p}_n(\mathbb{R}^3)} = \|f\|_{W^{m,p}(n\Gamma)}.
\]
We will also write \( H^m_n \) for \( W^{m,2}_n \). Moreover, define the periodic Coulomb space (homogeneous Sobolev space with index \(-1\)) \( \dot{H}^{-1}_n(\mathbb{R}^3) \) as
\[
\dot{H}^{-1}_n(\mathbb{R}^3) = \{ f \in \mathcal{S}'(\mathbb{R}^3) \mid \tau_R f = f \forall R \in n\mathbb{L}, \sum_{k \in L^*/n} \frac{1}{|k|^2} |\hat{f}(k)|^2 < \infty \}.
\]
Here, \( \{\hat{f}(k)\} \) denotes the Fourier coefficients of the \( n\Gamma \)-periodic function \( f \)
\[
\hat{f}(k) = (2\pi)^{-3/2} \int_{n\Gamma} f(x)e^{-ik \cdot x} \, dx.
\]
The space \( \dot{H}^{-1}_n(\mathbb{R}^3) \) is a Hilbert space with inner product
\[
\langle f, g \rangle_{\dot{H}^{-1}_n(\mathbb{R}^3)} = 4\pi \sum_{k \in L^*/n} \frac{1}{|k|^2} \overline{\hat{f}(k)} \hat{g}(k).
\]
Its dual space, the homogeneous Sobolev space, \( \dot{H}^1_n(\mathbb{R}^3) \) is given by
\[
\dot{H}^1_n(\mathbb{R}^3) = H^1_n(\mathbb{R}^3)/\mathbb{R},
\]
where the constant functions are factored out. \( \dot{H}^1_n(\mathbb{R}^3) \) is a Hilbert space with inner product
\[
\langle f, g \rangle_{\dot{H}^1_n(\mathbb{R}^3)} = \langle \nabla f, \nabla g \rangle_{L^2(\mathbb{R}^3)^3}.
\]
\[\|f\|_{\dot{H}^1_n(\mathbb{R}^3)} = \|\nabla f\|_{L^2(\mathbb{R}^3)^3} \]
then gives a norm on the space \( \dot{H}^1_n(\mathbb{R}^3) \). We also have higher order spaces \( \dot{H}^{m+1}_n \), defined by the norm
\[
\|f\|_{\dot{H}^{m+1}_n(\mathbb{R}^3)} = \|\nabla f\|_{H^m(\mathbb{R}^3)^3}.
\]
For electron density, we would use the function spaces that are rescaled versions of the spaces of periodic functions:
\[
W^{m,p}_\varepsilon = \{ f \mid \varepsilon^3 f(\varepsilon x) \in W^{m,p}_n, n = 1/\varepsilon \},
\]
and similarly for $L^p_\varepsilon$, $H^m_\varepsilon$, $\hat{H}^{-1}_\varepsilon$ and $\hat{H}^{m+1}_\varepsilon$. Note that the rescaling preserves the $L^1$ norm.

For Banach spaces $X$ and $Y$, $\mathcal{L}(X,Y)$ denotes the bounded linear operator from $X$ to $Y$ and $\|\cdot\|_{\mathcal{L}(X,Y)}$ denotes the operator norm. For a Hilbert space $H$, we use $\mathcal{S}_p(H)$ to denote the Schatten $p$-class operator on $H$, and $\|\cdot\|_{\mathcal{S}_p(H)}$ for the Schatten $p$-norm [23]. For $p = 1$, $\mathcal{S}_1(H)$ is the space of trace class operators; for $p = 2$, $\mathcal{S}_2(H)$ is the space of Hilbert-Schmidt operators.

Before ending this introduction, let us briefly summarize the main results of this paper. A central parameter in this paper is the ratio of the size of the unit cell and the size of the macroscopic domain of the crystal. We will denote this parameter by $\varepsilon$ and we are interested in the case when $\varepsilon \ll 1$. We will make the following assumptions about the electronic structure of the equilibrium (undeformed) state and the displacement field $u$:

1. the equilibrium state is an insulator;
2. charge density waves are stable at all scales;
3. the dielectric response tensor is positive definite;
4. $u$ is smooth and periodic over the macroscopic scale;
5. the gradients of $u$ are sufficiently small.

Under these assumptions, we prove that if $\varepsilon$ is sufficiently small, the Kohn-Sham equation has a locally unique solution and the solution can be approximated using an extension of the Cauchy-Born construction.

We should remark that the assumptions we made are quite physical and essentially sharp, except for the possibility of replacing some Sobolev norms by other norms. For example, if the crystal is a metal instead of an insulator, we expect its electronic structure to behave quite differently. If the displacement field is not periodic, then we expect to have new physical processes at the boundary, such as surface charge density waves, that have to be dealt with. If the deformation gradient is sufficiently large, we expect plastic deformation to take place.

2. Perfect crystal

We now consider the Kohn-Sham density functional theory for crystals. We assume that the system under consideration has a crystal structure in the equilibrium state: The nuclei positions form a lattice, denoted as $\mathbb{L}$, with unit cell $\Gamma$. Recall that the dual lattice and its unit cell are denoted as $\mathbb{L}^*$ and $\Gamma^*$ respectively.

The nuclei provide a background charge to the system. The contribution from each nucleus is represented by a compactly supported smooth or a fast decaying function $m_a(\cdot - X_i)$, where $X_i$ is the position of that nucleus. Here we are taking a pseudopotential approximation, treating the core electrons as part of the nuclei resulting in an effective charge distribution $m_a$, only the valence electrons are allowed to vary freely [18]. Therefore, the total charge contribution from the nuclei
is
\[
(m_e(x) = \sum_{x_i \in \mathbb{L}} m_u(x - X_i),
\]
where the subscript \(e\) signals the equilibrium state. We also assume that the function \(m_u\) respects the inversion symmetry: \(m_u(x) = m_u(-x)\). In addition, we assume
\[
\int_{\mathbb{R}^3} m_u = Z.
\]
This also implies \(\int_{\Gamma} m_e = Z\). We assume that there are \(Z\) (valence) electrons per unit cell.

In Kohn-Sham density functional theory, it is assumed that the electrons in the system follow an effective one-body Hamiltonian depending on the electron density. The effective Hamiltonian is given by
\[
\mathcal{H}_e(\rho) = -\Delta + V_e(\rho).
\]
The potential \(V_e\) depends on the electron density: If \(\rho\) is \(\Gamma\)-periodic, then
\[
V_e(\rho)(x) = \phi_e(x) + \eta(\rho(x)),
\]
where \(\phi_e\) is the Coulomb potential, given by
\[
-\Delta \phi_e = 4\pi (\rho - m_e),
\]
with the periodic boundary condition on \(\Gamma\) and the constraint that \(\int_{\Gamma} \phi_e = 0\). For the equation (2.4) to be solvable, we need the normalization constraint that
\[
\int_{\Gamma} \rho = Z.
\]
The current work is carried out under the assumption that the Kohn-Sham equation for the undeformed crystal lattice has a smooth, periodic solution. Furthermore, this equilibrium solution \(\rho_e\) satisfies some conditions that we will specify below.

It is obvious from the definition that \(V_e\) is also \(\Gamma\)-periodic. Therefore, \(\mathcal{H}_e\) is invariant under the translation with respect to the lattice. If \(V_e \in L^2_{\text{loc}}\) (which will always be satisfied by our assumption of regularity of \(\rho_e\) and \(m_e\)), by the standard Bloch-Floquet theory [22], we have
\[
\mathcal{H}_e = \int_{\Gamma^*} \mathcal{H}_{e, \xi} \, d\xi,
\]
where for each \(\xi \in \Gamma^*\), \(\mathcal{H}_{e, \xi}\) is an operator defined on \(L^2_\xi(\Gamma)\):
\[
L^2_\xi(\Gamma) = \{ f \in L^2(\Gamma) \mid \tau_R f = e^{-iR \xi} f, \forall R \in \mathbb{L} \},
\]
with spectral decomposition
\[
\mathcal{H}_{e, \xi} = \sum_{n \geq 1} E_n(\xi) |\psi_{n, \xi}\rangle \langle \psi_{n, \xi}|,
\]
where $E_n(\xi)$ is the $n$-th eigenvalue of $H_{e,\xi}$, and $\psi_{n,\xi}$ is the corresponding eigenfunction, the Bloch waves, with

$$u_{n,\xi}(x) = e^{-i\xi \cdot x} \psi_{n,\xi}(x)$$

being $\Gamma$-periodic. Moreover, the spectrum $\text{spec}(H_e)$ has the band structure:

$$\text{spec}(H_e) = \bigcup_{n \geq 1} \bigcup_{\xi \in \Gamma^*} E_n(\xi).$$

We will assume the following conditions on the equilibrium density $\rho_e$:

**Assumption A.** There exists an $\Gamma$-periodic density $\rho_e \in C^\infty(\Gamma)$ that satisfies the following conditions:

- $\rho_e$ is positive and bounded away from zero: There exists a constant $C_\rho > 0$, such that $\rho_e(x) \geq C_\rho$, for all $x \in \Gamma$.
- The Hamiltonian $H_e(\rho_e)$ satisfies the gap condition: Denote the spectrum for the first $Z$ bands by $\sigma_Z$,

$$\sigma_Z = \bigcup_{n=1}^Z \bigcup_{\xi \in \Gamma^*} E_n(\xi),$$

where $E_n(\xi)$ is the $n$-th eigenvalue of $H_{e,\xi}(\rho_e)$. We assume that

$$\text{dist}(\sigma_Z, \text{spec}(H_e(\rho_e)) \setminus \sigma_Z) = E_g.$$  

In physical terms, the system is a band insulator with band gap $E_g$.

- $\rho_e$ is a solution to the Kohn-Sham equation, i.e., let $\mathcal{C}$ be a contour (shown in Figure 1) around the first $Z$ bands in the resolvent set $\mathbb{C} \setminus \text{spec}(H_e(\rho_e))$ separating $\sigma_Z$ from the rest of the spectrum with $\text{dist}(\mathcal{C}, \text{spec}(H_e(\rho_e))) = E_g/2$, we have

$$\rho_e(x) = F_e(\rho_e)(x) = \frac{1}{2\pi i} \int_{\mathcal{C}} \frac{1}{\lambda - H_e(\rho_e)} d\lambda(x, x),$$

and $\rho_e$ satisfies the normalization constraint (2.5).

**Figure 1.** Schematic plot of the spectrum of $H_e(\rho_e)$ and a contour $\mathcal{C}$ (dash line). The filled rectangles denote the occupied bands, while the empty rectangles denote the unoccupied bands.

The right hand side of (2.10) defines the Kohn-Sham map for the system in equilibrium:

$$F_e(\rho)(x) = \frac{1}{2\pi i} \int_{\mathcal{C}} \frac{1}{\lambda - H_e(\rho)} d\lambda(x, x).$$
3. Stability condition

Consider the linearization of the Kohn-Sham map $F_e$ at the equilibrium density $\rho_e$. Formally, $\mathcal{L}_{e,\rho_e} : w \rightarrow \mathcal{L}_{e,\rho_e}(w)$, where

$$
\mathcal{L}_{e,\rho_e}(w) = \frac{1}{2\pi i} \int_{\mathbb{R}} \frac{1}{\lambda - \mathcal{H}_e(\rho_e)} \frac{1}{\lambda - \mathcal{H}_e(\rho_e)} d\lambda(x, x).
$$

Here $\delta_{\rho_e} V_e$ is the linearized operator of $V_e(\rho)$ at $\rho_e$. If $w$ is $\Gamma$-periodic, the operator $\delta_{\rho_e} V_e$ acting on $w$ is given by

$$
\delta_{\rho_e} V_e(w)(x) = \delta\phi_e(w)(x) + \eta'(\rho_e)w(x);
$$

$$
-\Delta\delta\phi_e(w)(x) = 4\pi w,
$$

with periodic boundary condition on $\Gamma$ and $\int_\Gamma \delta\phi_e = 0$ to fix the arbitrary constant.

In (3.1), $\delta_{\rho_e} V_e(w)$ is viewed as a multiplicative operator.

To simplify notations, we will denote $L_e = \mathcal{L}_{e,\rho_e}$.

Note that the domain of $L_e$ can be trivially extended to $n$-periodic functions.

The following proposition is a special case of Theorem 6.1 proved in Section 6.

**Proposition 3.1.** The operator $L_e$ defined in (3.1) is bounded on the spaces $\dot{H}^{-1}_n \cap H^1_n$ uniformly in $n$.

The operator $L_e$ can be analyzed by Bloch-Floquet theory. Consider the translation operators $\tau_R$ with $R \in n\mathbb{L}$. It is obvious that $\tau_R(\dot{H}^{-1}_n \cap H^1_n) = (\dot{H}^{-1}_n \cap H^1_n)$ as the functions in $(\dot{H}^{-1}_n \cap H^1_n)$ are $n\Gamma$-periodic. Moreover, it is also easy to check that $\tau_R L_e = L_e \tau_R$.

For $\xi \in \Gamma^*$, define the function space $D_\xi \subset L^2(\Gamma)$ by

$$
D_\xi = \left\{ w = g(x)e^{i\xi \cdot x} | g \text{ $\Gamma$-periodic}, \sum_{k \in \mathbb{L}^*} \left( \frac{1}{|k + \xi|^2} + |k + \xi|^4 \right) |\tilde{g}(k)|^2 < \infty \right\}.
$$

Here $\tilde{g}$ is the Fourier coefficients of the $\Gamma$-periodic function $g$. Consider the operator $L_{e,\xi}$ from $D_\xi$ to $D_\xi$, defined as

$$
L_{e,\xi}(w) = \frac{1}{2\pi i} \int_{\mathbb{R}} \frac{1}{\lambda - \mathcal{H}_e(\rho_e)} \frac{1}{\lambda - \mathcal{H}_e(\rho_e)} d\lambda(x, x),
$$

where $\delta_{\rho_e} V_{e,\xi}(w)$ is a multiplicative operator and the operator $\delta_{\rho_e} V_{e,\xi}$ acting on $w, w(x) = g(x)e^{i\xi \cdot x}$ is given by

$$
\delta_{\rho_e} V_{e,\xi}(w) = \delta_{\rho_e} \phi_{e,\xi}(we^{-i\xi \cdot x})e^{i\xi \cdot x} + \eta'(\rho_e)w
$$

$$
(-i\nabla + \xi)^2 \delta_{\rho_e} \phi_{e,\xi}(g) = 4\pi g \text{ in } \Gamma.
$$

It is clear that $\delta_{\rho_e} V_{e,\xi}(w)e^{-i\xi \cdot x}$ is $\Gamma$-periodic and $L_{e,\xi}(w) \in D_\xi$. 
Define the matrix $A_e = (A_{e,\alpha\beta})$ for $\alpha, \beta = 1, 2, 3$, where

$$A_{e,\alpha\beta} = -2\rho_e \sum_{n \leq Z} \sum_{m > Z} \int_{\Gamma^*} \frac{d\xi}{E_n(\xi) - E_m(\xi)} \times \langle u_{m,\xi}, \partial_{\xi^\alpha} u_{m,\xi} \rangle \langle u_{m,\xi}, \partial_{\xi^\beta} u_{m,\xi} \rangle$$

$$- \langle g_{e,\alpha,\xi}, V_e (I - L_e)^{-1} g_{e,\beta,\xi} \rangle,$$

and

$$g_{e,\alpha}(z) = 2\rho_e \sum_{n \leq Z} \sum_{m > Z} \int_{\Gamma^*} \frac{d\xi}{E_n(\xi) - E_m(\xi)} u_{n,\xi}^*(z) u_{m,\xi}(z) \langle u_{m,\xi}, i\partial_{\xi^\alpha} u_{m,\xi} \rangle;$$

$V_e = \delta_{\rho_e} V_e$ acting on $\Gamma$-periodic functions. The macroscopic dielectric tensor is given by $E_e = \frac{1}{2}(A_e + A_e^*) + \frac{1}{4} I$. As will be clear from (9.63), without deformation ($u = 0$), the macroscopic electric potential solves a macroscopic Poisson equation for dielectric media.

$$-\nabla \cdot (E_e \nabla U_0) = \rho_f,$$

where $\rho_f$ is the “free charge” in the system. $E_e$ characterizes the macroscopic response in electric potential to the perturbation in electron density.

We will assume that the electronic structure is stable, in the sense of the following two assumptions.

**Assumption B.** For every $\xi \in \Gamma^*$, the operator $I - L_e,\xi$, as an operator on $D_\xi$, is invertible and $\|(I - L_e,\xi)^{-1}\|_{L(H_{\xi})} \leq 1$.

**Assumption C.** The macroscopic dielectric tensor $E_e$ is positive definite.

From a physical viewpoint, Assumption B states that the system is stable with respect to plasmon excitation (charge density waves, for a physics-orientated discussion of plasmons, see for example [20]). Assumption C states that the system is stable with respect to the dielectric response to a macroscopic external potential.

The Assumption B actually states that the system is stable with charge density wave excitation for all scale, which can be seen from the following equivalent assumption.

**Assumption B’.** For every $n \in \mathbb{N}$, $I - L_e$ as an operator on $\dot{H}_n^{-1} \cap H_n^2$ is invertible, and the norm of its inverse is bounded independent of $n$:

$$\|(I - L_e)^{-1}\|_{L(\dot{H}_n^{-1} \cap H_n^2)} \lesssim 1.$$

The Assumption B can be described in more explicit terms using the Bloch-Floquet theory.

**Lemma 3.2.** Assumption B and Assumption B’ are equivalent.
Proof. Given $n \in \mathbb{N}$ and $f$ $n\Gamma$-periodic. For each $\xi \in \Gamma^* \cap n^{-1}\mathbb{L}^*$, define $$f_\xi(x) = \sum_{R \in \mathbb{L} \cap n\Gamma} f(x + R)e^{-i\xi \cdot R}.$$ It is easy to see that $f_\xi e^{-i\xi \cdot x}$ is $\Gamma$-periodic and $$f(x) = \frac{1}{n^3} \sum_{\xi \in \Gamma^* \cap n^{-1}\mathbb{L}^*} f_\xi(x).$$ Applying $(\mathcal{I} - \mathcal{L}_e)^{-1}$ on both sides, we have $$(\mathcal{I} - \mathcal{L}_e)^{-1} f = \frac{1}{n^3} \sum_{\xi \in \Gamma^* \cap n^{-1}\mathbb{L}^*} (\mathcal{I} - \mathcal{L}_{e,\xi})^{-1} f_\xi.$$ Taking the Fourier transform, we have for $\xi \in \Gamma^* \cap n^{-1}\mathbb{L}^*$ and $K \in \mathbb{L}^*$, $$\tilde{f}(\xi + K) = (f_\xi e^{-i\xi \cdot x})(K).$$ Hence, $$\|f\|^2_{H^{-1}_n \cap H^2_n} = \sum_{\xi \in \Gamma^* \cap n^{-1}\mathbb{L}^*} \|f_\xi\|^2_{\mathcal{D}_\xi}.$$ Similarly, we have $$\| (\mathcal{I} - \mathcal{L}_e)^{-1} f \|^2_{H^{-1}_n \cap H^2_n} = \sum_{\xi \in \Gamma^* \cap n^{-1}\mathbb{L}^*} \| (\mathcal{I} - \mathcal{L}_{e,\xi})^{-1} f_\xi \|^2_{\mathcal{D}_\xi}.$$ Therefore, $$\| (\mathcal{I} - \mathcal{L}_e)^{-1} f \|^2_{H^{-1}_n \cap H^2_n} \leq \sum_{\xi \in \Gamma^* \cap n^{-1}\mathbb{L}^*} \| (\mathcal{I} - \mathcal{L}_{e,\xi})^{-1} \|^2_{\mathcal{D}(\mathcal{D}_\xi)} \| f_\xi \|^2_{\mathcal{D}_\xi} \leq \sup_{\xi} \| (\mathcal{I} - \mathcal{L}_{e,\xi})^{-1} \|^2_{\mathcal{D}(\mathcal{D}_\xi)} \sum_{\xi \in \Gamma^* \cap n^{-1}\mathbb{L}^*} \| f_\xi \|^2_{\mathcal{D}_\xi} = \sup_{\xi} \| (\mathcal{I} - \mathcal{L}_{e,\xi})^{-1} \|^2_{\mathcal{D}(\mathcal{D}_\xi)} \| f \|^2_{H^{-1}_n \cap H^2_n}.$$ We arrive at $$\| (\mathcal{I} - \mathcal{L}_e)^{-1} \|_{\mathcal{L}(H^{-1}_n \cap H^2_n)} \leq \sup_{\xi \in \Gamma^* \cap n^{-1}\mathbb{L}^*} \| (\mathcal{I} - \mathcal{L}_{e,\xi})^{-1} \|_{\mathcal{L}(\mathcal{D}_\xi)}. $$ Conversely, if $\xi \in \Gamma^* \cap n^{-1}\mathbb{L}^*$ for some $n \in \mathbb{N}$, the function $f_\xi \in \mathcal{D}_\xi$ is then $n\Gamma$-periodic. Taking $f = f_\xi / n^3$, we have $$\| (\mathcal{I} - \mathcal{L}_{e,\xi})^{-1} f_\xi \|^2_{\mathcal{D}_\xi} = \| (\mathcal{I} - \mathcal{L}_e)^{-1} f \|^2_{H^{-1}_n \cap H^2_n} \leq \| (\mathcal{I} - \mathcal{L}_e)^{-1} \|_{\mathcal{L}(H^{-1}_n \cap H^2_n)} \| f \|^2_{H^{-1}_n \cap H^2_n} = \| (\mathcal{I} - \mathcal{L}_e)^{-1} \|^2_{\mathcal{D}(H^{-1}_n \cap H^2_n)} \| f_\xi \|^2_{\mathcal{D}_\xi}.$$ Hence $$\| (\mathcal{I} - \mathcal{L}_{e,\xi})^{-1} \|^2_{\mathcal{D}_\xi} \leq \| (\mathcal{I} - \mathcal{L}_e)^{-1} \|^2_{\mathcal{L}(H^{-1}_n \cap H^2_n)}.$$ This completes the proof since $\mathcal{L}_{e,\xi}$ depends continuously on $\xi$. \hfill \blacksquare
We also note that in Assumption B, the boundedness of the operator is characterized in $\hat{H}_n^{-1} \cap H_n^2$ norm. In particular, the norm $\hat{H}_n^{-1}$ is used to control the Coulomb operator. It is of interest to see whether it is possible to pose the stability condition in $L^2$ spaces:

**Assumption D.** For every $\xi \in \Gamma^*$, the operator $I - L_{c, \xi}$ as an operator on $L^2_\xi$ is invertible with norm bounded uniformly in $\xi$: $\|(I - L_{c, \xi})^{-1}\|_{L^2_\xi} \lesssim 1$.

Or, equivalently, **Assumption D’**. For every $n \in \mathbb{N}$, the operator $I - L_c$ as an operator on $L^2_n$ is invertible, and the norm of the inverse operator is bounded independent of $n$:

$$\|(I - L_c)^{-1}\|_{L^2(L^2_n)} \lesssim 1.$$  

One nice feature about the $L^2$ spaces is that on $L^2_n$, $L_c$ is similar to a self-adjoint operator. Therefore the spectral theory can be applied. In particular, Assumption D is valid if and only if the spectrum of $L_{c, \xi}$ is bounded away from 1 uniformly in $\xi$, or equivalently, the spectrum of $L_c$ on $L^2_n$ is bounded away from 1 uniformly in $n$.

Whether Assumption B is equivalent to Assumption D is open.

4. Homogeneously deformed crystal

Now we consider the electronic structure of a deformed crystal. Denote by $Y_i$ the position of the $i$-th nucleus after the deformation and write:

$$Y_i = X_i + U_i, \quad X_i \in \mathbb{L}.$$  

$U_i$ is the displacement of the $i$-th atom. We will be interested in the case when the displacement of the atoms follows a smooth vector field $u$, i.e., $U_i = u(X_i)$.

We will first consider the case when a homogeneous deformation is applied to the crystal, $u(x) = Ax, A \in \mathbb{R}^{3 \times 3}$. The position of the nuclei in the deformed crystal is given by

$$Y_i = (I + A)X_i, \quad X_i \in \mathbb{L}.$$  

The background charge density then becomes

$$m_A(y) = \sum_{X_i \in \mathbb{L}} m_a(y - Y_i),$$  

with the implicit assumption that the charge contribution of an individual ion to the pseudopotential does not change under deformation. This is also the working assumption in practical applications of the density functional theory.

The Kohn-Sham density functional theory is formulated naturally using the coordinates in the deformed configuration, the Eulerian coordinates. However, as will be clear later, it is more convenient for our purpose to pull back to the coordinates in the undeformed configuration, the Lagrangian coordinates.
For a $\Gamma$-periodic electron density $\rho$ (in Lagrangian coordinates) with total charge $Z$: $\int_\Gamma \rho = Z$, the Hamiltonian in the Lagrangian coordinates becomes

$$H_A(\rho) = -\Delta^A + V_A(\rho)$$

(4.4)

where $\Delta^A = a_{ij}^A \partial_i \partial_j$, $a_{ij}^A = ((I + A)^{-1}(I + A)^{-T})_{ij}$,

$$V_A(\rho) = \phi_A(\rho) + \eta(J_A^{-1}\rho).$$

The Coulomb part of the potential $\phi_A$ is given by the solution of

$$-J_A \Delta^A \phi_A = 4\pi(\rho - m_A),$$

(4.5)

with periodic boundary condition on $\Gamma$ and $\int_\Gamma \phi_A = 0$. Here $J_A = \det(I + A)$ is the Jacobian for the deformation map ($y = x + u(x)$) and we have pulled back $m_A$ to the Lagrangian coordinates:

$$m_A(x) = J_A \sum_{X_i \in L} m_u((I + A)(x - X_i)).$$

(4.6)

For a homogeneously deformed crystal, the Kohn-Sham map is formally defined by

$$F_A(\rho) = \frac{1}{2\pi i} \int_\Gamma \frac{1}{\lambda - H_A(\rho)} \mathrm{d}\lambda(x, x).$$

(4.7)

If the size of the deformation gradient $A$ is below a critical value, it can be shown that (4.7) is well-defined, and a self-consistent solution to the Kohn-Sham equation $\rho_A$ can be found in a neighborhood of $\rho_e$. We will defer the proof of the following theorem to Section 7.

**Theorem 4.1.** Under Assumptions A and B, there are positive constants $a$ and $\delta$, such that for $|A| \leq a$, there exists a unique $\Gamma$-periodic density $\rho_A(\cdot) \in H^6_{\text{per}}(\Gamma)$ with the property

1. $\rho_A$ is a self-consistent solution to the Kohn-Sham equation:

$$\rho_A = F_A(\rho_A).$$

2. $\|\rho_A - \rho_e\|_{H^6_{\text{per}}(\Gamma)} \leq \delta$ and $\rho_A$ satisfies the normalization constraint

$$\int_\Gamma \rho_A(x) \mathrm{d}x = Z.$$

Furthermore, the map from $A$ to $\rho_A \in H^6_{\text{per}}(\Gamma)$ is $C^\infty$.

In analogy with the Cauchy-Born rule for crystal lattices, we will call the density $\rho_A$ the Cauchy-Born electron density, and denote it by $\rho_{\text{CB}}(\cdot; A)$.

**Remark.** Here we prove the results in the space $H^6_{\text{per}}$. From the proof in Section 7, it is easy to see that it is straightforward to extend the result to spaces $H^m_{\text{per}}$ with positive integer $m \geq 2$. 
5. Deformed crystal and the extended Cauchy-Born rule

Now consider a smoothly deformed macroscopic crystal. We will assume that the size of the crystal is $O(1)$ and the lattice constant is $\varepsilon$, $\varepsilon \ll 1$. Here $\varepsilon$ is the ratio between the atomic length scale and the characteristic length scale of the smooth deformation. In this setup, the nuclei positions after deformation become

\begin{equation}
Y_i^\varepsilon = X_i^\varepsilon + u(X_i^\varepsilon) \equiv \tau(X_i^\varepsilon), \quad X_i^\varepsilon \in \varepsilon L.
\end{equation}

Here $X_i^\varepsilon$ is the equilibrium position of atoms: $X_i^\varepsilon = \varepsilon X_i$, $X_i \in \mathbb{L}$, $u$ is the displacement field. We will assume that $u(x) = B x + u_{\text{per}}(x)$, where $B$ is a $3 \times 3$ matrix and $u_{\text{per}}$ is a $\Gamma$-periodic function. Note that by the choice of the scaling, for the equilibrium undeformed state, the atoms lie on the lattice $\varepsilon L$ with unit cell $\varepsilon \Gamma$, while the macroscopic physical domain under consideration is $\Gamma$. There are $\varepsilon^{-3}$ atoms in the physical domain $\Gamma$.

Remark. By choosing $u$ to be of the form $B x + u_{\text{per}}$, we limit ourselves to studying the bulk behavior, and we have excluded surface effects. The latter is itself a subject of considerable interest and complexity.

Since we have rescaled the lattice constant to be $\varepsilon$, the charge contribution from each nucleus should be rescaled accordingly (so that the total charge of the nucleus is conserved):

\begin{equation}
m_a^\varepsilon(y) = \varepsilon^{-3} m_a(y/\varepsilon).
\end{equation}

The total background charge distribution (in Eulerian coordinates) becomes

\begin{equation}
m^\varepsilon(y) = \sum_{X_i \in L} m_a^\varepsilon(y - Y_i^\varepsilon).
\end{equation}

Again, we solve for the electronic structure in Lagrangian coordinates, instead of Eulerian coordinates. Given function $f$ defined on the deformed configuration, $\tau(\Gamma)$, the pull back of $f$ to the Lagrangian coordinates is

\begin{equation}
(\tau^* f)(x) = f(\tau(x)).
\end{equation}

For a function $g$ defined on the undeformed domain, the pushforward of $g$ is

\begin{equation}
(\tau_* g)(y) = g(\tau^{-1}(y)).
\end{equation}

We also denote the Jacobian of $\tau$ as $J(x) = \det \nabla \tau(x)$. For example, in the Lagrangian coordinates, the background charge becomes

\begin{equation}
m_a^\varepsilon(x) = J(x)(\tau^* m^\varepsilon)(x) = J(x)m^\varepsilon(\tau(x))
= J(x) \sum_{X_i \in L} \varepsilon^{-3} m_a\left(\frac{\tau(x) - \tau(X_i^\varepsilon)}{\varepsilon}\right),
\end{equation}

where the subscript $\tau$ is used to indicate the dependence on the displacement field.
In the rescaled variable, the Hamiltonian operator with potential $V$ is defined in the Eulerian coordinates by

$$\mathcal{H}^\varepsilon = -\varepsilon^2 \Delta + V(y).$$

The coefficient $\varepsilon^2$ in front of $\Delta$ comes from the rescaling of length. In Lagrangian coordinates, it becomes

$$\mathcal{H}^\varepsilon = -\varepsilon^2 J^{1/2} \Delta^\tau J^{-1/2} + (\tau^* V)(x)$$

where $\Delta^\tau = \tau^* \Delta$. Direct calculation gives

$$J^{1/2} \Delta^\tau J^{-1/2} = a_{ij}(x) \partial_i \partial_j + b_i(x) \partial_i + c(x),$$

where

$$a_{ij}(x) = \left( (I + \nabla u(x))^{-1} (I + \nabla u(x))^{-T} \right)_{ij};$$

$$b_i(x) = 2 J^{1/2}(x) \left( (I + \nabla u(x))^{-1} (I + \nabla u(x))^{-T} \nabla \left( J^{-1/2}(x) \right) \right)_i + \left( (I + \nabla u(x))^{-T} \nabla \cdot (I + \nabla u(x))^{-T} \right)_i;$$

$$c(x) = J^{1/2}(x) (I + \nabla u(x))^{-T} \nabla \cdot (I + \nabla u(x))^{-T} \nabla \left( J^{-1/2}(x) \right).$$

It is easy to check that when $u = 0$, $a_{ij}(x) = \delta_{ij}$, $b_i(x) = 0$ and $c(x) = 0$ for all $x \in \Gamma$.

Consistent with our choice of the displacement field $u$, we will consider $\Gamma$-periodic electron density. In Kohn-Sham density functional theory, the Hamiltonian depends on the density $\rho$ through the potential (written in Lagrangian coordinates):

$$V^\varepsilon_\phi(\rho)(x) = \phi^\varepsilon_\phi(\rho)(x) + \eta(J)^{-1} \varepsilon^3 \rho(x),$$

where $\phi^\varepsilon_\phi$ is the Coulomb potential that satisfies

$$-J(x) \Delta^\tau \phi^\varepsilon_\phi = 4\pi \varepsilon (\rho - m^\varepsilon_\phi),$$

with periodic boundary condition on $\Gamma$. We assume the average of $\phi^\varepsilon_\phi$ is zero to fix the arbitrary constant. Direct calculation yields

$$J(x) \Delta^\tau = a_{ij}(x) \partial_i \partial_j + b_i(x) \partial_i,$$

where

$$a_{ij}(x) = J(x) \left( (I + \nabla u(x))^{-1} (I + \nabla u(x))^{-T} \right)_{ij};$$

$$b_i(x) = J(x) \left( (I + \nabla u(x))^{-T} \nabla \cdot (I + \nabla u(x))^{-T} \right)_i.$$

The Kohn-Sham map in this case is defined by

$$\mathcal{F}^\varepsilon_\tau(\rho) = \frac{1}{2\pi i} \int_{\mathcal{C}} \frac{1}{\lambda - \mathcal{H}^\varepsilon_\tau(\rho)} \frac{d\lambda(x, x)}{d\lambda},$$

The right hand side is the diagonal of the kernel of the operator. We will show later that this map is well-defined.
In analogy with the spirit of the Cauchy-Born rule for crystal lattices, we expect that the electronic structure around a point \( x \) to be approximately given by the electronic structure of a homogeneously deformed crystal with deformation gradient \( \nabla u(x) \). As we have discussed in the last section, using Lagrangian coordinates, the electron density for the system with homogeneous deformation gradient \( \nabla u(x) \) is given by \( \rho_{\text{CB}}(x; \nabla u(x)) \). Therefore, the electron density constructed using the spirit of the Cauchy-Born rule is

\[
\rho_0(x) = \varepsilon^{-3} \rho_{\text{CB}}(x/\varepsilon; \nabla u(x)).
\]

Here, we have rescaled the Cauchy-Born density accordingly.

One main result of this paper is that under the stability conditions, the density constructed by the Cauchy-Born rule gives a good approximation to a solution to the Kohn-Sham equation. In other words, one can find a solution to the Kohn-Sham equation that is close to \( \rho_0 \).

**Theorem 5.1.** Under Assumptions A, B and C, there exist constants \( a, \varepsilon_0 \) and \( M \), such that if \( \varepsilon \leq \varepsilon_0 \) and if \( M_A = \sup_j \| \nabla^j u \|_{L^\infty} \leq a \), then there exists \( \rho^* \in L^\infty_\varepsilon \) with the property:

1. \( \rho^* \) is a solution to the Kohn-Sham equation:
   \[
   \rho^*(x) = F^*_\varepsilon(\rho^*)(x).
   \]

2. \( \| \rho^* - \varepsilon^{-3} \rho_{\text{CB}}(x/\varepsilon; \nabla u(x)) \|_{L^\infty_\varepsilon} \leq M \varepsilon^{1/2} \), i.e., \( \| \tilde{\rho}^* - \rho_{\text{CB}}(x; \nabla u(\varepsilon x)) \|_{L^\infty} \leq M \varepsilon^{1/2} \), where \( \tilde{\rho}^*(x) = \varepsilon^3 \rho(\varepsilon x) \), and \( \rho^* \) satisfies the normalization constraint:
   \[
   \int_{\Gamma} \rho^*(x) \, dx = Z \varepsilon^{-3}.
   \]

Recall that the space \( L^\infty_\varepsilon \) is the rescaled version of \( L^\infty_n \):

\[
L^\infty_\varepsilon = \{ f \mid \varepsilon^3 f(\varepsilon x) \in L^\infty_n, n = 1/\varepsilon \}.
\]

**Remark.** We will actually prove a stronger version of this result, see Theorem 5.5. Local uniqueness will also be established.

**Remark.** The result of Theorem 5.1 (Theorem 5.5) tells us that the effective Hamiltonian corresponding to the deformed case is of the form of the Hamiltonian considered in the previous work [10]. Hence, the results of [10] can be applied to obtain the characterization of the wave functions for the deformed crystal. In particular, the Cauchy-Born rule for the Wannier functions also holds (Theorem 9 in [10]).

**Remark.** We also remark that the stability assumptions B and C are essentially sharp (except that possibly a different norm might be used). The failure of these assumptions would lead to instabilities and breaking down of the Cauchy-Born approximation. This has been addressed for the classical atomistic potential model in [11, 12] and also for the nonlinear tight-binding model in [9]. The characterization of instabilities of electronic structure will be studied in future publications.
The overall strategy for the proof of the theorem is essentially the same as the one used in the previous work [9] where the nonlinear tight-binding model is considered: We first build an approximate solution to the Kohn-Sham equation. Starting from that approximate solution, we use the Newton-Raphson iteration to prove the existence of a solution in a neighborhood of the approximate solution. The convergence and uniformity of the iteration is guaranteed by the stability condition.

To be more specific, we will use the Newton-Raphson iteration to obtain the self-consistent solution of the Kohn-Sham equation

\[ \rho = F_\varepsilon^x(\rho). \]

We assume that we have an initial guess \( \rho^0 \) whose leading order is given by the Cauchy-Born approximation \( \varepsilon^{-3}\rho_{\text{CB}}(x/\varepsilon; \nabla u(x)) \), satisfying

\[ \|\rho^0 - F_\varepsilon^x(\rho^0)\|_{H^{-1}\cap H^1} \lesssim \varepsilon^{1/2}. \]

\( \rho^0 \) will be constructed later by asymptotics in Sections 9 and 10. Let us set up an iteration scheme by

\[ \rho^{n+1} = \rho^n - (I - L_{\varepsilon,\rho^0})^{-1}(\rho^n - F_\varepsilon^x(\rho^n)), \]

where \( L_{\varepsilon,\rho^0} = \frac{\partial F_\varepsilon^x}{\partial \rho}|_{\rho=\rho^0} \) is linearization of the Kohn-Sham map at displacement field \( \tau \) and density \( \rho^0 \). Equivalently, knowing \( \rho^n \), we let

\[ \rho^{n+1} = \rho^n + \delta \rho, \]

where \( \delta \rho \) satisfies

\[ \rho^n + \delta \rho = F_\varepsilon^x(\rho^n) + L_{\varepsilon,\rho^0}(\delta \rho). \]

The convergence of the iteration is guaranteed by the following elementary lemma.

**Lemma 5.2.** Let \( X \) be a Banach space with norm \( \|\cdot\| \). Consider the iteration scheme defined by

\[ \rho^{n+1} = \rho^n - (I - L)^{-1}(\rho^n - F(\rho^n)), \]

with initial iterate \( \rho^0 \) and \( L \) being a linear operator on \( X \). Assume there exist constants \( 0 < \eta \leq 1 \) and \( M \), such that \( F \) is defined on the set \( \{ \rho \in X \mid \|\rho - \rho^0\| \leq M \} \) and the following two conditions hold:

- \( \|(I - L)^{-1}(\rho^0 - F(\rho^0))\| \leq \eta M, \)

- If \( \|\tilde{\rho} - \rho^0\| \leq M \) and \( \|\tilde{\rho} - \rho^0\| \leq M, \) then

\[ \|(I - L)^{-1}(F(\tilde{\rho}) - F(\tilde{\rho}) - L(\tilde{\rho} - \tilde{\rho}))\| \leq (1 - \eta)\|\tilde{\rho} - \tilde{\rho}\|. \]
Then the sequence \( \{\rho^n\} \) defined in (5.18) converges in norm to a fixed point of \( F \) as \( n \) goes to infinity. The fixed point is unique in the set \( \{\rho \in X \mid \|\rho - \rho^0\| \leq M\} \).

**Proof.** Denote \( K = (I - L)^{-1} \). Subtracting (5.18) by the same equation with \( n \) replaced by \( n-1 \), we get

\[
\rho^{n+1} - \rho^n = \rho^n - \rho^{n-1} - K(\rho^n - \rho^{n-1} - (F(\rho^n) - F(\rho^{n-1})))
\]

Let us assume for the moment that \( \rho^{n-1} \) and \( \rho^n \) lie in a ball around \( \rho^0 \) with radius \( M \). Then by (5.20),

\[
\|\rho^{n+1} - \rho^n\| \leq (1 - \eta)\|\rho^n - \rho^{n-1}\|.
\]

Therefore,

\[
\|\rho^{n+1} - \rho^0\| \leq \sum_{k=0}^{n} \|\rho^{k+1} - \rho^k\| \leq \eta\|\rho^1 - \rho^0\|.
\]

Combined with (5.19),

\[
\|\rho^1 - \rho^0\| = \|K(\rho^0 - F(\rho^0))\| \leq \eta M.
\]

we obtain

\[
\|\rho^{n+1} - \rho^0\| \leq M.
\]

Hence, by induction, we have \( \|\rho^n - \rho^0\| \leq M \) for all \( n \). The convergence of the iteration to a fixed point follows directly from (5.21). The uniqueness follows (5.20) easily by contradiction.

To complete the proof of Theorem 5.1, we need two main lemmas. These two lemmas will be proved in Section 11.

**Lemma 5.3.** We have

\[
\|L^\varepsilon_{r,\rho} w - L^\varepsilon_{r,\rho^0} w\|_{H^{-1}_r \cap H^1_r} \lesssim (M_A + \varepsilon)\|w\|_{H^{-1}_r \cap H^1_r},
\]

where \( M_A = \sup_j \|\nabla^j u(x)\|_{L^\infty(r)} \).

**Lemma 5.4.** There exists a constant \( \delta_0 > 0 \) such that for any \( \tilde{\rho}, \tilde{\rho}^0 \) with \( \|\tilde{\rho} - \rho^0\|_{H^{-1}_r \cap H^1_r} \leq \delta_0 \), we have

\[
\|F^\varepsilon_{r}(\tilde{\rho}) - F^\varepsilon_{r}(\tilde{\rho}) - L^\varepsilon_{r,\rho^0}(\tilde{\rho} - \rho^0)\|_{H^{-1}_r \cap H^1_r} \lesssim \delta_0\|\tilde{\rho} - \rho^0\|_{H^{-1}_r \cap H^1_r}.
\]

Assuming these two lemmas, we are ready to prove the main result. We will actually prove a more refined version of Theorem 5.1:

**Theorem 5.5.** Under Assumptions A, B and C, there exist constants \( a, \varepsilon_0 \) and \( C \), such that if \( \varepsilon \leq \varepsilon_0 \) and if \( M_A = \sup_j \|\nabla^j u\|_{L^\infty} \leq a \), there exists a unique \( \rho^\varepsilon(x) \) with the property:

1. \( \rho^\varepsilon \) is a self-consistent solution to the Kohn-Sham equation:
   \[
   \rho^\varepsilon(x) = F^\varepsilon_{r}(\rho^\varepsilon)(x).
   \]
(2) \( \| \rho^\varepsilon - \rho^0 \|_{H^{-1}_\varepsilon \cap H^2_\varepsilon} \leq C \varepsilon^{1/2} \) and \( \rho^\varepsilon \) satisfies the normalization constraint:
\[
\int_\Gamma \rho^\varepsilon(x) \, dx = Z \varepsilon^{-3};
\]

Proof. We use Lemma 5.2 by taking \( \mathcal{F} = \mathcal{F}_\varepsilon^\varepsilon, \mathcal{L} = \mathcal{L}_{\varepsilon, \rho^0}^\varepsilon \) and the space \( H^{-1}_\varepsilon \cap H^2_\varepsilon \) with its natural norm. It then suffices to show (5.19) and (5.20).

By (5.15), there exists a constant \( C_1 \) such that
\[
\| \rho^0 - \mathcal{F}_\varepsilon^\varepsilon(\rho^0) \|_{H^{-1}_\varepsilon \cap H^2_\varepsilon} \leq C_1 \varepsilon^{1/2}.
\]
For \( w \in H^{-1}_\varepsilon \cap H^2_\varepsilon \), by Assumption B and a straightforward rescaling, we have
\[
\| (\mathcal{I} - \mathcal{L}_{\varepsilon, \rho^0})^{-1}(w) \|_{H^{-1}_\varepsilon \cap H^2_\varepsilon} \leq C_2 \| w \|_{H^{-1}_\varepsilon \cap H^2_\varepsilon}.
\]
From Lemma 5.3, we have
\[
\| (\mathcal{L}_{\varepsilon, \rho^0}^\varepsilon - \mathcal{L}_{\varepsilon, \rho^0}^\varepsilon)(w) \|_{H^{-1}_\varepsilon \cap H^2_\varepsilon} \leq \frac{1}{2C_2} \| w \|_{H^{-1}_\varepsilon \cap H^2_\varepsilon}
\]
by choosing \( \varepsilon_0 \) and \( \alpha \) sufficiently small. Hence, since
\[
(\mathcal{I} - \mathcal{L}_{\varepsilon, \rho^0})^{-1} = (\mathcal{I} - \mathcal{L}_{\varepsilon, \rho^0}^\varepsilon)^{-1}(\mathcal{I} - (\mathcal{L}_{\varepsilon, \rho^0}^\varepsilon - \mathcal{L}_{\varepsilon, \rho^0})(\mathcal{I} - (\mathcal{L}_{\varepsilon, \rho^0}^\varepsilon)^{-1})^{-1},
\]
we have
\[
\| (\mathcal{I} - \mathcal{L}_{\varepsilon, \rho^0})^{-1}(w) \|_{H^{-1}_\varepsilon \cap H^2_\varepsilon} \leq 2C_2 \| w \|_{H^{-1}_\varepsilon \cap H^2_\varepsilon}.
\]
Let \( w = \rho^0 - \mathcal{F}_\varepsilon^\varepsilon(\rho^0) \), we obtain, using (5.15),
\[
\| (\mathcal{I} - \mathcal{L}_{\varepsilon, \rho^0})^{-1}((\rho^0 - \mathcal{F}_\varepsilon^\varepsilon(\rho^0)) \|_{H^{-1}_\varepsilon \cap H^2_\varepsilon} \leq 2C_1 \varepsilon^{1/2}.
\]
Therefore, (5.19) is satisfied by letting \( \eta = 1/2 \) and \( M = 4C_1 \varepsilon^{1/2} \). We take \( \varepsilon_0 \) sufficiently small, so that \( M \leq \delta_0 \) in Lemma 5.4, we then have
\[
\| \mathcal{F}_\varepsilon^\varepsilon(\hat{\rho}) - \mathcal{F}_\varepsilon^\varepsilon(\tilde{\rho}) - \mathcal{L}_{\varepsilon, \rho^0}(\hat{\rho} - \tilde{\rho}) \|_{H^{-1}_\varepsilon \cap H^2_\varepsilon} \leq C_3 M \| \hat{\rho} - \tilde{\rho} \|_{H^{-1}_\varepsilon \cap H^2_\varepsilon}.
\]
Therefore, we obtain
\[
\| (\mathcal{I} - \mathcal{L}_{\varepsilon, \rho^0})^{-1}(\mathcal{F}_\varepsilon^\varepsilon(\hat{\rho}) - \mathcal{F}_\varepsilon^\varepsilon(\tilde{\rho}) - \mathcal{L}_{\varepsilon, \rho^0}(\hat{\rho} - \tilde{\rho})) \|_{H^{-1}_\varepsilon \cap H^2_\varepsilon} \leq C_3 M \| (\mathcal{I} - \mathcal{L}_{\varepsilon, \rho^0})^{-1} \|_{L^2(H^{-1}_\varepsilon \cap H^2_\varepsilon)} \| \hat{\rho} - \tilde{\rho} \|_{H^{-1}_\varepsilon \cap H^2_\varepsilon} \leq 2C_2 C_3 M \| \hat{\rho} - \tilde{\rho} \|_{H^{-1}_\varepsilon \cap H^2_\varepsilon}.
\]
The condition (5.20) follows by taking \( \varepsilon_0 \) sufficiently small such that
\[
2C_2 C_3 M = 8C_1 C_2^3 C_3 \varepsilon^{1/2} \leq (1 - \eta) = 1/2.
\]
We conclude using Lemma 5.2.

\[\square\]

The rest of the paper is devoted to the construction of approximate solution \( \rho^0 \) satisfying (5.15) and the proof of Lemmas 5.3 and 5.4. This is considerably more difficult than the corresponding estimates for the nonlinear tight-binding model in [9], due to the presence of the long range Coulomb potential and the continuous nature of the model. For example, to construct the approximate solution of the
Kohn-Sham equation, we have to exploit the localization properties of the electronic structure of an insulator. For that purpose, we need the results and tools developed in [10].

The proof is organized as follows. Section 6 is devoted to the study of the linearized Kohn-Sham operator which plays a major role in our analysis. The building blocks of the Cauchy-Born approximation is the homogeneously deformed system, which will be studied in Section 7. The analysis depends on the property that the Green’s function is exponentially localized for the system under consideration, the technical core of this is presented in Section 8. After these preparations, in Sections 9 and 10, we build a highly accurate approximate solution to the Kohn-Sham equation around the guess given by the Cauchy-Born rule. The final steps of the proof of Theorem 5.1 are given in Section 11. The proofs of some technical lemmas are delayed to the appendix.

6. The linearized Kohn-Sham operator

Given the displacement field \( \tau \) and lattice constant \( \varepsilon \), let \( \mathcal{H}_\tau^\varepsilon = \mathcal{H}_\varepsilon^\tau(\rho) \) be the effective Hamiltonian corresponding to the density \( \rho \)

\[
\mathcal{H}_\tau^\varepsilon(\rho) = -\varepsilon^2 (a_{ij}(x) \partial_i \partial_j + b_i(x) \partial_i + c(x)) + V_\tau^\varepsilon(\rho).
\]

We denote by \( \delta_\rho V_\tau^\varepsilon(w) \) the leading order perturbation in the potential generated by a density perturbation \( w \):

\[
\begin{align*}
\delta_\rho V_\tau^\varepsilon(w) &= \delta \phi_\tau^\varepsilon + \delta \eta_\tau^\varepsilon; \\
(-a_{ij}(x) \partial_i \partial_j - b_i(x) \partial_i) \delta \phi_\tau^\varepsilon &= 4\pi \varepsilon w; \\
\delta \eta_\tau^\varepsilon(x) &= \eta'(J(x)^{-1}(x)^3 \rho(x)) J(x)^{-1}(x)^3 w.
\end{align*}
\]

Here the equation for the Coulomb potential is solved with periodic boundary condition and the average of \( \delta \phi_\tau^\varepsilon \) is set to be 0 to fix the arbitrary constant. The Kohn-Sham map linearized at density \( \rho \) is formally given by

\[
\mathcal{L}_{\tau,\rho}^\varepsilon w = \frac{1}{2\pi i} \int_{\mathcal{C}} \frac{1}{\lambda - \mathcal{H}_\varepsilon^\tau} \delta_\rho V_\tau^\varepsilon(w) \frac{1}{\lambda - \mathcal{H}_\varepsilon^\tau} \, d\lambda(x, x).
\]

Here the function \( \delta_\rho V_\tau^\varepsilon(w) \) is viewed as a multiplicative operator.

We assume that the density \( \rho \) is periodic with respect to \( \Gamma \) (note that now \( \Gamma \) serves as the macroscopic domain on which our crystal is defined). Hence the same holds for \( V_\tau^\varepsilon = V_\varepsilon^\tau(\rho) \). Therefore, the Hamiltonian operator \( \mathcal{H}_\varepsilon^\tau \) commutes with translational operator \( \tau_R \) for \( R \in \mathbb{L} \). We will assume that the system is insulating, and we can choose compact contour \( \mathcal{C} \) around the occupied spectrum such that

\[
\text{dist}(\mathcal{C}, \text{spec}(\mathcal{H}_\varepsilon^\tau)) = E_g/2 > 0.
\]

This assumption will be justified when we apply the results in this section to a particular Hamiltonian.
Define the operator $\chi_{\tau, \rho}^\varepsilon$ formally by
\begin{equation}
(\chi_{\tau, \rho}^\varepsilon V)(x) = \frac{1}{2\pi^2} \int_{\partial \mathbb{C}} \frac{1}{\lambda - H_{\varepsilon}} V \left( \frac{1}{\lambda - H_{\varepsilon}} \right) d\lambda(x, x),
\end{equation}
then the linearized Kohn-Sham operator can be expressed as
\[ L_{\tau, \rho}^\varepsilon = \chi_{\tau, \rho}^\varepsilon \delta V_{\tau}^\varepsilon. \]
The definition of $\chi_{\tau, \rho}^\varepsilon$ will be made precise through Theorem 6.3.

The linearized Kohn-Sham operator is the composition of two operators: The operator $\delta V$ which maps density to potential, and the operator $\chi$ which maps potential to density. A key component of our analysis is the uniform estimates of these two operators for large crystals. This is carried out in Sections 6.1 and 6.2. As a corollary, we obtain the result that the linearized Kohn-Sham operator is a bounded operator on $L^2_{\varepsilon}$ uniformly in $\varepsilon$. In Section 6.3, the regularity of the operator $(I - L_e)^{-1}$ will be studied. In Section 6.4, we will compare Kohn-Sham operator linearized at different states and prove the stability of the Kohn-Sham operator with respect to the perturbation on the Hamiltonian.

6.1. From density to potential: Uniform estimates of the $\delta V$ operator.

For simplicity of notation, let us denote $V_{\varepsilon}(x) = V_{\varepsilon}^\varepsilon(\rho(\varepsilon x))$. We prove the uniform boundedness of the linearized Kohn-Sham operator.

**Theorem 6.1.** Assume $\rho \in W^{m, \infty}_\varepsilon$ and $V_{\varepsilon} \in W^m_n$ for $n = 1/\varepsilon$ and some integer $m \geq 0$, then the operator $L_{\tau, \rho}^\varepsilon$ is uniformly (with respect to $\varepsilon$) bounded on $H^{-1}_{\varepsilon} \cap H^m_{\varepsilon}$:
\[ \|L_{\tau, \rho}^\varepsilon\|_{L(H^{-1}_{\varepsilon} \cap H^m_{\varepsilon})} \leq C(E_g, \|\rho\|_{W^{m, \infty}_\varepsilon}, \|V_{\varepsilon}\|_{W^m_n}, \varepsilon). \]

**Remark.** We remark that we will apply the theorem to cases that $\|\rho\|_{W^{m, \infty}_\varepsilon}$ and $\|V_{\varepsilon}\|_{W^m_n}$ are bounded uniformly in $\varepsilon$, and hence, we have a uniform bound of the operator $L_{\tau, \rho}^\varepsilon$.

**Proof.** It is more convenient to use atomic unit scaling. Define $\delta V$ as (we suppress the dependence on $\rho$ and $\tau$ in the notation for simplicity)
\[
\begin{aligned}
\delta V(w) &= \delta \phi + \delta \eta; \\
(-a_{ij}(\varepsilon x)\partial_i \partial_j - \varepsilon b_i(\varepsilon x)\partial_i)\delta \phi = 4\pi w; \\
\delta \eta(x) &= \eta'(J(\varepsilon x)^{-1}e^3 \rho(\varepsilon x)J(\varepsilon x)^{-1})w(x),
\end{aligned}
\]
we then have
\begin{equation}
(\delta V w_{\varepsilon})(x/\varepsilon) = (\delta \rho V_{\varepsilon}^\varepsilon w)(x)
\end{equation}
where $w_{\varepsilon} = e^3 w(\varepsilon x)$. Further define $\chi$ as
\[ (\chi \nu)(x) = \frac{1}{2\pi i} \int_{\partial \mathbb{C}} \frac{1}{\lambda - H} \nu \frac{1}{\lambda - H} d\lambda(x, x), \]
where \( \nu \) is understood as a multiplicative operator on the right hand side, and the rescaled Hamiltonian \( \mathcal{H} \) is given by

\[
\mathcal{H} = a_{ij}(\varepsilon x) \partial_i \partial_j + \varepsilon b_i(\varepsilon x) \partial_i + \varepsilon^2 c(\varepsilon x) + V_\varepsilon.
\]

It is easy to check then

\[
(6.7) \quad (\chi \nu_\varepsilon)(x) = \varepsilon^3 (\chi_{\varepsilon, \rho}^\varepsilon \nu)(\varepsilon x),
\]

where \( \nu_\varepsilon(x) = \nu(\varepsilon x) \).

Thus the operator \( \mathcal{L} = \chi \delta V \) is related to \( \mathcal{L}_{\varepsilon, \rho} \) through

\[
(\mathcal{L} w_\varepsilon)(x) = \varepsilon^3 (\mathcal{L}_{\varepsilon, \rho}^\varepsilon w)(\varepsilon x),
\]

where \( w_\varepsilon = \varepsilon^3 w(\varepsilon x) \). Therefore, it suffices to consider the operator \( \mathcal{L} \). The Theorem is then a direct consequence of Lemma 6.2 and Theorem 6.3 proved below.

In the rest of this section, we establish the uniform estimate of \( \delta V \). The uniform estimate of \( \chi \) will be establish in Section 6.2.

**Lemma 6.2.** For any integer \( m \geq 0 \), we have

\[
(6.8) \quad \| \delta \phi \|_{H_n^{m+2}} \lesssim \| w \|_{H_n^{-1} \cap H_n^m}.
\]

Moreover, if \( \rho \in W^{m, \infty}_\varepsilon \), then

\[
(6.9) \quad \| \delta \eta \|_{H_n^m} \leq C(\| \rho \|_{W^{m, \infty}_\varepsilon}) \| w \|_{H_n^m}.
\]

Hence,

\[
(6.10) \quad \| \delta V(w) \|_{H_n^m + H_n^{m+2}} \leq C(\| \rho \|_{W^{m, \infty}_\varepsilon}) \| w \|_{H_n^{-1} \cap H_n^m}
\]

**Proof.** The argument for the exchange-correlation potential is straightforward. Recall \( \rho_\varepsilon(x) = \varepsilon^3 \rho(\varepsilon x) \), we have \( \rho_\varepsilon \in W^{m, \infty}_n \) since \( \rho \in W^{m, \infty}_\varepsilon \). Notice that

\[
\delta \eta(x) = \eta'(J(\varepsilon x) \rho_\varepsilon(x)) J(\varepsilon x) w(x),
\]

hence, by the smoothness of \( \eta \), we have

\[
\| \delta \eta \|_{H_n^m} \leq C(\| \rho \|_{W^{m, \infty}_\varepsilon}) \| w \|_{H_n^m}.
\]

Now consider the Coulomb potential that satisfies

\[
(-a_{ij}(\varepsilon x) \partial_i \partial_j - \varepsilon b_i(\varepsilon x) \partial_i) \delta \phi = 4\pi w,
\]

and \( \int \delta \phi_{\varepsilon} = 0 \) with periodic boundary condition on \( n \Gamma \). First assume that the operator is just the Laplacian (in other words, for the system without deformation). Then \( \delta \phi = \delta \phi_{\varepsilon} \), and

\[
-\Delta \delta \phi_{\varepsilon} = 4\pi w.
\]

In Fourier space, we have

\[
\delta \phi_{\varepsilon}(k) = \frac{4\pi}{|k|^2} \hat{w}(k),
\]
for $k \in \Gamma^*/n$. Notice that the above equation is well defined since $\hat{w}(0) = 0$ as a result of $w \in \dot{H}_n^{-1}$. By definition, 
\[
\|w\|_{\dot{H}_n^{-1} \cap \dot{H}_n^{m}} = \left( \sum_{k \in \Gamma^*/n} \left( \frac{1}{|k|^2} + |k|^{2m} \right) |\hat{w}|^2(k) \right)^{1/2}.
\]
Hence,
\[
||\delta \phi_c||_{\dot{H}_n^{m+2}}^2 = \sum_{k \in \Gamma^*/n} \left( 1 + |k|^{2m+2} \right) |\hat{w}|^2(k) \lesssim \sum_{k \in \Gamma^*/n} \left( \frac{1}{|k|^2} + |k|^{2m} \right) |\hat{w}|^2(k) = \|w\|_{\dot{H}_n^{-1} \cap \dot{H}_n^{m}}^2.
\]
Observe that in the case with deformation, the equation we are considering is simply the Poisson equation transformed to the Lagrangian coordinates. We will prove the desired estimate in two steps. The first is to prove that the estimate holds when the deformation is linear. The second is to show that the norms involved are equivalent for a general deformation and the linear part of that general deformation.

Denote by $\tau_\varepsilon$ as the displacement vector field in the atomic unit (for which the lattice parameter is 1): 
\[
\tau_\varepsilon(x) = \varepsilon^{-1} \tau(\varepsilon x), \; x \in n\Gamma.
\]
Write 
\[
\delta \phi_\tau(y) = \delta \phi_\tau(\tau_\varepsilon^{-1}(y)), \\
w_\tau(y) = J^{-1}(\varepsilon \tau_\varepsilon^{-1}(y))w(\tau_\varepsilon^{-1}(y)).
\]
Then we have the equation in Eulerian coordinates on the domain $\tau_\varepsilon(n\Gamma)$ (recall that $n = 1/\varepsilon$) 
(6.11) 
\[-\Delta \delta \phi_\tau(y) = 4\pi w_\tau(y).
\]

The domain $\tau_\varepsilon(n\Gamma)$ might have a complicated shape. Without loss of generality, let us assume that the vertices of $\Gamma$ are given by 
\[
\{X_\Gamma\} = \{n_1e_1 + n_2e_2 + n_3e_3 \mid n_i = 0 \text{ or } 1\},
\]
where the $e_i$’s are unit vectors of the lattice. Then the vertices of the cell $n\Gamma$ is $\{nX_\Gamma\}$ and after deformation, the positions become 
\[
\{\tau_\varepsilon(nX_\Gamma)\} = \{n(I + B)X_\Gamma\} + nu_{\text{per}}(0).
\]
Hence, due to periodicity, it is equivalent to solving for (6.11) in the convex hull spanned by $\{\tau_\varepsilon(nX_\Gamma)\}$.

We then map the $n(I + B)\Gamma$ periodic functions $w_\tau$ and $\delta \phi_\tau$ to $n\Gamma$ periodic functions by an affine transformation: 
\[
w_B(x) = w_\tau((I + B)x), \; \text{ and } \delta \phi_B(x) = \delta \phi_\tau((I + B)x).
\]
Now $w_B$ and $\delta \phi_B$ are $n\Gamma$ periodic, and they satisfy the equation 
\[-J_B \Delta B \delta \phi_B = 4\pi w_B.
\]
Since, in Fourier space,
\[ \tilde{\delta \phi_B}(k) = \frac{4\pi}{J_B[(I + B)^{-1}k]^2} \tilde{w}_B(k), \]
for \( k \in \Gamma^*/n \), similar to the estimate for \( \delta \phi_e \), we have
\[ \| \delta \phi_B \|_{H^{m+2}_n} \leq C \| w_B \|_{H^{m+2}_n}^2, \]
where the constant depends only on \( B \).

To arrive at the conclusion, it then suffices to prove
\[ \| w_B \|_{H^{m+1}_n} \lesssim \| w \|_{H^{m+1}_n} \quad \text{and} \quad \| \delta \phi \|_{H^{m+2}_n} \lesssim \| \delta \phi_B \|_{H^{m+2}_n}. \]

Let
\[ \tau_B(x) = \tau_e((I + B)^{-1}(x)). \]

As discussed above, we may limit to the case when \( \tau_B \) maps \( n\Gamma \) to \( n\Gamma \) by looking at the convex hull of the deformed crystal. Notice that
\[ \delta \phi(x) = \tau_B^*(\delta \phi_e)(x) = \delta \phi_e(\tau_e(x)) = \delta \phi_B(\tau_B(x)). \]

Hence,
\[ \nabla \delta \phi(x) = \nabla \tau_B \cdot \nabla \delta \phi_B(\tau_B(x)). \]

Since \( \nabla \tau_B(x) \) is a smooth function with uniformly bounded derivatives independent of \( \varepsilon \), we obtain
\[ \| \delta \phi \|_{H^{m+2}_n} = \| \nabla \delta \phi \|_{H^{m+1}_n} \lesssim \| \nabla \delta \phi_B(\tau_B(x)) \|_{H^{m+1}_n} \]
\[ \lesssim \| \nabla \delta \phi_B(x) \|_{H^{m+1}_n} = \| \delta \phi_B \|_{H^{m+1}_n}. \]

For the control of \( w_B \), using the dual characterization,
\[ \| w_B \|_{H^{-1}_n} = \sup_{\| f \|_{H^1_n} \leq 1} \int_{n\Gamma} w_B f \, dy \]
\[ = \sup_{\| f \|_{H^1_n} \leq 1} \int_{n\Gamma} J^{-1}((\varepsilon \tau_B^{-1}(y))w(\tau_B^{-1}(y)))f(y) \, dy \]
\[ = \sup_{\| f \|_{H^1_n} \leq 1} \int_{n\Gamma} w(x)\tau_B^*(f)(x) \, dx \leq \| w \|_{H^{-1}_n} \sup_{\| f \|_{H^1_n} \leq 1} \| \tau_B^*f \|_{H^*_n}. \]

As was shown above, we have \( \| \tau_B^*f \|_{H^*_n} \lesssim \| f \|_{H^*_n} \). Hence, we have the desired estimate \( \| w_B \|_{H^{-1}_n} \lesssim \| w \|_{H^{-1}_n}. \) The argument for the statement that \( \| w_B \|_{H^n} \lesssim \| w \|_{H^n} \) is similar and will be omitted. \( \square \)
6.2. From potential to density: Uniform estimates of the \( \chi \) operator.

**Theorem 6.3.** Assume \( V_\varepsilon \in W^{m,\infty}_n \) for some integer \( m \geq 0 \). There exists constant \( C \) depending only on \( E_g, \| V_\varepsilon \|_{W^{m,\infty}_n} \) and \( \mathcal{E} \), such that

\[
\chi_{\varepsilon_{\mu}} \rho \leq C(E_g, \| V_\varepsilon \|_{W^{m,\infty}_n}, \mathcal{E}) \| \rho \|_{H^{m}_{n}(\mathbb{R}^3)}, \quad \| \rho \|_{H^{m+2}_{n}(\mathbb{R}^3)}. \tag{6.12}
\]

In the following, we assume for simplicity of presentation that the Hamiltonian is given by

\[
\mathcal{H} = -\Delta + V_\varepsilon, \tag{6.13}
\]

where the kinetic term in \( \mathcal{H} \) takes the form of a Laplacian. All the argument presented below can be straightforwardly adapted to the deformed case in which the kinetic term in \( \mathcal{H} \) takes the form \( a_{ij}(\varepsilon x) \partial_i \partial_j + b_i(\varepsilon x) \partial_i + c(\varepsilon x) \).

We will decompose the proof into several steps: the conclusion of the theorem is proved by combining Propositions 6.8, 6.9, 6.13 and Corollary 6.12, established below.

First let us note the following lemma about the regularity of the kernels of bounded operators, which will be often used in the rest of the paper.

**Lemma 6.4.** Let \( T \) be a bounded linear operator on \( L^2(\mathbb{R}^3) \) satisfying

\[
\| Tf \|_{H^m} \leq C \| f \|_{H^{-m}}, \quad \forall f \in L^2(\mathbb{R}^3)
\]

for some constant \( C \) and integer \( m \geq 2 \). Then \( T \) is an integral operator with a kernel \( K(\cdot, \cdot) \in C^{n-2, \alpha}(\mathbb{R}^3 \times \mathbb{R}^3) \) for \( 0 \leq \alpha < 1/2 \), such that

\[
\| K(\cdot, \cdot) \|_{C^{n-2, \alpha}(\mathbb{R}^3 \times \mathbb{R}^3)} \leq \gamma_m C, \tag{6.14}
\]

where \( \gamma_m \) is a constant depending only on \( m \). In particular, the diagonal of the kernel: \( K_d: K_d(x) = K(x, x) \) is well-defined, and

\[
\| K_d \|_{C^{n-2, \alpha}(\mathbb{R}^3)} \leq \gamma_m C. \tag{6.15}
\]

**Proof.** We extend a technique used by Agmon for the regularity estimates of Green’s function for elliptic operators in [1].

Let \( g = Tf \) for \( f \in L^2(\mathbb{R}^3) \). Since \( g \in H^m(\mathbb{R}^3) \) with \( m \geq 2 \), \( g \) is in the Hölder space \( C^{n-2, \alpha}(\mathbb{R}^3) \) for \( 0 \leq \alpha < 1/2 \). Hence for each \( x \), the mapping \( f \mapsto g(x) \) defines a bounded linear functional on \( L^2(\mathbb{R}^3) \). Thus by the Riesz representation theorem, there exists a function \( K(x, \cdot) \in L^2(\mathbb{R}^3) \), such that

\[
(T f)(x) = g(x) = \int K(x, y) f(y) \, dy. \tag{6.16}
\]

Take \( f_\varepsilon(y) = \overline{K(x, y)} \), then using the Sobolev inequality, we have

\[
\| f_\varepsilon \|_{L^2}^2 = \int K(x, y) f_\varepsilon(y) \, dy = (T f_\varepsilon)(x) \leq \| T \|_{L^2(\mathbb{R}^3)} \| f_\varepsilon \|_{L^2}.
\]
Hence, \( \|f_x\|_{L^2}^2 \lesssim \|T\|_{\mathcal{L}(L^2, H^2)}^2 \). Moreover, let \( f_{x,x'} = f_x - f_{x'} \), we have
\[
\|f_x - f_{x'}\|_{L^2}^2 = (Tf_{x,x'})(x) - (Tf_{x,x'})(x') \\
\leq |x - x'|\|Tf_{x,x'}\|_{C^{0,\alpha}} \\
\lesssim \|x - x'|\|Tf_{x,x'}\|_{H^2} \\
\leq |x - x'|\|T\|_{\mathcal{L}(L^2, H^2)} \|f_x - f_{x'}\|_{L^2},
\]
which implies that \( K(x, \cdot) \) as a function from \( x \) to \( f_x \) in \( L^2(\mathbb{R}^3) \) is Hölder continuous with exponent \( \alpha \in [0, 1/2) \). For the case when \( m \geq 3 \), we apply the above argument to the operator \( \nabla^{m-2} T \). Its kernel, \( \nabla^{m-2} K(\cdot, \cdot) \), considered as a function of \( x \) to functions in \( L^2(\mathbb{R}^3) \), is also Hölder continuous
\[
\|\nabla^{m-2} K(x, \cdot)\|_{C^{0,\alpha}(\mathbb{R}^3; L^2(\mathbb{R}^3))} \lesssim \gamma_m \|T\|_{\mathcal{L}(L^2, H^m)}.
\]
Therefore, we have
\[
(6.17) \quad \|K(x, \cdot)\|_{C^{m-2,\alpha}(\mathbb{R}^3; L^2(\mathbb{R}^3))} \lesssim \gamma_m \|T\|_{\mathcal{L}(L^2, H^m)}
\]
with the constant depending only on \( m \).

Define the operator \( \Lambda^s \) acting on functions in the Schwartz class \( \mathcal{S} \) by
\[
(\Lambda^s g)(x) = (2\pi)^{-3/2} \int \hat{g}(k) (1 + |k|^2)^{s/2} e^{ik \cdot x} \, d\xi.
\]
Set \( g = T(\Lambda^m f) \) for \( f \in \mathcal{S} \), then by the Sobolev inequality, \( g \in C^{m-2,\alpha}(\mathbb{R}^3) \), and \( \|g\|_{C^{m-2,\alpha}} = \|T(\Lambda^m f)\|_{C^{m-2,\alpha}} \lesssim \|T(\Lambda^m f)\|_{H^m} \leq \|T\|_{\mathcal{L}(H^{-m}, H^m)} \|f\|_{L^2} \),
\[
\text{where we have used } \|\Lambda^m f\|_{H^{-m}} = \|f\|_{L^2}. \text{ This is equivalent to saying}
\]
\[
\sup_{f \in \mathcal{S}, \|f\|_{L^2} = 1} \left\| \int K(\cdot,y)(\Lambda^m f)(y) \, dy \right\|_{C^{m-2,\alpha}(\mathbb{R}^3)} \leq \gamma_m \|T\|_{\mathcal{L}(H^{-m}, H^m)},
\]
which implies by the dual characterization of the Sobolev space
\[
\|K(\cdot, \cdot)\|_{C^{m-2,\alpha}(\mathbb{R}^3; H^m(\mathbb{R}^3))} \leq \gamma_m \|T\|_{\mathcal{L}(H^{-m}, H^m)}.
\]
Applying again the Sobolev inequality, we have
\[
\|K(\cdot, \cdot)\|_{C^{m-2,\alpha}(\mathbb{R}^3 \times \mathbb{R}^3)} \leq \gamma_m \|T\|_{\mathcal{L}(H^{-m}, H^m)}
\]
with the constant \( \gamma_m \) depending only on \( m \). \( \square \)

**Proposition 6.5.** Assume \( V_\varepsilon \in L^\infty_\varepsilon \). There exists constant \( C \) depending only on \( E_\varepsilon, \|V_\varepsilon\|_{L^\infty} \) and \( \mathcal{C} \), such that
\[
(6.18) \quad \|\chi\nu\|_{L^\infty} \leq C(E_\varepsilon, \|V_\varepsilon\|_{L^\infty}, \mathcal{C}) \|\nu\|_{L^\infty}.
\]

**Proof.** Let
\[
Q_\nu = \frac{1}{2\pi^4} \int_{\mathbb{R}^3} \frac{1}{|\lambda - \mathcal{H}|} \nu \frac{1}{\lambda - \mathcal{H}} \, d\lambda,
\]
\[
Q_{\lambda, \nu} = \frac{1}{\lambda - \mathcal{H}} e^{\lambda - \mathcal{H}} \frac{1}{\lambda - \mathcal{H}}
\]
It is easy to see that for $C$, 
\[ \| (\lambda - H)^{-1} (1 - \Delta) \|_{L^2(L^2)} \leq C(E_g, \| V_\varepsilon \|_{L^\infty}), \]
where the constant depends on $E_g$ and $\| V_\varepsilon \|_{L^\infty}$. Therefore, since $\nu \in L^\infty$, $Q_{\lambda, \nu}$ is a bounded operator from $H^{-2}(\mathbb{R}^3)$ to $H^2(\mathbb{R}^3)$
\[ \| Q_{\lambda, \nu} \|_{L^2(H^{-2}, H^2)} \leq C(E_g, \| V_\varepsilon \|_{L^\infty}) \| \nu \|_{L^\infty}. \]
Furthermore, since $C$ is a compact contour, we have
\[ \| Q_{\nu} \|_{L^2(H^{-2}, H^2)} \leq C(E_g, \| V_\varepsilon \|_{L^\infty}, C) \| \nu \|_{L^\infty}. \]
We conclude using Lemma 6.4 that
\[ \| \nu \|_{L^\infty} \leq C(E_g, \| V_\varepsilon \|_{L^\infty}, C) \| \nu \|_{L^\infty}. \]
Periodicity of $\chi \nu$ is an easy consequence of the invariance of $Q_{\nu}$ under translations with respect to the lattice $n\mathbb{L}$:
\[ \tau R Q_{\nu} = Q_{\nu} \tau R, \quad R \in n\mathbb{L}. \]
Hence,
\[ (\chi \nu)(x + R) = Q_{\nu}(x + R, x + R) = \tau R Q_{\nu} \tau R(x, x) = Q_{\nu}(x, x) = (\chi \nu)(x), \]
for almost every $x \in n\Gamma$.

**Remark.** Notice that the argument of periodicity applies as long as the function $\chi \nu$ is well-defined. Therefore, in the following, we will not repeat this part of the proof.

**Proposition 6.6.** Assume $V_\varepsilon \in L^\infty_n$. There exists a constant $C$ depending only on $E_g$, $\| V_\varepsilon \|_{L^\infty}$ and $C$, such that
\[ (6.19) \quad \| \nu \|_{L^\infty_n} \leq C(E_g, \| V_\varepsilon \|_{L^\infty}, C) \| \nu \|_{L^1_n}. \]

**Proof.** Let us first consider $\nu \in L^1_n \cap L^\infty_n$. Then $Q_{\nu}$ is a bounded operator on $L^2$. Taking the Bloch decomposition of $Q_{\nu}$ with respect to the lattice $n\mathbb{L}$ [22], we obtain
\[ Q_{\nu} = \int_{\Gamma^*/n} (Q_{\nu})_\xi d\xi. \]
For $\xi \in \Gamma^*/n$, the operator $(Q_{\nu})_\xi$ is given by
\[ (Q_{\nu})_\xi = \frac{1}{2\pi i} \int_{\mathbb{C}} (Q_{\lambda, \nu})_\xi \lambda d\lambda = \frac{1}{2\pi i} \int_{\mathbb{C}} \frac{1}{\lambda - \mathcal{H}_\xi} \nu \frac{1}{\lambda - \mathcal{H}_\xi} d\lambda. \]
Here $\mathcal{H}_\xi$ is the Bloch decomposition of $\mathcal{H}$ with respect to the lattice $n\mathbb{L}$ (note that $\mathcal{H}$ is invariant under translations by assumption):
\[ \mathcal{H} = \int_{\Gamma^*/n} \mathcal{H}_\xi d\xi. \]
Since $\text{spec}(\mathcal{H}_\xi) \subset \text{spec}(\mathcal{H})$, the gap of $\mathcal{H}_\xi$ is no smaller than $E_g$. 

Write
\[ (Q_{\lambda, \nu})_\xi = \frac{1}{\lambda - \mathcal{H}_\xi} (1 - \Delta_\xi)(1 - \Delta_\xi)^{-1} \nu (1 - \Delta_\xi)^{-1} (1 - \Delta_\xi)^{-1} \frac{1}{\lambda - \mathcal{H}_\xi}. \]

Note that we have
\[ (6.20) \| f(x) g(-i\nabla_\xi) \|_{\mathcal{O}_{p}(L^2_\mathbb{Z})} \lesssim \| f \|_{L^p_\mathbb{Z}} \| g \|_{p(L^\mathbb{Z}/n)}, \]

where
\[ \| g \|_{p(L^\mathbb{Z}/n)} = \left( \sum_{k \in L^p} |g(k/n)|^p \right)^{1/p}. \]

This is the periodic version of [23, Theorem 4.1], and follows easily by adapting the proof there to the periodic case. Using (6.20), we conclude that the operator
\[ (1 - \Delta_\xi)^{-1} \nu (1 - \Delta_\xi)^{-1} \]
is in trace class, and
\[ \| (1 - \Delta_\xi)^{-1} \nu (1 - \Delta_\xi)^{-1} \|_{\mathcal{O}_{1}(L^2_\mathbb{Z})} \leq \| (1 - \Delta_\xi)^{-1} \nu \|_{1/2}^2 \|_{\mathcal{O}_{2}(L^2_\mathbb{Z})} \]
\[ \lesssim \| \nu \|_{1/2}^2 \|_{L^2_\mathbb{Z}} = \| \nu \|_{L^1_\mathbb{Z}}. \]

Therefore, since the operators \((\lambda - \mathcal{H}_\xi)^{-1} (1 - \Delta_\xi)\) and \((1 - \Delta_\xi)(\lambda - \mathcal{H}_\xi)^{-1}\) are bounded, we obtain
\[ \| (Q_{\lambda, \nu})_\xi \|_{\mathcal{O}_{1}(L^2_\mathbb{Z})} \leq C \| \nu \|_{L^1_\mathbb{Z}}. \]

Since the contour is compact, we have
\[ \| (Q_{\nu})_\xi \|_{\mathcal{O}_{1}(L^2_\mathbb{Z})} \leq C \| \nu \|_{L^1_\mathbb{Z}}, \]

where the constant is independent of \(n\) or \(\xi\). Therefore, the diagonal of the kernel of the operator \((Q_{\nu})_\xi\) is well-defined. Now,
\[ Q_{\nu}(x, x) = \int_{\Gamma \Gamma / n} (Q_{\nu})_\xi(x, x) \, d\xi, \quad x \in n\Gamma, \]
is well-defined since for each \(\xi\), \((Q_{\nu})_\xi\) is trace class. Moreover, we have the estimates
\[ \| \chi \nu \|_{L^1_\mathbb{Z}(\mathbb{R}^3)} = \| Q_{\nu}(x, x) \|_{L^1(n\Gamma)} \leq \sup_{\xi \in \Gamma \Gamma / n} \| (Q_{\nu})_\xi \|_{\mathcal{O}_{1}(L^2(n\Gamma))} \]
\[ \leq C \| \nu \|_{L^1_\mathbb{Z}(\mathbb{R}^3)}. \]

The desired result follows since \(L^1_\mathbb{Z} \cap L^\infty_\mathbb{Z}\) is dense in \(L^1_\mathbb{Z}\).

\[ \square \]

From Propositions 6.5 and 6.6, using interpolation, we have

**Corollary 6.7.** Assume \(V_\varepsilon \in L^\infty_\mathbb{Z}\). There exists constant \(C\) depending only on \(E_g\), \(\| V_\varepsilon \|_{L^\infty} \) and \(\mathcal{E}\), such that
\[ (6.21) \| \chi \nu \|_{L^1_\mathbb{Z}} \leq C(E_g, \| V_\varepsilon \|_{L^\infty}, \mathcal{E}) \| \nu \|_{L^1_\mathbb{Z}}. \]

The derivatives of \(\chi \nu\) can also be controlled, if \(V_\varepsilon\) has additional regularity:
Proposition 6.8. Assume $V_\varepsilon \in W_{n,\infty}^m$ for some $m \geq 0$. There exists constant $C$ depending only on $E_g$, $\|V_\varepsilon\|_{W_{n,\infty}^m}$ and $\mathcal{C}$, such that

$$
\|\chi \nu\|_{H_n^m} \leq C(E_g, \|V_\varepsilon\|_{W_{n,\infty}^m}, \mathcal{C})\|\nu\|_{H_n^m}.
$$

Proof. The case $m = 0$ is proved in Corollary 6.7. Let us assume $m \geq 1$. Observe that

$$
\nabla (\chi \nu)(x) = (\nabla Q_\nu)(x, x) - (Q_\nu \nabla)(x, x),
$$

where the terms on the right hand side mean the diagonal part of the kernel of the operators $\nabla Q_\nu$ and $Q_\nu \nabla$ respectively. Furthermore notice that

$$
\nabla Q_\lambda \nu - Q_\lambda \nu \nabla = \left[\nabla, \frac{1}{\lambda - \mathcal{H}}\right] \nu \frac{1}{\lambda - \mathcal{H}} + \frac{1}{\lambda - \mathcal{H}} (\nabla \nu) \frac{1}{\lambda - \mathcal{H}} + \frac{1}{\lambda - \mathcal{H}} \nu \left[\nabla, \frac{1}{\lambda - \mathcal{H}}\right].
$$

For the second term, notice that $\nabla \nu$ is a $H_n^{m-1}$ function (as $\nu$ is in $H_n^m$), by Corollary 6.7, the second term gives a $L_2^n$ function with the desired bound. The analysis for the first and third terms are the same. Therefore we only consider the first term. We have

$$
\left[\nabla, \frac{1}{\lambda - \mathcal{H}}\right] \nu \frac{1}{\lambda - \mathcal{H}} = \frac{1}{\lambda - \mathcal{H}} (\nabla V_\varepsilon) \frac{1}{\lambda - \mathcal{H}} \nu \frac{1}{\lambda - \mathcal{H}}.
$$

Consider the right hand side as an operator

$$
(\chi_1 \nu)(x) = \left(\frac{1}{\lambda - \mathcal{H}} (\nabla V_\varepsilon) \frac{1}{\lambda - \mathcal{H}} \nu \frac{1}{\lambda - \mathcal{H}}\right)(x, x).
$$

Using the similar techniques as in the proof of Propositions 6.5, 6.6, and the fact that

$$
\|((\lambda - \mathcal{H})^{-1}(\nabla V_\varepsilon))\|_{L^2} \leq \|((\lambda - \mathcal{H})^{-1})\|_{L^2} \|\nabla V_\varepsilon\|_{L^\infty} \lesssim E_g \|V_\varepsilon\|_{W_{1,\infty}^1},
$$

we conclude that $\chi_1$ is a bounded operator on $L_2^n$. Therefore, we have

$$
\|\nabla (\chi \nu)\|_{L_2^n} \leq C(E_g, \|V_\varepsilon\|_{W_{1,\infty}^1}, \mathcal{C})\|\nu\|_{H_1^n}.
$$

The argument is analogous for the higher order derivatives, and we obtain

$$
\|\chi \nu\|_{H_n^m(\mathbb{R}^3)} \leq C(E_g, \|V_\varepsilon\|_{W_{n,\infty}^m}, \mathcal{C})\|\nu\|_{H_n^m(\mathbb{R}^3)}.
$$

□

Proposition 6.9. Assume $V_\varepsilon \in L_{n,\infty}^\infty$. There exists constant $C$ depending only on $E_g$, $\|V_\varepsilon\|_{W_{n,\infty}^m}$ and $\mathcal{C}$, such that

$$
\|\chi \nu\|_{H_n^{m-1}} \leq C(E_g, \|V_\varepsilon\|_{L^\infty}, \mathcal{C})\|\nabla \nu\|_{L_2^n(\mathbb{R}^3)}.
$$
Proof. Consider the Bloch decomposition of the operator $Q_\nu$ with respect to the lattice $nL$:  

\[ Q_\nu = \int_{\Gamma^n/\nu} (Q_\nu)_{\xi} \, d\xi, \]

\[ (Q_\nu)_{\xi} = \frac{1}{2\pi i} \int_{C} \frac{1}{\lambda - \mathcal{H}_\xi} \nu \frac{1}{\lambda - \mathcal{H}_\xi} \, d\lambda, \]

where $\mathcal{H}_\xi$ is the Bloch decomposition of $\mathcal{H}$ with respect to the lattice $nL$ (by assumption, $\mathcal{H}$ is invariant under translations of the lattice vectors in $nL$). Assume for the moment that the following holds: For each $\xi \in \Gamma^n/\nu$, define $\rho_\xi$ by $\rho_\xi(x) = (Q_\nu)_{\xi}(x,x)$. $\rho_\xi$ is well-defined as a function in $\mathcal{H}^{-1}(\mathbb{R}^3)$, with the estimate

\[ \|\rho_\xi\|_{\mathcal{H}^{-1}} \leq C(E_g, \|V_c\|_{L^\infty}, \mathcal{C}) \|\nu\|_{\mathcal{H}^1}. \]

Then since

\[ \tilde{\chi}_\nu(k) = \int_{\Gamma^n/\nu} \rho_\xi(k) \, d\xi, \]

using Minkowski inequality, we have

\[ \left( \sum_{k \in \Lambda \cap \Gamma^n/\nu} \frac{1}{|k|^2} |\tilde{\chi}_\nu(k)|^2 \right)^{1/2} \leq \int_{\Gamma^n/\nu} \left( \sum_{k \in \Lambda \cap \Gamma^n/\nu} \frac{1}{|k|^2} |\tilde{\rho}_\xi(k)|^2 \right)^{1/2} \, d\xi \]

\[ \leq \int_{\Gamma^n/\nu} \|\rho_\xi\|_{\mathcal{H}^{-1}(\mathbb{R}^3)} \, d\xi \]

\[ \leq C(E_g, \|V_c\|_{L^\infty}, \mathcal{C}) \|\nu\|_{\mathcal{H}^1(\mathbb{R}^3)}. \]

We then obtain

\[ \|\chi_\nu\|_{\mathcal{H}^{-1}(\mathbb{R}^3)} \leq C(E_g, \|V_c\|_{L^\infty}, \mathcal{C}) \|\nu\|_{\mathcal{H}^1(\mathbb{R}^3)}. \]

Therefore, it suffices to prove (6.24).

Consider the Bloch wave decomposition for the density matrix

\[ \mathcal{P} = \frac{1}{2\pi i} \int_{C} \frac{1}{\lambda - \mathcal{H}} \, d\lambda = \int_{\Gamma^n/\nu} \frac{1}{2\pi i} \int_{C} \frac{1}{\lambda - \mathcal{H}_\xi} \, d\lambda \, d\xi = \int_{\Gamma^n/\nu} \mathcal{P}_\xi \, d\xi. \]

The operator $\mathcal{P}_\xi$ as defined by the last equality is an orthogonal projection on $L^2_\xi(n\Gamma)$. Following [4, 5], let us introduce the spaces

\[ \mathcal{H}_\xi = \mathcal{H}_{1,\nu}(L^2_\xi(n\Gamma)) = \{ Q_\xi \in \mathcal{H}_2(L^2_\xi(n\Gamma)) \mid Q_\xi^{-}, Q_\xi^{++} \in \mathcal{H}_1(L^2_\xi(n\Gamma)) \}. \]

\[ \mathcal{Q}_\xi = \{ Q_\xi \in \mathcal{H}_\xi \mid Q_\xi = Q_\xi; |\nabla|Q_\xi \in \mathcal{H}_2(L^2_\xi(n\Gamma)) \}; \]

\[ |\nabla|Q_\xi^{-}|\nabla|, |\nabla|Q_\xi^{++}|\nabla| \in \mathcal{H}_1(L^2_\xi(n\Gamma))). \]
The space $\mathcal{D}_\xi$ is endowed with its natural norm

$$
\|Q_\xi\|_{\mathcal{D}_\xi} = \|Q_\xi\|_{\mathcal{D}_2} + \|Q_\xi^-\|_{\mathcal{D}_1} + \|Q_\xi^+\|_{\mathcal{D}_1}
+ \|\nabla|Q_\xi|\|_{\mathcal{D}_2} + \|\nabla|Q_\xi^-|\|_{\mathcal{D}_1} + \|\nabla|Q_\xi^+|\|_{\mathcal{D}_1}.
$$

Here we have introduced the shorthand notations

$$
Q_\xi^- = p_\xi Q_\xi p_\xi, \quad Q_\xi^+ = p_\xi Q_\xi p_\xi^+, \\
Q_\xi^{+-} = p_\xi Q_\xi p_\xi^{++}, \quad Q_\xi^{++} = p_\xi^+ Q_\xi p_\xi^+,
$$

where $p_\xi^+ = 1 - p_\xi$. Notice that the meaning of the shorthand notations depends on $\xi$. Operators in $\mathcal{D}_\xi$ can be associated with a generalized trace

$$
\text{tr}_\xi(Q_\xi) = \text{tr}(Q_\xi^-) + \text{tr}(Q_\xi^+).
$$

The following lemma is an adaptation of [4, Proposition 1] to the periodic case, and can be proved using essentially the same argument.

**Lemma 6.10.** Assume that $Q_\xi \in \mathcal{D}_\xi$. Then for any $\nu \in \dot{H}^1_0(\mathbb{R}^3)$, we have $Q_\xi \nu \in \mathcal{S}_1^\dagger$, and

$$
|\text{tr}_\xi(Q_\xi \nu)| \lesssim \|Q_\xi\|_{\mathcal{D}_\xi} \|\nu\|_{\dot{H}^1_0}.
$$

with constant independent of $n$ and $\xi$. Thus, there exists a uniquely defined function $\rho_{Q_\xi} \in \dot{H}^{-1}_n(\mathbb{R}^3)$ such that

$$
\langle \rho_{Q_\xi}, \nu \rangle_{\dot{H}^{-1}_n, \dot{H}^1_0} = \text{tr}(Q_\xi \nu),
$$

for every $\nu \in \dot{H}^1_0(\mathbb{R}^3)$. The linear map from $Q_\xi \in \mathcal{D}_\xi$ to $\rho_{Q_\xi} \in \dot{H}^{-1}_n(\mathbb{R}^3)$ is bounded

$$
\|\rho_{Q_\xi}\|_{\dot{H}^{-1}_n} \lesssim \|Q_\xi\|_{\mathcal{D}_\xi}.
$$

Using Lemma 6.10, we have

$$
\|\rho_\xi\|_{\dot{H}^{-1}_n} = \|\rho_{Q_\xi}\|_{\dot{H}^{-1}_n} \lesssim \|Q_\xi\|_{\mathcal{D}_\xi}.
$$

Hence, to show (6.24), it suffices to bound $\|\rho_{Q_\xi}\|_{\mathcal{D}_\xi}$. One can easily check that $(Q_\nu)^{-+} = 0$ and $(Q_\nu)^{+-} = 0$. The argument for $(Q_\nu)^{-+}$ and $(Q_\nu)^{+-}$ is the same and we only consider the former.

$$
(Q_\nu)^{-+} = \frac{1}{2\pi i} \int_{\mathbb{C}} \frac{1}{\lambda - H_\xi} \rho_\xi \frac{1}{\lambda - H_\xi} d\lambda = \frac{1}{2\pi i} \int_{\mathbb{C}} \frac{1}{\lambda - H_\xi} \rho_\xi \rho_\xi^+ \frac{1}{\lambda - H_\xi} d\lambda = \frac{1}{2\pi i} \int_{\mathbb{C}} \frac{1}{\lambda - H_\xi} \rho_\xi \rho_\xi^+ \frac{1}{\lambda - H_\xi} d\lambda.
$$

since

$$
\rho_\xi[\rho_\xi, \nu] \rho_\xi^+ = \rho_\xi \rho_\xi^+ \rho_\xi^+ - \rho_\xi \rho_\xi^+ \rho_\xi^+ = \rho_\xi \rho_\xi^+.
$$
Putting in the expression of $P$, we have

\[
\left[ P, \nu \right] = \frac{1}{2\pi i} \int_{\mathcal{C}} \left( \frac{1}{\lambda - H_{\xi}} \nu - \nu \frac{1}{\lambda - H_{\xi}} \right) \, d\lambda
\]

\[
= \frac{1}{2\pi i} \int_{\mathcal{C}} \frac{1}{\lambda - H_{\xi}} \left[ H_{\xi}, \nu \right] \frac{1}{\lambda - H_{\xi}} \, d\lambda
\]

\[
= \frac{1}{2\pi i} \int_{\mathcal{C}} \frac{1}{\lambda - H_{\xi}} \left[ -\Delta, \nu \right] \frac{1}{\lambda - H_{\xi}} \, d\lambda
\]

\[
= \sum_{j=1}^{3} \frac{1}{2\pi i} \int_{\mathcal{C}} \frac{1}{\lambda - H_{\xi}} \frac{\partial \nu}{\partial x_j} \frac{1}{\lambda - H_{\xi}} \, d\lambda
\]

Consider the first term (the argument for the other term is similar)

\[
\frac{1}{\lambda - H_{\xi}} \frac{\partial \nu}{\partial x_j} \frac{1}{\lambda - H_{\xi}}.
\]

Since $\|(\lambda - H_{\xi})^{-1}(1 - \Delta)\|$ and $\|(1 - \Delta)(\lambda - H_{\xi})^{-1}\|$ are bounded by a constant that depends only on $E_g$ and the $L^\infty$ norm of the potential in the Hamiltonian, it suffices to consider

\[
(1 - \Delta_{\xi})^{-1} \frac{\partial \nu}{\partial x_j} (1 - \Delta_{\xi})^{-1}.
\]

Since $(1 - \Delta_{\xi})^{-1} \frac{\partial \nu}{\partial x_j}$ is bounded, we have

\[
\left\| \frac{1}{\lambda - H_{\xi}} \frac{\partial \nu}{\partial x_j} \frac{1}{\lambda - H_{\xi}} \right\|_{L^2(\mathbb{R}^3)} \leq C(E_g, \| V_c \|_{L^\infty}) \|(1 - \Delta_{\xi})^{-1}\|_{L^2(\mathbb{R}^3)}
\]

\[
\leq C(E_g, \| V_c \|_{L^\infty}) \| \nabla \nu \|_{L^2(\mathbb{R}^3)^3}
\]

\[
= C(E_g, \| V_c \|_{L^\infty}) \| \nu \|_{H^1(\mathbb{R}^3)}
\]

where we have used the inequality (6.20). Hence, we have

\[
\| [P, \nu] \|_{L^2(\mathbb{R}^3)} \leq C(E_g, \| V_c \|_{L^\infty}, \mathcal{C}) \| \nu \|_{H^1(\mathbb{R}^3)},
\]

with constant independent of $n$ and $\xi$. Therefore,

\[
\| (Q_{\nu})_{\xi}^{-\top} \|_{L^2(\mathbb{R}^3)} \| \nabla [(Q_{\nu})_{\xi}^{-\top}] \|_{L^2(\mathbb{R}^3)} \leq C(E_g, \| V_c \|_{L^\infty}, \mathcal{C}) \| \nu \|_{H^1(\mathbb{R}^3)}.
\]

We conclude using Lemma 6.10.

\[\square\]

We prove the following lemma used below in the proof of Corollary 6.12.

**Lemma 6.11.** Let $A, B$ be self-adjoint operators on a Hilbert space $\mathcal{H}$. Assume that $B$ is positive and bounded, and $ABA$ is bounded. Then $AB$ and $BA$ are bounded, and we have

\[
\| AB \| \leq \| B \|^{1/2} \| ABA \|^{1/2}, \quad \| BA \| \leq \| B \|^{1/2} \| ABA \|^{1/2}.
\]
Proof. Denote the square root of the positive operator $B$ as $B^{1/2}$. For $f, g \in \mathcal{H}$, we have
\[
\langle f, BA g \rangle = \langle B^{1/2} f, B^{1/2} A g \rangle \leq \langle B^{1/2} f, B^{1/2} f \rangle^{1/2} \langle B^{1/2} A g, B^{1/2} A g \rangle^{1/2} \leq \langle f, B f \rangle^{1/2} \langle A B A g, A B A g \rangle^{1/2} \leq \|B\|^{1/2} \|A B A\|^{1/2} \|f\| \|g\|.
\]
Therefore
\[
\|B A\| \leq \|B\|^{1/2} \|A B A\|^{1/2}.
\]
The argument for $A B$ is analogous. \hfill \Box

**Corollary 6.12.** Assume $V \in L_n^\infty$. There exists constant $C$ depending only on $E_g, \|V\|_{L^\infty}$ and $\mathcal{C}$, such that
\[
(6.31) \quad \|\chi \nu\|_{H_n^{-1}} \leq C(E_g, \|V\|_{L^\infty}, \mathcal{C}) \|\nu\|_{L_n^2}.
\]

Proof. $\chi$ is a bounded operator from $\dot{H}_n^1(\mathbb{R}^3)$ to $\dot{H}_n^{-1}(\mathbb{R}^3)$ if and only if $\phi^{1/2} \chi \phi^{1/2}$ is a bounded operator on $L_n^2(\mathbb{R}^3)$. Here $\phi$ is the Coulomb operator from $\dot{H}_n^{-1}$ to $\dot{H}_n^1$. $\chi$ is also a bounded operator on $L_n^2(\mathbb{R}^3)$. In addition, it is also easy to see that $\chi$ is a negative self-adjoint operator.

Therefore, by Lemma 6.11 (applied to $-\chi$ and $-\phi^{1/2} \chi \phi^{1/2}$), $\phi^{1/2} \chi$ is a bounded operator from $L^2(\mathbb{R}^3)$ to $L^2(\mathbb{R}^3)$, which is equivalent to saying that $\chi$ is a bounded operator from $L_n^2(\mathbb{R}^3)$ to $\dot{H}_n^{-1}(\mathbb{R}^3)$. \hfill \Box

**Proposition 6.13.** Assume $V \in W_n^{1,\infty}$ for some $m \geq 0$. There exists constant $C$ depending only on $E_g, \|V\|_{W_n^{1,\infty}}$ and $\mathcal{C}$, such that
\[
(6.32) \quad \|\chi \nu\|_{H_{\nu}^{-\infty}(\mathbb{R}^3)} \leq C(E_g, \|V\|_{W_n^{1,\infty}}, \mathcal{C}) \|\nabla \nu\|_{H_{\nu}^{-\infty}(\mathbb{R}^3)}.
\]

Proof. Using the spectral projection $\mathcal{P}$ and $\mathcal{P}^\perp = \mathcal{I} - \mathcal{P}$, we have
\[
Q_\nu = \frac{1}{2\pi i} \int_{\mathcal{C}} \frac{1}{\lambda - \mathcal{H}} \nu \frac{1}{\lambda - \mathcal{H}} d\lambda
= \frac{1}{2\pi i} \int_{\mathcal{C}} \mathcal{P} \frac{1}{\lambda - \mathcal{H}} \nu \frac{1}{\lambda - \mathcal{H}} \mathcal{P}^\perp d\lambda
+ \frac{1}{2\pi i} \int_{\mathcal{C}} \mathcal{P}^\perp \frac{1}{\lambda - \mathcal{H}} \nu \frac{1}{\lambda - \mathcal{H}} \mathcal{P} d\lambda
= Q_\nu^+ + Q_\nu^-.
\]
Here we have used the shorthand notation $Q_\nu^+ = \mathcal{P} Q_\nu \mathcal{P}^\perp$ and $Q_\nu^- = \mathcal{P}^\perp Q_\nu \mathcal{P}$.

Since $\mathcal{P}$ commutes with $(\lambda - \mathcal{H})^{-1}$, we have
\[
Q_\nu^+ = \frac{1}{2\pi i} \int_{\mathcal{C}} \frac{1}{\lambda - \mathcal{H}} [\mathcal{P}, \nu] \mathcal{P}^\perp \frac{1}{\lambda - \mathcal{H}} d\lambda.
\]
Substituting into the expression of \([P, \nu]\), we obtain
\[
Q^{-}_\nu = \frac{1}{4\pi^2} \iint_{\mathcal{E} \times \mathcal{E}} \frac{1}{\lambda - \mathcal{H}_{\mu - \mathcal{H}}} \left[ -\Delta, \nu \right] \frac{1}{\mu - \mathcal{H}} \mathcal{P} \frac{1}{\lambda - \mathcal{H}} \mathrm{d}\mu \mathrm{d}\lambda
\]
\[
= -\frac{1}{4\pi^2} \iint_{\mathcal{E} \times \mathcal{E}} \frac{1}{\lambda - \mathcal{H}_{\mu - \mathcal{H}}} \nabla \nu \cdot \nabla \frac{1}{\mu - \mathcal{H}} \mathcal{P} \frac{1}{\lambda - \mathcal{H}} \mathrm{d}\mu \mathrm{d}\lambda
\]
\[
- \frac{1}{4\pi^2} \iint_{\mathcal{E} \times \mathcal{E}} \frac{1}{\lambda - \mathcal{H}_{\mu - \mathcal{H}}} \nabla \cdot \nabla \frac{1}{\mu - \mathcal{H}} \mathcal{P} \frac{1}{\lambda - \mathcal{H}} \mathrm{d}\mu \mathrm{d}\lambda.
\]
Let us consider the first term on the right hand side. Take the \(x_1\) component (other components follow the same argument)
\[
\frac{1}{4\pi^2} \iint_{\mathcal{E} \times \mathcal{E}} \frac{1}{\lambda - \mathcal{H}_{\mu - \mathcal{H}}} \partial_{x_1} \nu \partial_{x_1} \frac{1}{\mu - \mathcal{H}} \mathcal{P} \frac{1}{\lambda - \mathcal{H}} \mathrm{d}\mu \mathrm{d}\lambda.
\]
Define the operator \(\chi'\) by
\[
(\chi'(W))(x) = \frac{1}{4\pi^2} \iint_{\mathcal{E} \times \mathcal{E}} \frac{1}{\lambda - \mathcal{H}_{\mu - \mathcal{H}}} \partial_{x_1} \nu \partial_{x_1} \frac{1}{\mu - \mathcal{H}} \mathcal{P} \frac{1}{\lambda - \mathcal{H}} \mathrm{d}\mu \mathrm{d}\lambda.
\]
Notice that \(\chi'\) is quite similar to the original operator \(\chi\). Indeed, it is not hard to see that using the similar argument as in the proof of Proposition 6.8, we can obtain
\[
\|\chi' W\|_{H^m_\mu} \leq C(E_g, \|V\|_{W^{m,\infty}_\mu}, \mathcal{E}) \|W\|_{H^m_\mu}.
\]
Replacing \(W\) by \(\partial_{x_1} \nu\) and using similar considerations for the other terms in the expression of \(Q_\nu\), we arrive at
\[
\|\chi \nu\|_{H^m_\mu} \leq C(E_g, \|V\|_{W^{m,\infty}_\mu}, \mathcal{E}) \|\nabla \nu\|_{H^m_\mu}.
\]

6.3. Regularity of \((\mathcal{I} - \mathcal{L}_c)^{-1}\). The stability Assumption B guarantees that \((\mathcal{I} - \mathcal{L}_c)^{-1}\) is a bounded operator on \(H^2_{\text{per},0}\), where
\[
H^m_{\text{per},0} = \{ f \in \mathcal{S}'(\mathbb{R}^3) \mid \tau_R f = f, \forall R \in \mathbb{L}, f \in H^m(\Gamma); \int_{\Gamma} f \, dx = 0 \},
\]
for any non-negative integer \(m\). Note that it is easy to see that the norm associated with \(H^m_{\text{per},0}\) is equivalent to the norm of \(H^m_1 \cap H^1_{\text{per}}\), the spaces of periodic function with period 1.

Let us first prove the lemma on the commutator \([\nabla, \mathcal{L}_c]\), which will be used below in the proof of Proposition 6.15.

Lemma 6.14. \([\nabla, \mathcal{L}_c]\) is a bounded operator on \(H^m_{\text{per},0}\) for any integer \(m \geq 2\).

Proof. Note that \(\mathcal{L}_c = \chi_c V_c\), where
\[
(\chi_c V_c)(x) = \frac{1}{2\pi i} \int_{\mathcal{E}} \frac{1}{\lambda - \mathcal{H}_c} V_c \frac{1}{\lambda - \mathcal{H}_c} \mathrm{d}\lambda(x, x),
\]
and
\[
\begin{align*}
\mathcal{V}_e w(z) &= \phi(z) + \eta(z); \\
-\Delta \phi(z) &= 4\pi w(z), \quad \text{with} \quad \langle \phi(\cdot) \rangle = 0; \\
\eta(z) &= \eta'(\rho_e(z)) w(z).
\end{align*}
\]
It follows that
\[
[\nabla, \mathcal{L}_e] = [\nabla, \chi_e] \mathcal{V}_e + \chi_e [\nabla, \mathcal{V}_e].
\]
We first study the commutator $[\nabla, \mathcal{V}_e]$. By the definition of $\mathcal{V}_e$, it is easy to see that
\[
([\nabla, \mathcal{V}_e] w)(z) = (\nabla \mathcal{V}_e w)(z) - (\mathcal{V}_e (\nabla w))(z) = \nabla_z (\eta'(\rho_e(z))) w(z).
\]
By the smoothness of $\rho_e$ and $\eta$, we get
\[
\| [\nabla, \mathcal{V}_e] w \|_{H^m_{\text{per}}} \lesssim \| w \|_{H^m_{\text{per}}}.
\]
Then, using Proposition 6.8, we obtain
\[
\| \chi_e [\nabla, \mathcal{V}_e] w \|_{H^m_{\text{per}}} \lesssim \| w \|_{H^m_{\text{per}}}.
\]
Next, consider the term $[\nabla, \chi_e] \mathcal{V}_e$. We have
\[
([\nabla, \chi_e] \mathcal{V})(x) = \nabla (\chi_e \mathcal{V})(x) - \chi_e (\nabla \mathcal{V})(x)
\]
\[
= \frac{1}{2\pi i} \int_{\mathcal{E}} \left[ \nabla, \frac{1}{\lambda - \mathcal{H}_e} \right] V \frac{1}{\lambda - \mathcal{H}_e} \, d\lambda(x, x)
\]
\[
+ \frac{1}{2\pi i} \int_{\mathcal{E}} \frac{1}{\lambda - \mathcal{H}_e} \left[ \nabla, \frac{1}{\lambda - \mathcal{H}_e} \right] V \, d\lambda(x, x).
\]
Notice that since $\mathcal{H}_e = -\Delta + \mathcal{V}_e$, we have
\[
\left[ \nabla, \frac{1}{\lambda - \mathcal{H}_e} \right] = \frac{1}{\lambda - \mathcal{H}_e} (\nabla \mathcal{V}_e) \frac{1}{\lambda - \mathcal{H}_e}.
\]
Define $\chi_1$ to be the operator
\[
(\chi_1 \mathcal{V})(x) = \frac{1}{2\pi i} \int_{\mathcal{E}} \frac{1}{\lambda - \mathcal{H}_e} (\nabla \mathcal{V}_e) \frac{1}{\lambda - \mathcal{H}_e} V \frac{1}{\lambda - \mathcal{H}_e} \, d\lambda(x, x).
\]
Then, using the similar argument as in the proof of Proposition 6.8 and Proposition 6.13, we have
\[
\| \chi_1 \mathcal{V} \|_{H^m_{\text{per},0}} \leq C(E_g, \mathcal{V}_e, \mathcal{E}) \| \mathcal{V} \|_{H^{m+1}_{\text{per}} + H^m_{\text{per}}},
\]
Therefore similar estimate for $[\nabla, \chi_e]$ also holds. Now the lemma follows from the fact that
\[
\| \mathcal{V}_e w \|_{H^{m+1}_{\text{per}} + H^m_{\text{per}}} \lesssim \| w \|_{H^m_{\text{per},0}},
\]
and
\[
\| [\nabla, \chi] \mathcal{V}_e w \|_{H^m_{\text{per}}} \lesssim \| w \|_{H^m_{\text{per}}}.
\]

We can then prove the main results of this subsection:
Proposition 6.15. \((\mathcal{I} - \mathcal{L}_c)^{-1}\) is a bounded operator on \(H^m_{\text{per}, 0}\) for any integer \(m \geq 2\).

Proof. We will use induction. Suppose \((\mathcal{I} - \mathcal{L}_c)^{-1}\) is bounded on \(H^{m-1}_{\text{per}, 0}\) with norm \(M_{m-1}\), let us show its boundedness on \(H^m_{\text{per}, 0}\). For any \(w \in H^m_{\text{per}, 0}\), we want to control

\[\| (\mathcal{I} - \mathcal{L}_c)^{-1} w \|_{H^m_{\text{per}, 0}}.\]

By assumption, we already have

\[\| (\mathcal{I} - \mathcal{L}_c)^{-1} w \|_{H^{m-1}_{\text{per}, 0}} \leq M_{m-1} \| w \|_{H^{m-1}_{\text{per}, 0}} \leq M_{m-1} \| w \|_{H^m_{\text{per}, 0}}.\]

Hence, it suffices to consider

\[\| \nabla (\mathcal{I} - \mathcal{L}_c)^{-1} w \|_{H^{m-1}_{\text{per}, 0}}.\]

Using the commutator identities

\[\nabla (\mathcal{I} - \mathcal{L}_c)^{-1} = (\mathcal{I} - \mathcal{L}_c)^{-1} \nabla + [\nabla, (\mathcal{I} - \mathcal{L}_c)^{-1}];\]

\[[\nabla, (\mathcal{I} - \mathcal{L}_c)^{-1}] = (\mathcal{I} - \mathcal{L}_c)^{-1} [\nabla, \mathcal{L}_c](\mathcal{I} - \mathcal{L}_c)^{-1},\]

we arrive at

\[\| \nabla (\mathcal{I} - \mathcal{L}_c)^{-1} w \|_{H^{m-1}_{\text{per}, 0}} \leq \| (\mathcal{I} - \mathcal{L}_c)^{-1} \nabla w \|_{H^{m-1}_{\text{per}, 0}} + \| [\nabla, (\mathcal{I} - \mathcal{L}_c)^{-1}] w \|_{H^{m-1}_{\text{per}, 0}}\]

\[\leq M_{m-1} \| \nabla w \|_{H^{m-1}_{\text{per}, 0}} + M^2_{m-1} \| [\nabla, \mathcal{L}_c]\|_{L^2(H^{m-1}_{\text{per}, 0})} \| w \|_{H^{m-1}_{\text{per}, 0}}.\]

The conclusion follows from the boundedness of the commutator \([\nabla, \mathcal{L}_c]\), which is guaranteed by the Lemma 6.14.

\(\square\)

6.4. Comparison of two linearized Kohn-Sham operators. In the proof of Theorem 5.1, we will need to compare two linearized Kohn-Sham operators. This subsection is devoted to the technical results that will be used.

Consider two \(\chi\) operators corresponding to different Hamiltonians:

\[(\chi \nu)(x) = \frac{1}{2\pi i} \int_{\mathbb{R}} \frac{1}{\lambda - H} \nu \frac{1}{\lambda - \tilde{H}} \, d\lambda(x, x);\]

\[(\tilde{\chi} \nu)(x) = \frac{1}{2\pi i} \int_{\mathbb{R}} \frac{1}{\lambda - \tilde{H}} \nu \frac{1}{\lambda - H} \, d\lambda(x, x).\]

with

\[H = -a_{ij}(x) \partial_i \partial_j + V_c,\]

\[\tilde{H} = -\tilde{a}_{ij}(x) \partial_i \partial_j + \tilde{V}_c.\]

We assume that the two Hamiltonians correspond to insulators with gap bigger than \(E_g\), the estimates below are in terms of the difference between \(a\) and \(\tilde{a}\), and between \(V_c\) and \(\tilde{V}_c\). The constants below depend on \(E_g\).

We will prove the following result:
Proposition 6.16. For $V_\varepsilon, \hat{V}_\varepsilon \in W^{2,\infty}_n + H^2_n$, we have
\begin{equation}
\| \chi - \hat{x} \|_{L^2(H^1_n, H^{-1}_n, n)} \lesssim \| a - \tilde{a} \|_{W^{2,\infty}} + \| V_\varepsilon - \hat{V}_\varepsilon \|_{W^{2,\infty}_n + H^2_n}.
\end{equation}

This follows from the following lemmas.

Lemma 6.17. For $V_\varepsilon, \hat{V}_\varepsilon \in L^\infty_n$, we have
\begin{equation}
\| \chi - \hat{x} \|_{L^2(H^1_n, H^{-1}_n)} \lesssim \| a - \tilde{a} \|_{L^\infty} + \| V_\varepsilon - \hat{V}_\varepsilon \|_{L^\infty}.
\end{equation}

Proof. As before, let us consider the Bloch decomposition of the operators
\[
Q = \frac{1}{2\pi i} \int_\theta \frac{1}{\lambda - H} \frac{1}{\lambda - \hat{H}} \, d\lambda;
\]
\[
\hat{Q} = \frac{1}{2\pi i} \int_\theta \frac{1}{\lambda - \hat{H}} \frac{1}{\lambda - H} \, d\lambda.
\]
For each $\xi \in \Gamma^* / n$, let
\[
Q_\xi = \frac{1}{2\pi i} \int_\theta \frac{1}{\lambda - H_\xi} \frac{1}{\lambda - \hat{H}_\xi} \, d\lambda;
\]
\[
\hat{Q}_\xi = \frac{1}{2\pi i} \int_\theta \frac{1}{\lambda - \hat{H}_\xi} \frac{1}{\lambda - H_\xi} \, d\lambda.
\]
Denote by $\rho_\xi$ and $\hat{\rho}_\xi$ the density that corresponds to $Q_\xi$ and $\hat{Q}_\xi$ respectively. As before, it suffices to estimate $\| \rho_\xi - \hat{\rho}_\xi \|_{H^{-1}_\xi}$ for each $\xi$.

Using the dual characterization of the space $H^{-1}_\xi$, we have
\[
\| \rho_\xi - \hat{\rho}_\xi \|_{H^{-1}_\xi} = \sup_{\| W \|_{H^1} \leq 1} \langle W, \rho_\xi - \hat{\rho}_\xi \rangle_{H^1_n, H^{-1}_n}.
\]
Take $W \in H^1$ with $\| W \|_{H^1} \leq 1$. By definition, we have
\[
\langle W, \rho_\xi - \hat{\rho}_\xi \rangle_{H^1_n, H^{-1}_n} = \langle W, \rho_\xi \rangle_{H^1_n, H^{-1}_n} - \langle W, \hat{\rho}_\xi \rangle_{H^1_n, H^{-1}_n} = \text{tr}_{P_\xi} WQ_\xi - \text{tr}_{\hat{P}_\xi} W\hat{Q}_\xi.
\]
We suppress the dependence on $\xi$ in the notation for simplicity. By definition,
\[
\text{tr}_{P} WQ - \text{tr}_{\hat{P}} W\hat{Q} = (\text{tr} PWQP + \text{tr} P^\perp WQP^\perp) - (\text{tr} \hat{P} W\hat{Q}\hat{P} + \text{tr} P^\perp W\hat{Q}\hat{P}^\perp) = (\text{tr} PWP^\perp QP - \text{tr} PWP^\perp \hat{Q}\hat{P}) + (\text{tr} P^\perp WQP^\perp - \text{tr} P^\perp W\hat{Q}\hat{P}^\perp)
\]
Let us consider only the first term, the argument for the second term is analogous,
\[
\text{tr} PWP^\perp QP - \text{tr} PWP^\perp \hat{Q}\hat{P} = \text{tr} [P, W] P^\perp QP - \text{tr} [\hat{P}, W] P^\perp \hat{Q}\hat{P}
\]
\begin{equation}
= \text{tr} (P - \hat{P}) [P, W] P^\perp QP + \text{tr} [\hat{P}, W] P^\perp QP + \text{tr} [\hat{P}, W] (P^\perp QP - P^\perp \hat{Q}\hat{P})
\end{equation}
Consider the first term, we have shown in the proof of Proposition 6.9 that
\[ \| [ \mathcal{P}_\xi, W ] \|_{\mathfrak{S}_2 (L^2_{\xi}(\alpha \Gamma))} \lesssim \| \nabla W \|_{L^2(\alpha \Gamma)} \leq 1, \]
and
\[ \| \mathcal{P}_\xi \mathcal{Q}_\xi \mathcal{P}_\xi \|_{\mathfrak{S}_2 (L^2_{\xi}(\alpha \Gamma))} \lesssim \| \nabla \nu \|_{L^2(\alpha \Gamma)}. \]
Combined with the fact that
\[ \| \mathcal{P}_{\xi} - \hat{\mathcal{P}}_{\xi} \|_{\mathfrak{S}_2 (L^2_{\xi}(\alpha \Gamma))} \lesssim \| a - \hat{a} \|_{L^\infty} + \| V_{\xi} - \hat{V}_{\xi} \|_{L^\infty}, \]
we have
\[ |\text{tr}(\mathcal{P} - \hat{\mathcal{P}})[\mathcal{P}, W]\mathcal{P} \mathcal{Q} \|_{\mathfrak{S}_2 (\alpha \Gamma)} \lesssim (\| a - \hat{a} \|_{L^\infty} + \| V_{\xi} - \hat{V}_{\xi} \|_{L^\infty}) \| \nu \|_{H^1}. \]
Consider then the second term in the right hand side of (6.38), we have
\[
\begin{align*}
[\mathcal{P} - \hat{\mathcal{P}}, W] &= \frac{1}{2\pi i} \int_{\epsilon} [R_\lambda - \hat{R}_\lambda, W] \, d\lambda \\
&= \frac{1}{2\pi i} \int_{\epsilon} R_\lambda [\mathcal{H}, W] R_\lambda - \hat{R}_\lambda [\hat{\mathcal{H}}, W] \hat{R}_\lambda \, d\lambda \\
&= \frac{1}{2\pi i} \int_{\epsilon} (R_\lambda - \hat{R}_\lambda) [\mathcal{H}, W] R_\lambda \, d\lambda \\
&\quad + \frac{1}{2\pi i} \int_{\epsilon} \hat{R}_\lambda [\mathcal{H} - \hat{\mathcal{H}}, W] R_\lambda \, d\lambda \\
&\quad + \frac{1}{2\pi i} \int_{\epsilon} \hat{R}_\lambda [\hat{\mathcal{H}}, W] (R_\lambda - \hat{R}_\lambda) \, d\lambda.
\end{align*}
\]
The first and third term on the right hand side can be controlled in the $\mathfrak{S}_2$ norm since $[\mathcal{H}, W] \in \mathfrak{S}_2$, $[\hat{\mathcal{H}}, W] \in \mathfrak{S}_2$ with norm controlled by $\| W \|_{H^1}$ and the difference of the resolvent is bounded by $(\| a - \hat{a} \|_{L^\infty} + \| V_{\xi} - \hat{V}_{\xi} \|_{L^\infty})$ in operator norm. Let us consider the second term, we have
\[ [\mathcal{H} - \hat{\mathcal{H}}, W] = -(a_{ij} - \hat{a}_{ij}) \partial_i (\partial_j W) - (a_{ij} - \hat{a}_{ij}) (\partial_i W) \partial_j. \]
Hence, we obtain
\[ \| \hat{R}_\lambda [\mathcal{H} - \hat{\mathcal{H}}, W] R_\lambda \|_{\mathfrak{S}_2 (L^2_{\xi}(\alpha \Gamma))} \leq \| a - \hat{a} \|_{L^\infty} \| \nabla W \|_{L^2(\alpha \Gamma)}. \]
From this, we get
\[ \| [\mathcal{P} - \hat{\mathcal{P}}, W] \|_{\mathfrak{S}_2 (L^2_{\xi}(\alpha \Gamma))} \lesssim \| a - \hat{a} \|_{L^\infty} + \| V_{\xi} - \hat{V}_{\xi} \|_{L^\infty}. \]
Therefore, we have
\[ |\text{tr}(\hat{\mathcal{P}})[\mathcal{P} - \hat{\mathcal{P}}, W]\mathcal{P} \mathcal{Q} \|_{\mathfrak{S}_2 (\alpha \Gamma)} \lesssim (\| a - \hat{a} \|_{L^\infty} + \| V_{\xi} - \hat{V}_{\xi} \|_{L^\infty}) \| \nu \|_{H^1}. \]
Now consider the last term in (6.38), we have
\[
\begin{align*}
\mathcal{P} \mathcal{Q} - \hat{\mathcal{P}} \mathcal{Q} &= \frac{1}{2\pi i} \int_{\epsilon} R_\lambda \mathcal{P} \mathcal{Q} R_\lambda - \hat{R}_\lambda \hat{\mathcal{P}} \mathcal{Q} \hat{R}_\lambda \, d\lambda \\
&= -\frac{1}{2\pi i} \int_{\epsilon} R_\lambda \mathcal{P} \mathcal{Q} [\mathcal{P}, \nu] R_\lambda - \hat{R}_\lambda \hat{\mathcal{P}} \mathcal{Q} [\hat{\mathcal{P}}, \nu] \hat{R}_\lambda \, d\lambda,
\end{align*}
\]
\[ R_{\lambda} \mathcal{P}^\perp [\mathcal{P}, \nu] \mathcal{P} R_{\lambda} - \tilde{R}_{\lambda} \mathcal{P}^\perp [\tilde{\mathcal{P}}, \nu] \tilde{\mathcal{P}} R_{\lambda} = (R_{\lambda} - \tilde{R}_{\lambda}) \mathcal{P}^\perp [\mathcal{P}, \nu] \mathcal{P} R_{\lambda} + \tilde{R}_{\lambda} (\mathcal{P}^\perp - \tilde{\mathcal{P}}^\perp) [\mathcal{P}, \nu] \mathcal{P} R_{\lambda} + \tilde{R}_{\lambda} \mathcal{P}^\perp [\tilde{\mathcal{P}}, \nu] (\mathcal{P} - \tilde{\mathcal{P}}) R_{\lambda} + \tilde{R}_{\lambda} \mathcal{P}^\perp [\tilde{\mathcal{P}}, \nu] (R_{\lambda} - \tilde{R}_{\lambda}). \]

Using (6.40) for the third term and the bound of the difference of the resolvent for the other terms, we obtain
\[
\| \mathcal{P}^\perp Q \mathcal{P} - \tilde{\mathcal{P}}^\perp \tilde{\mathcal{Q}} \tilde{\mathcal{P}} \|_{\mathcal{A}(L_2^0(\omega \Gamma))} \lesssim (\| a - \tilde{a} \|_{L^\infty} + \| V_{\epsilon} - \tilde{V}_{\epsilon} \|_{L^\infty}) \| \nu \|_{H_1^1}. \]

Therefore
\[
| \text{tr} \tilde{\mathcal{P}} [\tilde{\mathcal{P}}, W] (\mathcal{P}^\perp Q \mathcal{P} - \tilde{\mathcal{P}}^\perp \tilde{\mathcal{Q}} \tilde{\mathcal{P}}) | \lesssim (\| a - \tilde{a} \|_{L^\infty} + \| V_{\epsilon} - \tilde{V}_{\epsilon} \|_{L^\infty}) \| \nu \|_{H_1^1}. \]

We arrive at the estimate
\[
| \text{tr}_P W Q - \text{tr}_P W \tilde{Q} | \lesssim (\| a - \tilde{a} \|_{L^\infty} + \| V_{\epsilon} - \tilde{V}_{\epsilon} \|_{L^\infty}) \| \nu \|_{H_1^1}. \]

Hence
\[
\| \rho_{\epsilon} - \tilde{\rho}_{\epsilon} \|_{H_{-1}^1} \lesssim (\| a - \tilde{a} \|_{L^\infty} + \| V_{\epsilon} - \tilde{V}_{\epsilon} \|_{L^\infty}) \| \nu \|_{H_1^1}. \]

\[ \square \]

**Lemma 6.18.** For \( V_{\epsilon}, \tilde{V}_{\epsilon} \in W_{n_{\infty}}^2 + H_{n_{\infty}}^2 \), we have
\[
\| \chi - \tilde{\chi} \|_{\mathcal{A}(H_2^0, H_2^2)} \lesssim \| a - \tilde{a} \|_{W^{2, \infty}} + \| V_{\epsilon} - \tilde{V}_{\epsilon} \|_{W_{n_{\infty}}^2 + H_{n_{\infty}}^2}. \]

**Proof.** Using the resolvent identity, we have
\[
Q - \tilde{Q} = \frac{1}{2\pi i} \int_{\mathcal{E}} (R_\lambda \nu R_\lambda - \tilde{R}_\lambda \nu \tilde{R}_\lambda) d\lambda \]
\[
= \frac{1}{2\pi i} \int_{\mathcal{E}} R_\lambda (\mathcal{H} - \tilde{\mathcal{H}}) \tilde{R}_\lambda \nu R_\lambda + \tilde{R}_\lambda \nu R_\lambda (\mathcal{H} - \tilde{\mathcal{H}}) \tilde{R}_\lambda d\lambda \]

It follows from the same argument as in the proof of Propositions 6.5 and 6.6 as well as an interpolation argument that
\[
\| \rho_Q - \rho_{\tilde{Q}} \|_{L_2^2} \lesssim (\| a - \tilde{a} \|_{L^\infty} + \| V_{\epsilon} - \tilde{V}_{\epsilon} \|_{L^\infty}) \| \nu \|_{L_2^2}. \]

For derivatives, let us focus on the density given by the first term in (6.42), the consideration for the other term is similar:
\[
\delta \rho_1(x) = \frac{1}{2\pi i} \int_{\mathcal{E}} R_\lambda (\mathcal{H} - \tilde{\mathcal{H}}) \tilde{R}_\lambda \nu R_\lambda d\lambda(x, x). \]
Taking the derivative, we obtain
\[
\nabla \delta \rho_1(x) = \frac{1}{2\pi i} \int_G [\nabla, R_\lambda](H - \tilde{H}) \tilde{R}_\lambda \nu R_\lambda \, d\lambda(x, x)
\]
\[
+ \frac{1}{2\pi i} \int_G R_\lambda [\nabla, (H - \tilde{H})] \tilde{R}_\lambda \nu R_\lambda \, d\lambda(x, x)
\]
\[
(6.44)
\]
\[
+ \frac{1}{2\pi i} \int_G R_\lambda (H - \tilde{H}) \tilde{R}_\lambda (\nabla \nu) R_\lambda \, d\lambda(x, x)
\]
\[
+ \frac{1}{2\pi i} \int_G R_\lambda (H - \tilde{H}) \tilde{R}_\lambda \nu R_\lambda \, d\lambda(x, x)
\]
\]

Let us consider the first and second terms of (6.44). The argument for the third and fifth terms is similar to the first term, and the fourth term can be bounded using a similar argument as the one used to prove (6.43).

For the first term in (6.44), direct calculation yields
\[
[\nabla, R_\lambda] = R_\lambda (-\nabla (a_{ij}) \partial_i \partial_j + \nabla V_\varepsilon) R_\lambda
\]

Hence, the first term can be rewritten as
\[
I_1(x) = \frac{1}{2\pi i} \int_G R_\lambda (-\nabla (a_{ij}) \partial_i \partial_j + \nabla V_\varepsilon) R_\lambda (H - \tilde{H}) \tilde{R}_\lambda \nu R_\lambda \, d\lambda(x, x).
\]

The $L^2_n$ estimate of $I_1$ follows a similar argument used in the proof of Corollary 6.7. Indeed, taking the Bloch decomposition, we have
\[
I_1(x) = \int_{\Gamma^*/n} I_{1, \xi}(x) \, d\xi,
\]

where for $\xi \in \Gamma^*/n$, $I_{1, \xi}$ is given by
\[
I_{1, \xi}(x) = \frac{1}{2\pi i} \int_G R_{\lambda, \xi} (-\nabla (a_{ij}) \partial_i \partial_j + \nabla V_\varepsilon) R_{\lambda, \xi} (H_\xi - \tilde{H}_\xi) \tilde{R}_{\lambda, \xi} \nu R_{\lambda, \xi} \, d\lambda(x, x).
\]

Using Jensen’s inequality, the estimate of $I_1$ will follow from the one for $I_{1, \xi}$. Define the operator
\[
Q_{\lambda, \xi, \nu} = R_{\lambda, \xi} (-\nabla (a_{ij}) \partial_i \partial_j + \nabla V_\varepsilon) R_{\lambda, \xi} (H_\xi - \tilde{H}_\xi) \tilde{R}_{\lambda, \xi} \nu R_{\lambda, \xi}.
\]

If $\nu \in L^1_n$, we have
\[
\|Q_{\lambda, \xi, \nu}\|_{\Omega_n(L^2_n)} \leq \|R_{\lambda, \xi} (-\nabla (a_{ij}) \partial_i \partial_j + \nabla V_\varepsilon)\|_{\mathcal{L}(L^2_n)} \times \|R_{\lambda, \xi} (H_\xi - \tilde{H}_\xi)\|_{\mathcal{L}(L^2_n)} \|\tilde{R}_{\lambda, \xi} \nu R_{\lambda, \xi}\|_{\Omega_n(L^2_n)}.
\]

Note that
\[
\|R_{\lambda, \xi} (-\nabla (a_{ij}) \partial_i \partial_j + \nabla V_\varepsilon)\|_{\mathcal{L}(L^2_n)} \leq \sum_{ij} \|\nabla a_{ij}\|_{L^\infty} \|R_{\lambda, \xi} \partial_i \partial_j\|_{\mathcal{L}(L^2_n)} + \|R_{\lambda, \xi} \nabla V_\varepsilon\|_{\mathcal{L}(L^2_n)}
\]
\[
\lesssim \|a\|_{W^{1, \infty}} + \|V_\varepsilon\|_{W^{1, \infty}_0} + H^1_\varepsilon,
\]
where in the last inequality we have used the fact that
\[ \| R_{\lambda,\xi} W \|_{L^2} \leq \| R_{\lambda,\xi} W \|_{\mathcal{A}^1} \lesssim \| W \|_{L^2} \]
using (6.20). Therefore, we have
\[ \| Q_{\lambda,\xi,\nu} \|_{\mathcal{A}^1} \lesssim (\| a \|_{W^{1,\infty}} + \| V_\nu \|_{W^{1,\infty}_n+H^1_2}) (\| a - \bar{a} \|_{L^\infty} + \| V_\nu - \bar{V}_\nu \|_{L^\infty}) \| \nu \|_{L^1}. \]

On the other hand, if \( \nu \in L^\infty_n \), then
\[ \| Q_{\lambda,\xi,\nu} \|_{L^2(\mu,\nu)} \lesssim \| R_{\lambda,\xi} \|_{L^2(\mu,\nu)} \| (\nabla(a_{ij}) \partial_i \partial_j + \nabla V_\nu) R_{\lambda,\xi} \|_{L^2(\mu,\nu)} \| \nu R_{\lambda,\xi} \|_{L^2(\mu,\nu,\nu)}. \]

It follows that
\[ \| Q_{\lambda,\xi,\nu} \|_{L^2(\mu,\nu)} \lesssim (\| a \|_{W^{1,\infty}} + \| V_\nu \|_{W^{1,\infty}_n+H^1_2}) (\| a - \bar{a} \|_{L^\infty} + \| V_\nu - \bar{V}_\nu \|_{L^\infty}) \| \nu \|_{L^\infty}. \]

Hence, we can use the argument in the proof of Propositions 6.5, 6.6 and interpolation to conclude that
\[ \| I_1,\xi \|_{L^2_\nu} \lesssim (\| a \|_{W^{1,\infty}} + \| V_\nu \|_{W^{1,\infty}_n+H^1_2}) (\| a - \bar{a} \|_{L^\infty} + \| V_\nu - \bar{V}_\nu \|_{L^\infty}) \| \nu \|_{L^2_\mu}. \]

For the second term of (6.44), we use
\[ [\nabla, \mathcal{H} - \tilde{\mathcal{H}}] = -\nabla(a_{ij}(x) - \bar{a}_{ij}(x)) \partial_i \partial_j + \nabla(V_\nu - \bar{V}_\nu). \]

Therefore, by similar argument as the one used for the first term, we obtain
\[ \left\| \frac{1}{2\pi} \int_{\mathbb{R}} \nabla(V_\nu - \bar{V}_\nu) R_{\lambda,\xi,\nu} R_{\lambda} d\lambda(x, x) \right\|_{L^2_\mu} \lesssim (\| \nabla a - \nabla \bar{a} \|_{L^\infty} + \| \nabla V_\nu - \nabla \bar{V}_\nu \|_{L^\infty}) \| \nu \|_{L^2_\mu}. \]

Hence, taking into account the estimates for the other terms that we have omitted, we arrive at
\[ \| \nabla(\rho_Q - \rho_\tilde{Q}) \|_{L^2_\mu} \lesssim (\| a - \bar{a} \|_{W^{1,\infty}} + \| V_\nu - \bar{V}_\nu \|_{W^{1,\infty}_n+H^1_2}) \| \nu \|_{H^1_2}. \]

For the second derivative, let us focus on one term that arises from the expression of \( \nabla^2 \rho_1 \):
\[ I_2(x) = \frac{1}{2\pi} \int_{\mathbb{R}} \nabla(V_\nu - \bar{V}_\nu) \tilde{R}_{\lambda,\nu} \tilde{R}_\lambda d\lambda(x, x). \]

The other terms can be treated using similar arguments. Again using the Bloch decomposition, it suffices to bound for each \( \xi \in \Gamma^*/n, \)
\[ I_{2,\xi}(x) = \frac{1}{2\pi} \int_{\mathbb{R}} \nabla(V_\nu - \bar{V}_\nu) \tilde{R}_{\lambda,\xi} \tilde{R}_\lambda d\lambda(x, x). \]

Following a similar argument as the one above for \( I_{1,\xi} \), we have
\[ \| I_{2,\xi}(x) \|_{L^2_\mu} \lesssim \| \nabla(V_\nu - \bar{V}_\nu) \|_{L^\infty} \| \nabla \nu \|_{L^2_\mu} \lesssim \| \nabla(V_\nu - \bar{V}_\nu) \|_{L^\infty} \| \nu \|_{H^1_2}. \]
Taking into account the consideration for other terms that we have omitted, we conclude with the estimate
\[ \| \nabla^2 (Q - \tilde{Q}) \|_{L^2} \lesssim (\| a - \tilde{a} \|_{W^2,\infty} + \| V_\varepsilon - \tilde{V}_\varepsilon \|_{W^2,\infty + H^2_n}) \| \nu \|_{H^2_n}. \]

Following Lemmas 6.17, 6.18 and 6.11 as in the proof of Corollary 6.12, we have

**Corollary 6.19.** For \( V_\varepsilon, \tilde{V}_\varepsilon \in W^{2,\infty}_n + H^2_n \), we have
\[ (6.45) \| \lambda - \tilde{\lambda} \|_{X(H^2_n, H^2_n)} \lesssim \| a - \tilde{a} \|_{W^2,\infty} + \| V_\varepsilon - \tilde{V}_\varepsilon \|_{W^2,\infty + H^2_n}. \]

Finally, we prove

**Lemma 6.20.** For \( V_\varepsilon, \tilde{V}_\varepsilon \in W^{2,\infty}_n + H^2_n \), we have
\[ (6.46) \| \lambda - \tilde{\lambda} \|_{X(H^2_n, H^2_n)} \lesssim \| a - \tilde{a} \|_{W^2,\infty} + \| V_\varepsilon - \tilde{V}_\varepsilon \|_{W^2,\infty + H^2_n}. \]

**Proof.** Write
\[ (6.47) Q - \tilde{Q} = \frac{1}{2\pi i} \int_{\mathcal{P}} \left( R_\lambda [\mathcal{P}, \nu] \mathcal{P} R_\lambda - \tilde{R}_\lambda [\tilde{\mathcal{P}}, \nu] \tilde{\mathcal{P}} \right) d\lambda \]
\[ - \frac{1}{2\pi i} \int_{\mathcal{P}} \left( R_\lambda [\mathcal{P}, \nu] R_\lambda - \tilde{R}_\lambda \tilde{\mathcal{P}} \right) d\lambda \]

where we have inserted some projection operators in the expressions. Consider only the first term and substitute in the expression of \([\mathcal{P}, \nu]\) and \([\tilde{\mathcal{P}}, \nu]\), we obtain
\[ - \frac{1}{4\pi^2} \int_{\mathcal{P} \times \mathcal{P}} R_\lambda R_\mu [\mathcal{H}, \nu] \mathcal{P} R_\lambda d\mu d\lambda \]
\[ + \frac{1}{4\pi^2} \int_{\mathcal{P} \times \mathcal{P}} \tilde{R}_\lambda \tilde{R}_\mu [\tilde{\mathcal{H}}, \nu] \tilde{\mathcal{P}} \tilde{R}_\mu \tilde{R}_\lambda d\mu d\lambda \]

The remaining argument is similar to that in the proof of Proposition 6.13, Lemma 6.17 and Lemma 6.18. We omit the details here.

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7. **Proof of the Results for the Homogeneously Deformed Crystal**

In this section, we study the case when the deformation is homogeneous.

**Lemma 7.1.** There exist constants \( a_0, \delta_0 > 0 \), such that for \( |A| \leq a_0 \), \( \rho \in H^6_{\text{per}} \),
\[ \| \rho - \rho_c \|_{H^0_{\text{per}}} \leq \delta_0 \] and \( \int \rho = Z \), we have
\[ \| V_\lambda \rho - V_\varepsilon \rho_c \|_{H^0_{\text{per}}} \lesssim |A| + \| \rho - \rho_c \|_{H^0_{\text{per}}}. \]

**Proof.** Consider the difference between \( V_\lambda \rho \) and \( V_\varepsilon \rho_c \):
\[ V_\lambda \rho - V_\varepsilon \rho_c = (\phi_\lambda \rho - \phi_\varepsilon \rho_c) + (\eta(J^{-1}_A \rho - \eta(\rho_c)). \]
For the Coulomb part, since
\[ -J_A \Delta^A \phi_A[\rho] = 4\pi (\rho - m_A), \]
\[ -\Delta \phi_e[\rho_e] = 4\pi (\rho_e - m_e), \]
we have
\[ -\Delta (\phi_e[\rho_e] - \phi_A[\rho]) = -\Delta \phi_e[\rho_e] + J_A \Delta^A \phi_A[\rho] + (\Delta - J_A \Delta^A) \phi_A[\rho] \]
\[ = 4\pi (\rho_e - m_e) - 4\pi (\rho - m_A) + (\Delta - J_A \Delta^A) \phi_A[\rho], \]
where \( J_A = \det(I + A), \Delta^A = \alpha^A_{ij} \partial_i \partial_j \) and
\[ \alpha^A_{ij} = ((I + A)^{-1}(I + A)^{-T})_{ij}, \]
It is easy to see that
\[ |J_A \alpha^A_{ij} - \delta_{ij}| \lesssim |A|, \]
when \(|A|\) is sufficiently small. Therefore, by standard elliptic estimates, we have
\[ \|\phi_A[\rho] - \phi_e[\rho_e]\|_{H^6_{per}} \lesssim |A| + \|\rho - \rho_e\|_{H^6_{per}}. \]
For the exchange-correlation part, by the smoothness of \( \eta \) on \((0, \infty)\), we have
\[ \|\eta (J_A^{-1} \rho) - \eta(\rho_e)\|_{H^6_{per}} \lesssim \|J_A^{-1} \rho - \rho_e\|_{H^6_{per}} \lesssim |A| + \|\rho - \rho_e\|_{H^6_{per}}, \]
if \(|A|\) and \(\|\rho - \rho_e\|_{H^6_{per}}\) are sufficiently small. \( \square \)

**Lemma 7.2.** There exist constants \( a_0, \delta_0 > 0 \), such that for \(|A| \leq a_0, \rho \in H^6_{per}, \)
\(\|\rho - \rho_e\|_{H^6_{per}} \leq \delta_0\) and \(\int \rho = Z\), we have
\[ \text{dist}(\mathcal{E}, \text{spec}(\mathcal{H}_A[\rho])) \geq E_a/4. \]

**Proof.** By definition,
\[ \mathcal{H}_e[\rho_e] = -\Delta + V_e[\rho_e]; \]
\[ \mathcal{H}_A[\rho] = -a^A_{ij} \partial_i \partial_j + V_A[\rho]. \]
Since \(|a^A_{ij} - \delta_{ij}| \lesssim |A|\), for \( f \in \mathcal{D}(\mathcal{H}_e[\rho_e]) = H^2(\mathbb{R}^3)\), we have
\[ \| (\Delta - \Delta^A) f \|_{L^2} \lesssim |A| \| \Delta f \|_{L^2}. \]
Hence, for \( \lambda \in \mathcal{E}\),
\[ \| (\Delta - \Delta^A)(\lambda - \mathcal{H}_e[\rho_e])^{-1}\|_{L^2(L^2)} \lesssim |A|. \]
Combined with Lemma 7.1, we arrive at the estimate
\[ \|(\mathcal{H}_A[\rho] - \mathcal{H}_e[\rho_e])(\lambda - \mathcal{H}_e[\rho_e])^{-1}\|_{L^2(L^2)} \lesssim |A| + \|\rho - \rho_e\|_{H^6_{per}}. \]
Since
\[ (\lambda - \mathcal{H}_A[\rho])^{-1} = (\lambda - \mathcal{H}_e[\rho_e])^{-1} (I - (\mathcal{H}_A[\rho] - \mathcal{H}_e[\rho_e])(\lambda - \mathcal{H}_e[\rho_e])^{-1})^{-1}, \]
by choosing $a_0$ and $\delta_0$ sufficiently small that the left hand side of (7.1) is bounded by 1/2 uniformly with respect to $\lambda \in \mathcal{C}$ ($\mathcal{C}$ is a compact set), we obtain for any $\lambda \in \mathcal{C}$,

$$\|(\lambda - \mathcal{H}_A[\rho])^{-1}\|_{L^1(\mathcal{L})} \leq 2\|(\lambda - \mathcal{H}_e[\rho])^{-1}\|_{L^1(\mathcal{L})} \leq 4/E_g.$$ 

Hence if $|\mu - \lambda| < E_g/2$, the inverse of $\mu - \mathcal{H}_A[\rho]$ is bounded. Hence we have $\text{dist}(\mathcal{C}, \text{spec} \mathcal{H}_A[\rho]) \geq E_g/4$. □

**Proposition 7.3.** Under the same assumption as in Lemma 7.2, the Kohn-Sham map

$$F_A(\rho)(x) = \frac{1}{2\pi i} \int_{\mathcal{C}} \frac{1}{\lambda - \mathcal{H}_A[\rho]} \, d\lambda(x, x)$$

is well-defined from $\mathcal{D}_\rho$ to $H^6_{\text{per}, Z}$, where

$$H^6_{\text{per}, Z} = \{ \rho \in H^6_{\text{per}} \mid \int_{\Gamma} \rho = Z \};$$

$$\mathcal{D}_\rho = \{ \rho \in H^6_{\text{per}, Z} \mid \|\rho - \rho_e\|_{H^6_{\text{per}}} \leq \delta_0 \}.$$ 

Consequently, the map

(7.2) 

$$F(\rho, A) = F_A(\rho) = \frac{1}{2\pi i} \int_{\mathcal{C}} \frac{1}{\lambda - \mathcal{H}_A[\rho]} \, d\lambda(x, x),$$

is well-defined from $\mathcal{D}_\rho \times \mathcal{D}_A$ to $H^6_{\text{per}, Z}$, where

$$\mathcal{D}_A = \{ A \in \mathbb{R}^{3x3} \mid |A| \leq a_0 \}.$$ 

**Proof.** By Lemma 7.2, the projection operator

$$\mathcal{P} = \frac{1}{2\pi i} \int_{\mathcal{C}} \frac{1}{\lambda - \mathcal{H}_A[\rho]} \, d\lambda$$

is well-defined since the contour lies in the resolvent set. We consider the Bloch decomposition

$$\mathcal{P} = \int_{\Gamma^*} \mathcal{P}_\xi \, d\xi = \int_{\Gamma^*} \frac{1}{2\pi i} \int_{\mathcal{C}} \frac{1}{\lambda - \mathcal{H}_A[\rho]} \, d\lambda.$$ 

Since $V_A(\rho) \in H^6_{\text{per}}$, by standard elliptic theory [14], $(\lambda - \mathcal{H}_{A,\xi}[\rho])^{-1}$ is a bounded operator from $H^m_{\text{per}}(\mathbb{R}^3)$ to $H^{m+2}_{\text{per}}(\mathbb{R}^3)$, if $0 \leq m \leq 6$. In addition, since $(\lambda - \mathcal{H}_{A,\xi}[\rho])^{-1}$ is self-adjoint, it is also bounded from $H^{m-2}_{\text{per}}(\mathbb{R}^3)$ to $H^{-m}_{\text{per}}(\mathbb{R}^3)$, if $0 \leq m \leq 6$. Since the contour $\mathcal{C}$ is compact, the same is true for $\mathcal{P}_\xi$, uniformly with respect to $\xi \in \Gamma^*$. Moreover, using the idempotency property, $\mathcal{P}_\xi = \mathcal{P}_\xi^m$, we have

$$\|\mathcal{P}_\xi\|_{L^1(H^{-m}, H^m)} \leq C,$$

with the bound depending only on the gap $E_g$ and the norm of $V_A$. Hence, from the regularity of the kernel of $\mathcal{P}_\xi$ (Lemma 6.4), we conclude that

$$\rho_\xi(x) = \mathcal{P}_\xi(x, x)$$

is a $C^6(\Gamma)$ function. Therefore, by the compactness of $\Gamma^*$, we have the desired regularity estimate for $F_A(\rho)$. 

The normalization identity follows from the Bloch decomposition:
\[
\frac{1}{2\pi i} \int_{\Gamma} dx \int \frac{1}{\lambda - \mathcal{H}_A[\rho]} d\lambda(x, x) = \int_{\Gamma^*} d\xi \text{tr}_{L_\xi^2(\Gamma)} \left( \frac{1}{2\pi i} \int_{\mathcal{E}} \frac{1}{\lambda - (\mathcal{H}_A[\rho])_\xi} d\lambda \right) = Z.
\]

**Lemma 7.4.** The map \( \mathcal{F} \) from \( \mathcal{D}_\rho \times \mathcal{D}_A \) to \( H^6_{\text{per}, Z} \) is \( C^\infty \).

**Proof.** It is easy to see that the dependence of \( a_{ij} \) and \( \mathcal{V}_A[\rho] \) on \( A \) and \( \rho \) is smooth. The conclusion then follows from the resolvent identity as well as the similar arguments used in the proof of Proposition 7.3 applied to the derivatives of \( \mathcal{F} \). Let us consider one representative term in the first derivative, the argument for other terms and for higher order derivatives are analogous. Differentiating (7.2) with respect to \( a_{ij}^A \), using the idempotency property, we have for any \( b \)
\[
\frac{\partial \mathcal{F}}{\partial a_{ij}^A}(b)(x) = \int_{\Gamma^*} \frac{\partial}{\partial a_{ij}^A} \mathcal{P}_\xi^A(b)(x, x) d\xi = \int_{\Gamma^*} \sum_{l=0}^7 \left( \mathcal{P}_\xi^{l-1} \frac{\partial \mathcal{P}_\xi}{\partial a_{ij}^A}(b) \mathcal{P}_\xi^l \right)(x, x) d\xi.
\]
Here the eighth power of \( \mathcal{P}_\xi \) is used to provide sufficient regularity. By the resolvent identity, we have
\[
\frac{\partial \mathcal{P}_\xi}{\partial a_{ij}^A}(b) = \frac{1}{2\pi i} \int_{\mathcal{E}} \frac{1}{\lambda - \mathcal{H}_A[\rho]} (-b\partial_i \partial_j) \frac{1}{\lambda - \mathcal{H}_A[\rho]} d\lambda.
\]
Hence, it is a bounded operator from \( H^m_{\text{per}} \) to \( H^{m+2}_{\text{per}} \) for integer \( m \) between \(-8 \) and \( 6 \). Therefore, \( \partial \mathcal{P}_\xi^A/\partial a_{ij}^A \) is a bounded operator from \( H^8_{\text{per}} \) to \( H^6_{\text{per}} \). By Lemma 6.4, the kernel is in \( C^0(\Gamma) \). Thus, \( \partial \mathcal{F}/\partial a_{ij}^A(b) \) is a \( H^6_{\text{per}} \) function for any number \( b \). \( \square \)

**Proof of Theorem 4.1.** We will use the implicit function theorem. Define map \( \mathcal{T} \) by
\[
(7.3) \quad \mathcal{T}(\rho, A) = \rho - \mathcal{F}(\rho, A)
\]
from \( \mathcal{D}_\rho \times \mathcal{D}_A \) to \( H^6_{\text{per}, 0} \), where
\[
H^6_{\text{per}, 0} = \{ \rho \in H^6_{\text{per}} \mid \int_{\Gamma} \rho = 0 \}.
\]
Then, by Lemma 7.4, \( \mathcal{T} \) is a \( C^\infty \) map, and we have
\[
(7.4) \quad \mathcal{T}(\rho_e, 0) = \rho_e - \mathcal{F}(\rho_e, 0) = 0.
\]
Notice that
\[
(7.5) \quad \frac{\delta}{\delta \rho} \mathcal{T}(\rho, A)|_{\rho=\rho_e, A=0} = \mathcal{L}_e
\]
is invertible and the inverse is bounded as an operator on \( H^6_{\text{per}, 0}(\mathbb{R}^3) \) due to the stability assumption and Proposition 6.15. Applying the implicit function theorem on \( \mathcal{T} \), we arrive at the desired result.
Let
\[ \mathcal{L}_A = \frac{1}{2\pi i} \int \frac{1}{\lambda - \mathcal{H}_A(\rho_A)} \delta_{\rho_A} V_A(w) \frac{1}{\lambda - \mathcal{H}_A(\rho_A)} \, d\lambda(x,x). \]

Note that since \( \rho_A = \rho_{\text{CB}}(:,A) \in H^6_{\text{per},Z} \), we have \( V_{\text{CB}}(:,A) = V_A(\rho_A) \in W^4_{\text{per}} \). Therefore, following the same argument as in Section 6.3, we have

**Proposition 7.5.** \((\mathcal{I} - \mathcal{L}_A)^{-1}\) is a bounded operator on \( H^m_{\text{per},0} \) for \( m = 2, 3, 4 \).

8. Exponential decay of the resolvent

Recall the following Combes-Thomas type of estimate [6] proved in [10]:

**Proposition 8.1.** Given the Hamiltonian \( \mathcal{H} = -\Delta + V \) with a \( \Delta \)-bounded potential \( V \).\(^1\) For any \( \lambda \in \mathbb{C} \setminus \text{spec}(\mathcal{H}) \), let \( \text{dist}(\lambda, \text{spec}(\mathcal{H})) = d \). Then there exist constants \( \gamma_{\text{max}} > 0 \) and \( M \), such that for all \( x_0 \) and all \( \gamma < \gamma_{\text{max}} \), we have

\[ \| E_{x_0}^{-1}(\lambda - \mathcal{H})^{-1} E_{x_0} \|_{L^2} \leq M/d, \]

where \( E_{x_0} \) is a multiplicative operator

\[ (E_{x_0} f)(x) = e^{-\gamma((x-x_0)^2+1)^{1/2}} f(x), \]

and \( \gamma_{\text{max}} \) depends only on \( d, |\lambda|, M \) and the relative bound of \( V \) with respect to \( \Delta \).

In addition, from the proof of [10, Theorem 9], we also have:

**Corollary 8.2.** Under the assumption of Proposition 8.1, we have for all \( x_0, 1 \leq i, j \leq 3 \) and \( \gamma < \gamma_{\text{max}} \),

\[ \| \partial_i \partial_j E_{x_0}^{-1}(\lambda - \mathcal{H})^{-1} E_{x_0} \|_{L^2} \lesssim M, \]

and

\[ \| E_{x_0}^{-1} \partial_i \partial_j (\lambda - \mathcal{H})^{-1} E_{x_0} \|_{L^2} \lesssim M. \]

Consequently, we have:

**Corollary 8.3.** Let
\[ \mathcal{G}_\lambda(x,x') = (\lambda - \mathcal{H})^{-1}(x,x'). \]

Under the assumption of Proposition 8.1, we have for all \( x_0 \) and \( \gamma < \gamma_{\text{max}} \),

\[ \| e^{-\gamma((x-x_0)^2+1)^{1/2}} \mathcal{G}_\lambda(x,x_0) \|_{L^2_x} \lesssim M. \]

Moreover, for any positive integer \( n \)

\[ \| |x - x_0|^n \mathcal{G}_\lambda(x,x_0) \|_{L^2} \leq C(n) M, \]

uniformly in \( x_0 \).

\(^1\) \( V \) is \( \Delta \)-bounded if there exist constant \( C_1 \) and \( C_2 \), such that for \( f \in \mathcal{D}(\Delta) \),

\[ \| Vf \|_{L^2} \leq C_1 \| f \|_{L^2} + C_2 \| \Delta f \|_{L^2}. \]
Remark. Note that the constant $C(n)$ might depend on $n$.

Proof. The first statement results from a combination of Lemma 6.4, Proposition 8.1 and Corollary 8.2.

The second statement is an easy consequence of the first, since

$$\|x - x_0\|^n G_\lambda(x, x_0) \leq \left\| x - x_0 \right\| e^{-\gamma((x - x_0)^2 + 1)^{1/2}} \times \left\| e^{\gamma((x - x_0)^2 + 1)^{1/2}} G_\lambda(x, x_0) \right\|_{L^2}$$

From the corollary, it is easy to see that the kernel of the density matrix decays exponentially fast away from diagonal. Note that this should not be confused with the exponential decay of the density $\rho$, the diagonal of the density matrix. As we are considering crystalline systems, $\rho$ does not decay. The main application of the above exponential decay property of the Green’s function will be the following type of estimates. As usual, we assume that the contour $\mathcal{C}$ is compact and separates the occupied spectrum of $\mathcal{H}$ from the rest of the spectrum with a gap.

**Proposition 8.4.** We have for any $x$

$$\left| \frac{1}{2\pi i} \int_{\rho} \frac{1}{\lambda - \mathcal{H}} (x' - x)^\alpha \frac{1}{\lambda - \mathcal{H}} \, d\lambda(x, x) \right| \leq C(|\alpha|) M,$$

for any multi-index $\alpha$. Here and in the sequel, $(x' - x)^\alpha$ is understood as a multiplicative operator, i.e., for each fixed $x$,

$$(x' - x)^\alpha f(x') = (x' - x)^\alpha f(x'), \quad \forall x'.$$

Proof. For any $x$, define the function $f_x$ by

$$f_x(x') = (x' - x)^\alpha \frac{1}{\lambda - \mathcal{H}}(x', x).$$

From Corollary 8.3, $f_x$ is a $L^2$ function. Notice that

$$\frac{1}{\lambda - \mathcal{H}}(x' - x)^\alpha \frac{1}{\lambda - \mathcal{H}}(x, x) = \left( \frac{1}{\lambda - \mathcal{H}} f_x \right)(x).$$

By elliptic regularity and the Sobolev inequality, we have

$$\|(\lambda - \mathcal{H})^{-1} f_x\|_{L^\infty} \leq \|(\lambda - \mathcal{H})^{-1} f_x\|_{L^2} \leq \|(\lambda - \mathcal{H})^{-1}\|_{Z(L^2, H^2)} \|f_x\|_{L^2}.$$

This proves the proposition.

**Proposition 8.5.**

$$\left| \frac{1}{2\pi i} \int_{\rho} \frac{1}{\lambda - \mathcal{H}} \partial_i \partial_j (x' - x)^\alpha \frac{1}{\lambda - \mathcal{H}} \, d\lambda(x, x) \right| \leq C(|\alpha|) M,$$

and

$$\left| \frac{1}{2\pi i} \int_{\rho} \frac{1}{\lambda - \mathcal{H}} (x' - x)^\alpha \partial_i \partial_j \frac{1}{\lambda - \mathcal{H}} \, d\lambda(x, x) \right| \leq C(|\alpha|) M,$$

for any indices $i, j$ and multi-index $\alpha$. 
Proof. We only prove the first inequality. The second inequality is an easy corollary.

Let
\[ A_x = \frac{1}{2\pi i} \int_\mathbb{C} \frac{1}{\lambda - \mathcal{H}} \partial_i \partial_j (x' - x)^\alpha \frac{1}{\lambda - \mathcal{H}} \, d\lambda, \]
\[ P = \frac{1}{2\pi i} \int_\mathbb{C} \frac{1}{\lambda - \mathcal{H}} \, d\lambda. \]

Using the spectral representation and the Cauchy theorem, it is easy to see that
\[ PA_x P = 0 \quad \text{and} \quad P^\perp A_x P^\perp = 0. \]

Hence,
\[ A_x = PA_x P + P^\perp A_x P^\perp = PA_x + A_x P. \]

Therefore,
\[ A_x(x, x) = -\frac{1}{4\pi^2} \int_\mathbb{C} \frac{1}{\mu - \mathcal{H}} \frac{1}{\lambda - \mathcal{H}} \partial_i \partial_j (x' - x)^\alpha \frac{1}{\lambda - \mathcal{H}} \, d\lambda \, d\mu(x, x) \]
\[ - \frac{1}{4\pi^2} \int_\mathbb{C} \frac{1}{\lambda - \mathcal{H}} \partial_i \partial_j (x' - x)^\alpha \frac{1}{\lambda - \mathcal{H}} \frac{1}{\mu - \mathcal{H}} \, d\lambda \, d\mu(x, x). \]

For the first term, define
\[ f_x(x') = (x' - x)^\alpha \frac{1}{\lambda - \mathcal{H}}(x', x). \]

We have
\[ \left\| \frac{1}{\mu - \mathcal{H}} \frac{1}{\lambda - \mathcal{H}} \partial_i \partial_j f_x \right\|_{L^\infty} \lesssim \left\| \frac{1}{\lambda - \mathcal{H}} \partial_i \partial_j f_x \right\|_{L^2} \lesssim \left\| \frac{1}{\lambda - \mathcal{H}} \partial_i \partial_j \right\|_{\mathcal{L}(L^2)} \| f_x \|_{L^2}. \]

Hence the first term is bounded. For the second term, let
\[ g_x(x') = \partial_i \partial_j (x' - x)^\alpha \frac{1}{\lambda - \mathcal{H}} \frac{1}{\mu - \mathcal{H}}(x', x), \]
and
\[ h_x(x') = e^{\gamma((x'-x)^2+1)^{1/2}} \frac{1}{\mu - \mathcal{H}}(x', x) \]
then
\[ \| g_x \|_{L^2} \leq \left\| \partial_i \partial_j (x' - x)^\alpha \frac{1}{\lambda - \mathcal{H}} e^{-\gamma((x'-x)^2+1)^{1/2}} \right\|_{\mathcal{L}(L^2)} \| h_x \|_{L^2}, \]
where \((x' - x)^\alpha\) and \(e^{-\gamma((x'-x)^2+1)^{1/2}}\) are understood as multiplicative operators with \(x\) as parameter as usual. Therefore, \(g_x\) is a \(L^2\) function. The boundedness of the second term then follows
\[ \left\| \left( \frac{1}{\lambda - \mathcal{H}} g_x \right)(x) \right\|_{H^2} \leq \left\| \frac{1}{\lambda - \mathcal{H}} g_x \right\|_{H^2} \leq \| (\lambda - \mathcal{H})^{-1} \|_{\mathcal{L}(L^2, H^2)} \| g_x \|_{L^2}. \]
\[ \square \]

Proposition 8.6.
\[ \left| \frac{1}{2\pi i} \int_\mathbb{C} \frac{1}{\lambda - \mathcal{H}} (x' - x)^\alpha \partial_i \partial_j \frac{1}{\lambda - \mathcal{H}} (x' - x)^\beta \partial_k \partial_l \frac{1}{\lambda - \mathcal{H}} \, d\lambda(x, x) \right| \leq C(|\alpha|, |\beta|) M, \]
for any indices \(i, j, k, l\) and multi-indices \(\alpha\) and \(\beta\).
Proof. Let

\[ A_x = \frac{1}{2\pi i} \int_{\mathcal{C}} \frac{1}{\lambda - \mathcal{H}} (x' - x)^\alpha \partial_i \partial_j \frac{1}{\lambda - \mathcal{H}} (x' - x)^\beta \partial_k \partial_l \frac{1}{\lambda - \mathcal{H}} \, d\lambda. \]

Inserting \( I = \mathcal{P} + \mathcal{P}^\perp \), we have

\[ (8.2) \quad A_x = A_{x}^{++} + A_{x}^{-+} + A_{x}^{+-} + A_{x}^{--}. \]

Here we have used the short-hand notation

\[ A_{x}^{++} = \frac{1}{2\pi i} \int_{\mathcal{C}} \mathcal{P}^\perp \frac{1}{\lambda - \mathcal{H}} (x' - x)^\alpha \partial_i \partial_j \mathcal{P} \frac{1}{\lambda - \mathcal{H}} (x' - x)^\beta \partial_k \partial_l \mathcal{P}^\perp \frac{1}{\lambda - \mathcal{H}} \, d\lambda, \]

and similarly for the other terms. We have also used the fact that

\[ A_{x}^{++} = 0 \quad \text{and} \quad A_{x}^{--} = 0, \]

which follows from the spectral representation and the Cauchy theorem.

Let us analyze one typical term in (8.2), say \( A_{x}^{+-} \). The arguments for other terms are similar. We have

\[ A_{x}^{+-}(x, x) = (A_{x}^{+-} \delta_x)(x), \]

where \( \delta_x \) is the Dirac-delta function centered at \( x \). We have

\[ \|A_{x}^{+-} \delta_x\|_{L^\infty} \leq \left\| \frac{1}{\lambda - \mathcal{H}} \right\|_{L^\infty(L^2; H^2)} \left\| (x' - x)^\alpha \partial_i \partial_j \frac{1}{\lambda - \mathcal{H}} e^{-\gamma((x' - x)^2 + 1)} \right\|_{L^2}\]

\[ \times \left\| e^{\gamma((x' - x)^2 + 1)} \mathcal{P} e^{-\gamma((x' - x)^2 + 1)} \right\|_{L^2(H^2; L^2)} \]

\[ \times \left\| e^{\gamma((x' - x)^2 + 1)} (x' - x)^\beta \partial_k \partial_l \frac{1}{\lambda - \mathcal{H}} e^{-\gamma((x' - x)^2 + 1)} \right\|_{L^2(H^2; L^2)} \]

\[ \times \left\| e^{\gamma((x' - x)^2 + 1)} \delta_x(x') \right\|_{H^2} \lesssim M. \]

Here the boundedness of the second and fourth terms follows from Corollary 8.2, the boundedness of the third term is an easy corollary of Corollary 8.2, and the boundedness of the fifth term follows by noticing that \( \mathcal{P}^\perp = I - \mathcal{P} \). Therefore, \( A_x(x, x) \) is bounded.

\[ \square \]

Similar argument can be used to establish the boundedness of higher order terms:

**Proposition 8.7.**

\[ \left| \frac{1}{2\pi i} \int_{\mathcal{C}} \frac{1}{\lambda - \mathcal{H}} \prod_{n=1}^{N} (x' - x)^{\alpha_n} \partial_{i_n} \partial_{j_n} \frac{1}{\lambda - \mathcal{H}} \, d\lambda(x, x) \right| \leq C(\{\|\alpha_n\|\}) M, \]

for any positive integer \( N \), indices \( i_n, j_n \) and multi-indices \( \alpha_n, n = 1, \ldots, N. \)
9. Asymptotic analysis of the Kohn-Sham equation

To construct a solution to the self-consistent equation

\[ \rho(x) = \frac{1}{2\pi i} \int e^{-i(\lambda - \mathcal{H}_\tau[\rho])} d\lambda(x,x), \]

we will first construct approximate solutions of the form:

\[ \rho^\varepsilon(x) = \epsilon^3 \rho_0(x,x/\epsilon) + \epsilon^{-2} \rho_1(x,x/\epsilon) + \epsilon^{-1} \rho_2(x,x/\epsilon) + \rho_3(x,x/\epsilon) \]

where \( \rho_j(\cdot, \cdot), j = 0, 1, 2, 3, \) are smooth in the first variable and \( \Gamma \)-periodic in the second variable. For this purpose, we need to understand the asymptotic structure of the Kohn-Sham map. In the following, we will often deal with two-scale functions such as the \( \rho_j \)'s. If \( f \) is such a function, we denote by \( \langle f(x, \cdot) \rangle \) a function of \( x \) defined by:

\[ \langle f(x, \cdot) \rangle = \frac{1}{|\Gamma|} \int_{\Gamma} f(x,z) \, dz. \]

Sometimes, when it is more convenient, we will also use the notation \( \langle f \rangle \) or \( \langle f(x, z) \rangle \) where \( z \) is understood as a dummy variable.

When there is no danger of confusion, we will suppress the dependence of \( \mathcal{H}_\tau \) and \( V^\varepsilon \) on \( \rho \) in the notations in this section.

Let us also remark that the purpose of this section is to construct a candidate approximate solution using asymptotic analysis. The constructed density \( \rho^\varepsilon \) will be proved to be indeed close to the its image under Kohn-Sham map in the next section. In particular, in this section, we sometimes do not give explicitly control of the higher order terms.

9.1. Two-scale structure of the potential. Recall that the Hamiltonian associated with \( \rho \) is given by

\[ \mathcal{H}_\tau = -\varepsilon^2 J^{1/2} \Delta_J J^{-1/2} + V^\varepsilon \]

\[ = -\varepsilon^2 a_{ij}(x) \partial_i \partial_j - \varepsilon^2 b_i(x) \partial_i - \varepsilon^2 c(x) + V^\varepsilon \]

where \( V^\varepsilon = \phi^\varepsilon + \eta(J(x)^{-1} \varepsilon^3 \rho(x)) \),

and \( \phi^\varepsilon \) solves

\[ (-a_{ij}(x) \partial_i \partial_j - b_i(x) \partial_i) \phi^\varepsilon = 4\pi \varepsilon (\rho - m^\varepsilon), \quad \langle \phi^\varepsilon \rangle = 0, \]

with periodic boundary condition on \( \Gamma \). We will study the two-scale structure of \( V^\varepsilon \) in this subsection.

First, let us write the deformed position of the atoms in a Taylor series around \( x \),

\[ \tau(X_i^\varepsilon) = \tau(x) + \sum_{k = 1}^{K} \sum_{|\beta| = k} \frac{1}{\beta!} \frac{\partial^\beta \tau(x)}{\partial x^\beta} (X_i^\varepsilon - x)^\beta + O(\|X_i^\varepsilon - x\|)^{K+1}. \]
Then,
\[
m_i^\varepsilon(x) = J(x) \frac{1}{\varepsilon^3} \sum_{X_i \in L} m_a \left( \frac{\tau(x) - \tau(X_i^\varepsilon)}{\varepsilon} \right)
\]
\[
= J(x) \frac{1}{\varepsilon^3} \sum_{X_i \in L} m_a \left( (I + A) \left( \frac{x - X_i}{\varepsilon} \right) \right)
\]
\[
- \sum_{k=2}^{K} \sum_{|\beta|=k} \frac{1}{\beta!} \frac{\partial^\beta \tau(x)}{\partial x^\beta} \left( \frac{X_i^\varepsilon - x}{\varepsilon} \right)^\beta + O(\varepsilon^K)
\]
\[
= J(x) \frac{1}{\varepsilon^3} \sum_{X_i \in L} m_a ((I + A)(x/\varepsilon - X_i))
\]
\[
- J(x) \frac{1}{\varepsilon^3} \sum_{X_i \in L} m'_a \sum_{|\beta|=2} \frac{1}{\beta!} \frac{\partial^\beta \tau(x)}{\partial x^\beta} (X_i - x/\varepsilon)^\beta
\]
\[
+ J(x) \frac{1}{\varepsilon^3} \sum_{X_i \in L} m''_a \left( \sum_{|\beta|=2} \frac{1}{\beta!} \frac{\partial^\beta \tau(x)}{\partial x^\beta} (X_i - x/\varepsilon)^\beta \right)^2
\]
\[
- J(x) \frac{1}{\varepsilon^3} \sum_{X_i \in L} m'_a \sum_{|\beta|=4} \frac{1}{\beta!} \frac{\partial^\beta \tau(x)}{\partial x^\beta} (X_i - x/\varepsilon)^\beta + O(1).
\]

Here $m'_a$ and $m''_a$ are evaluated at $(I + A)(x/\varepsilon - X_i)$, $A$ is the short hand notation for $\nabla u(x)$. Hence, we can express $m_i^\varepsilon(x)$ as
\[
m_i^\varepsilon(x) = \varepsilon^{-3} m_0(x, x/\varepsilon) + \varepsilon^{-2} m_1(x, x/\varepsilon) + \varepsilon^{-1} m_2(x, x/\varepsilon) + O(1),
\]
with
\[
m_0(x, z) = J(x) \sum_{X_i \in L} m_a((I + \nabla u(x))(z - X_i));
\]
\[
m_1(x, z) = -J(x) \sum_{X_i \in L} m'_a \sum_{|\beta|=2} \frac{1}{\beta!} \frac{\partial^\beta \tau(x)}{\partial x^\beta} (X_i - z)^\beta;
\]
\[
m_2(x, z) = J(x) \frac{1}{2} \sum_{X_i \in L} m''_a \left( \sum_{|\beta|=2} \frac{1}{\beta!} \frac{\partial^\beta \tau(x)}{\partial x^\beta} (X_i - z)^\beta \right)^2
\]
\[
- J(x) \sum_{X_i \in L} m'_a \sum_{|\beta|=4} \frac{1}{\beta!} \frac{\partial^\beta \tau(x)}{\partial x^\beta} (X_i - z)^\beta.
\]

Notice that the functions $m_i(\cdot, \cdot)$ are smooth and periodic in both variables. It is also important to note that terms in the form $O(\cdot)$ can be easily controlled using the smoothness assumptions.

We summarize the properties of $m_i$ in the following lemma

**Lemma 9.1.**

(a) $\langle m_0(x, \cdot) \rangle = Z$ and $\langle m_1(x, \cdot) \rangle = 0$ for all $x \in \Gamma$. 
(b) As $M_A = \sup_j \| \nabla^j u \|_{L^\infty} \rightarrow 0$

\[
\| \nabla u_0 \|_{L^\infty(\Gamma \times \Gamma)} = O(M_A);
\]

\[
\| m_i \|_{L^\infty(\Gamma \times \Gamma)} = O(M_A), \quad i \geq 1.
\]

(c) For $i \geq 1$, we have

\[
\int_{\Gamma} \int_{\Gamma} m_i(x, z) \, dz \, dx = 0.
\]

**Proof.** The proof for (a) and (b) is straightforward by definition. For (c), notice that by definition, we have

\[
\int_{\Gamma} m_\xi(x) \, dx = Z/\varepsilon^{-3},
\]

and by (a),

\[
\int \int \varepsilon^{-3} m_0(x, z) \, dx \, dz = Z/\varepsilon^{-3}.
\]

Since

\[
m_\xi(x) = \varepsilon^{-3} m_0(x, x/\varepsilon) + \varepsilon^{-2} m_1(x, x/\varepsilon) + \varepsilon^{-1} m_2(x, x/\varepsilon) + O(1),
\]

we have

\[
Z/\varepsilon^{-3} = \int_{\Gamma} \varepsilon^{-3} m_0(x, x/\varepsilon) + \varepsilon^{-2} m_1(x, x/\varepsilon) + \varepsilon^{-1} m_2(x, x/\varepsilon) + O(1).
\]

As $\varepsilon$ goes to zero, we have

\[
\lim_{\varepsilon \to 0} \int_{\Gamma} m_i(x, x/\varepsilon) \, dx = \int_{\Gamma} \int_{\Gamma} m_i(x, z) \, dz \, dx.
\]

Therefore, since (9.13) must be satisfied at every order, we obtain

\[
\int_{\Gamma} \int_{\Gamma} m_i(x, z) \, dz \, dx = 0.
\]

□

Next, we look for an approximation of the Coulomb potential $\phi_\xi$ in the form:

\[
\tilde{\phi}_\xi(x) = \phi_0(x, x/\varepsilon) + \varepsilon \phi_1(x, x/\varepsilon) + \varepsilon^2 \phi_2(x, x/\varepsilon),
\]

where $\phi_i(x, z)$ are periodic in the $z$ variable. The action of $-a_{ij} \partial_i \partial_j - b_i \partial_i$ on a two scale function $f(x, x/\varepsilon)$ can be written as

\[
(-a_{ij} \partial_i \partial_j - b_i \partial_i) f(x, x/\varepsilon) = -\varepsilon^{-2} a_{ij}(x) \partial_i \partial_j f(x, x/\varepsilon)
\]

\[
- 2\varepsilon^{-1} a_{ij}(x) \partial_i \partial_z f(x, x/\varepsilon) - \varepsilon^{-1} b_i(x) \partial_z f(x, x/\varepsilon)
\]

\[
- a_{ij}(x) \partial_z \partial_j f(x, x/\varepsilon) - b_i(x) \partial_z f(x, x/\varepsilon)
\]

\[
= -\varepsilon^{-2} L_0 f(x, x/\varepsilon) - \varepsilon^{-1} L_1 f(x, x/\varepsilon) - L_2 f(x, x/\varepsilon)
\]
where the last equality serves as the definition for $L_0, L_1$ and $L_2$. Substituting into equation (9.6) and collecting orders, we have

\begin{align}
(9.14) & \quad -L_0 \phi_0(x, z) = 4\pi (\rho_0(x, z) - m_0(x, z)), \\
(9.15) & \quad -L_0 \phi_1(x, z) = 4\pi (\rho_1(x, z) - m_1(x, z)) + L_1 \phi_0(x, z), \\
(9.16) & \quad -L_0 \phi_2(x, z) = 4\pi (\rho_2(x, z) - m_2(x, z)) + L_1 \phi_1(x, z) + L_2 \phi_0(x, z), \\
(9.17) & \quad -L_0 \phi_3(x, z) = 4\pi (\rho_3(x, z) - m_3(x, z)) + L_1 \phi_2(x, z) + L_2 \phi_1(x, z).
\end{align}

Therefore the leading order term $\phi_0(x, z)$ is determined by (9.14) and the solvability condition of (9.16):

\begin{align}
(9.18) & \quad \begin{cases}
-L_0 \phi_0(x, z) = 4\pi (\rho_0(x, z) - m_0(x, z)), \\
-L_2 \langle \phi_0(x, \cdot) \rangle = 4\pi (\langle \rho_2(x, \cdot) \rangle - \langle m_2(x, \cdot) \rangle).
\end{cases}
\end{align}

Similarly

\begin{align}
(9.19) & \quad \begin{cases}
-L_0 \phi_1(x, z) = 4\pi (\rho_1(x, z) - m_1(x, z)) + L_1 \phi_0(x, z), \\
-L_2 \langle \phi_1(x, \cdot) \rangle = 4\pi (\langle \rho_3(x, \cdot) \rangle - \langle m_3(x, \cdot) \rangle).
\end{cases}
\end{align}

\begin{align}
(9.20) & \quad \begin{cases}
-L_0 \phi_2(x, z) = 4\pi (\rho_2(x, z) - m_2(x, z)) + L_1 \phi_1(x, z) + L_2 \phi_0(x, z), \\
-L_2 \langle \phi_2(x, \cdot) \rangle = 4\pi (\langle \rho_4(x, \cdot) \rangle - \langle m_4(x, \cdot) \rangle).
\end{cases}
\end{align}

Moreover, the solvability condition for (9.14) and (9.15) implies the constraints

\[ \langle \rho_0(x, \cdot) \rangle = \langle m_0(x, \cdot) \rangle = Z, \quad \langle \rho_1(x, \cdot) \rangle = \langle m_1(x, \cdot) \rangle = 0. \]

for all $x \in \Gamma$.

The exchange-correlation potential can be expressed using Taylor expansion as

\begin{align}
\eta(J(x)^{-1} \varepsilon^3 \rho(x)) = & \eta(J(x)^{-1} \rho_0(x, x/\varepsilon) + \varepsilon J(x)^{-1} \rho_1(x, x/\varepsilon) \\
& + \varepsilon^2 J(x)^{-1} \rho_2(x, x/\varepsilon) + \mathcal{O}(\varepsilon^3)) \\
& \quad + \frac{1}{2} \varepsilon^2 \psi(J(x)^{-1} \rho_1(x, x/\varepsilon))^2 + \mathcal{O}(\varepsilon^3) \\
& \quad + \frac{1}{2} \varepsilon \eta''(J(x)^{-1} \rho_0(x, x/\varepsilon)) J(x)^{-1} \rho_1(x, x/\varepsilon) + \mathcal{O}(\varepsilon^3) \\
& \quad = \eta_0(x, x/\varepsilon) + \varepsilon \eta_1(x, x/\varepsilon) + \varepsilon^2 \eta_2(x, x/\varepsilon) + \mathcal{O}(\varepsilon^3),
\end{align}

where $\eta'$ and $\eta''$ are evaluated at $J(x)^{-1} \rho_0(x, x/\varepsilon)$. The last equality defines $\eta_i(x, z)$:

\begin{align}
(9.22) & \quad \eta_0(x, z) = \eta(J(x)^{-1} \rho_0(x, z)); \\
(9.23) & \quad \eta_1(x, z) = \eta'(J(x)^{-1} \rho_0(x, z)) J(x)^{-1} \rho_1(x, z); \\
(9.24) & \quad \eta_2(x, z) = \eta''(J(x)^{-1} \rho_0(x, z)) J(x)^{-1} \rho_1(x, z) \\
& \quad + \frac{1}{2} \eta''(J(x)^{-1} \rho_0(x, z))(J(x)^{-1} \rho_1(x, z))^2.
\end{align}
Hence, the potential $V_\varepsilon^\varepsilon$ can be approximated by
\begin{equation}
V_\varepsilon^\varepsilon(x) = V_\varepsilon(x, x/\varepsilon) + \varepsilon V_1(x, x/\varepsilon) + \varepsilon^2 V_2(x, x/\varepsilon)
\end{equation}
where
\begin{equation}
V_i(x, z) = \phi_i(x, z) + \eta_i(x, z).
\end{equation}
The $V_i$'s are $\Gamma$-periodic in the second variable. Higher order approximations can be constructed accordingly.

### 9.2. Two-scale structure of the Kohn-Sham map.

In this subsection, we construct the two scale approximation for the image of the Kohn-Sham map, assuming that the effective potential $V_\varepsilon^\varepsilon$ is given in a two-scale form
\begin{equation}
V_\varepsilon^\varepsilon(x) = V_0(x, x/\varepsilon) + \varepsilon V_1(x, x/\varepsilon) + \varepsilon^2 V_2(x, x/\varepsilon) + \varepsilon^3 V_3(x, x/\varepsilon) + O(\varepsilon^4).
\end{equation}
The asymptotic analysis is based on the resolvent expansion and the localization property of the Green’s functions.

The Hamiltonian takes the following form
\begin{equation}
H_\varepsilon^\varepsilon = -\varepsilon^2 a_{ij}(x) \partial_i \partial_j - \varepsilon^2 b_i(x) \partial_i - \varepsilon^2 c(x) + V_\varepsilon^\varepsilon.
\end{equation}
Given $x_0$, define the leading order Hamiltonian by
\begin{equation}
H_0^\varepsilon(x_0) = -\varepsilon^2 a_{ij}(x_0) \partial_i \partial_j + V_0(x_0, x/\varepsilon)
\end{equation}
and let $\delta H_\varepsilon(x_0)$ be the difference between $H_\varepsilon^\varepsilon$ and $H_0^\varepsilon(x_0)$
\begin{equation}
\delta H_\varepsilon(x_0) = -\varepsilon^2 (a_{ij}(x) - a_{ij}(x_0)) \partial_i \partial_j - \varepsilon^2 b_i(x) \partial_i - \varepsilon^2 c(x) + V_\varepsilon^\varepsilon(x) - V_0(x_0, x/\varepsilon).
\end{equation}
Further expand $\delta H_\varepsilon(x_0)$ as
\begin{equation}
\delta H_\varepsilon(x_0) = \delta H_1^\varepsilon(x_0) + \delta H_2^\varepsilon(x_0) + \delta H_3^\varepsilon(x_0) + \text{h.o.t.},
\end{equation}
where the higher order terms are omitted and
\begin{align}
\delta H_1^\varepsilon(x_0) &= -\varepsilon^2 ((x - x_0) \cdot \partial_\varepsilon a_{ij}(x_0)) \partial_i \partial_j - \varepsilon^2 b_i(x_0) \partial_i \\
&\quad + \varepsilon^2 (c(x_0) + \frac{1}{2} ((x - x_0) \cdot \partial_\varepsilon b_i(x_0)) \partial_i \\
&\quad + \varepsilon ((x - x_0) \cdot \partial_\varepsilon V_1(x_0, x/\varepsilon) + \varepsilon^2 V_2(x_0, x/\varepsilon));
\end{align}
\begin{align}
\delta H_2^\varepsilon(x_0) &= -\varepsilon^2 \frac{1}{2} ((x - x_0) \cdot \partial_\varepsilon)^2 a_{ij}(x_0) \partial_i \partial_j - \varepsilon^2 ((x - x_0) \cdot \partial_\varepsilon b_i(x_0)) \partial_i \\
&\quad - \varepsilon^2 c(x_0) + \frac{1}{2} ((x - x_0) \cdot \partial_\varepsilon)^2 V_0(x_0, x/\varepsilon) \\
&\quad + \varepsilon ((x - x_0) \cdot \partial_\varepsilon V_1(x_0, x/\varepsilon) + \varepsilon^2 V_2(x_0, x/\varepsilon));
\end{align}
\begin{align}
\delta H_3^\varepsilon(x_0) &= -\varepsilon^2 \frac{1}{6} ((x - x_0) \cdot \partial_\varepsilon)^3 a_{ij}(x_0) \partial_i \partial_j - \varepsilon^2 \frac{1}{2} ((x - x_0) \cdot \partial_\varepsilon)^2 b_i(x_0) \partial_i \\
&\quad - \varepsilon^2 ((x - x_0) \cdot \partial_\varepsilon c(x_0) + \frac{1}{2} ((x - x_0) \cdot \partial_\varepsilon)^3 V_0(x_0, x/\varepsilon) \\
&\quad + \varepsilon \frac{1}{2} ((x - x_0) \cdot \partial_\varepsilon)^2 V_1(x_0, x/\varepsilon) + \varepsilon^2 (x - x_0) \cdot \partial_\varepsilon V_2(x_0, x/\varepsilon) \\
&\quad + \varepsilon^3 V_3(x_0, x/\varepsilon)).
\end{align}
Using the resolvent identity, we have

\[
\frac{1}{\lambda - H_\varepsilon} = \frac{1}{\lambda - H_0^\varepsilon(x_0)} + \frac{1}{\lambda - H_0^\varepsilon(x_0)} \delta H^\varepsilon(x_0) \frac{1}{\lambda - H_0^\varepsilon(x_0)}
\]

\[
+ \frac{1}{\lambda - H_0^\varepsilon(x_0)} \delta H^\varepsilon(x_0) \frac{1}{\lambda - H_0^\varepsilon(x_0)} \delta H^\varepsilon(x_0) \frac{1}{\lambda - H_0^\varepsilon(x_0)}
\]

\[
+ \frac{1}{\lambda - H_0^\varepsilon(x_0)} \left( \delta H^\varepsilon(x_0) \frac{1}{\lambda - H_0^\varepsilon(x_0)} \right)^3 + \mathcal{O}(\varepsilon^4).
\]

Substituting in the expression of \(H_0^\varepsilon\) and \(\delta H^\varepsilon\), we obtain the following form for the density corresponding to \(H_\varepsilon\):

\[
\frac{1}{2\pi i} \int_{\mathcal{C}} \frac{1}{\lambda - H_\varepsilon} d\lambda(x,x) = \frac{1}{2\pi i} \int_{\mathcal{C}} \frac{1}{\lambda - H_0(x)} d\lambda(x,x)
\]

\[
+ \frac{1}{2\pi i} \int_{\mathcal{C}} \frac{1}{\lambda - H_0(x)} \delta H_1^\varepsilon(x) \frac{1}{\lambda - H_0(x)} d\lambda(x,x)
\]

\[
+ \frac{1}{2\pi i} \int_{\mathcal{C}} \frac{1}{\lambda - H_0(x)} \delta H_2^\varepsilon(x) \frac{1}{\lambda - H_0(x)} d\lambda(x,x)
\]

\[
+ \frac{1}{2\pi i} \int_{\mathcal{C}} \frac{1}{\lambda - H_0(x)} \left( \delta H_1^\varepsilon(x) \frac{1}{\lambda - H_0(x)} \right)^2 d\lambda(x,x)
\]

+ h.o.t.

Substituting in the expression for \(\delta H_1^\varepsilon\), \(\delta H_2^\varepsilon\) and \(\delta H_3^\varepsilon\), we get

\[
\frac{1}{2\pi i} \int_{\mathcal{C}} \frac{1}{\lambda - H_\varepsilon} d\lambda(x,x) = \varepsilon^{-3} w_0(x,x/\varepsilon) + \varepsilon^{-2} w_1(x,x/\varepsilon)
\]

\[
+ \varepsilon^{-1} w_2(x,x/\varepsilon) + w_3(x,x/\varepsilon) + \mathcal{O}(\varepsilon),
\]

where

(9.35) \( w_0(x,z) = \frac{1}{2\pi i} \int_{\mathcal{C}} \frac{1}{\lambda - H_0(x)} d\lambda(z,z), \quad H_0(x) = -a_{ij}(x) \partial_j \partial_j + V_0(x,z) \)

the latter is viewed as an operator on \(L^2_z(\mathbb{R}^3)\) with \(x\) as a parameter,

(9.36) \( w_1(x,z) = \frac{1}{2\pi i} \int_{\mathcal{C}} \frac{1}{\lambda - H_0(x)} \delta H_1(x,z) \frac{1}{\lambda - H_0(x)} d\lambda(z,z), \)

(9.37) \( w_2(x,z) = \frac{1}{2\pi i} \int_{\mathcal{C}} \frac{1}{\lambda - H_0(x)} \delta H_2(x,z) \frac{1}{\lambda - H_0(x)} d\lambda(z,z)
\]

\[
+ \frac{1}{2\pi i} \int_{\mathcal{C}} \frac{1}{\lambda - H_0(x)} \left( \delta H_1(x,z) \frac{1}{\lambda - H_0(x)} \right)^2 d\lambda(z,z),
\]
with
\[ w_3(x, z) = \frac{1}{2\pi i} \int_{\ell} \frac{1}{\lambda - H_0(x)} \delta H_3(x, z) \frac{1}{\lambda - H_0(x)} \, d\lambda(z, z) \]
\[ + \frac{1}{2\pi i} \int_{\ell} \frac{1}{\lambda - H_0(x)} \delta H_1(x, z) \frac{1}{\lambda - H_0(x)} \, d\lambda(z, z) \times \delta H_2(x, z) \frac{1}{\lambda - H_0(x)} \, d\lambda(z, z) \]
\[ + \frac{1}{2\pi i} \int_{\ell} \frac{1}{\lambda - H_0(x)} \left( \delta H_1(x, z) \frac{1}{\lambda - H_0(x)} \right)^2 \, d\lambda(z, z), \]
(9.38)

the \( \delta H_i \)'s are operators on \( L^2(\Gamma) \) with \( x \) and \( z \) as parameters:
\[ \delta H_1(x, z) = -(\zeta - z) \cdot \partial_x a_{ij}(x) \partial_{\zeta i} \partial_{\zeta j} - b_i(x) \partial_{\zeta i} + (\zeta - z) \cdot \partial_x V_0(x, \zeta) + V_1(x, \zeta); \]
\[ \delta H_2(x, z) = -\frac{1}{2}((\zeta - z) \cdot \partial_x)^2 a_{ij}(x) \partial_{\zeta i} \partial_{\zeta j} - (\zeta - z) \cdot \partial_x b_i(x) \partial_{\zeta i} - c(x) \]
\[ + \frac{1}{2}((\zeta - z) \cdot \partial_x)^2 V_0(x, \zeta) + (\zeta - z) \cdot \partial_x V_1(x, \zeta) + V_2(x, \zeta); \]
\[ \delta H_3(x, z) = -\frac{1}{6}((\zeta - z) \cdot \partial_x)^3 a_{ij}(x) \partial_{\zeta i} \partial_{\zeta j} - \frac{1}{2}((\zeta - z) \cdot \partial_x)^2 b_i(x) \partial_{\zeta i} \]
\[ - (\zeta - z) \cdot \partial_x e(x) + \frac{1}{6}((\zeta - z) \cdot \partial_x)^3 V_0(x, \zeta) \]
\[ + \frac{1}{2}((\zeta - z) \cdot \partial_x)^2 V_1(x, \zeta) + (\zeta - z) \cdot \partial_x V_2(x, \zeta) + V_3(x, \zeta). \]
Here and in the following \( \zeta \) is a dummy variable and the operators act on functions in \( \zeta \).

9.3. Asymptotic analysis of the Kohn-Sham equation. Now we are ready to construct asymptotic solutions to the Kohn-Sham equation.

9.3.1. The leading order term. For the leading order, we have
\[ \rho_0(x, z) = \frac{1}{2\pi i} \int_{\ell} \frac{1}{\lambda + a_{ij}(x) \partial_{\zeta i} \partial_{\zeta j} - V_0(x, \zeta)} \, d\lambda(z, z); \]
\[ V_0(x, z) = \phi_0(x, z) + \eta(J(x)^{-1} \rho_0(x, z)); \]
\[ -L_0 \phi_0(x, z) = 4\pi(\rho_0(x, z) - m_0(x, z)); \]
\[ -L_2 \phi_0(x, \cdot) = 4\pi(\rho_2(x, \cdot) - m_2(x, \cdot)). \]
(9.40)

The set of equations are not closed since \( \phi_0 \) depends on \( \langle \rho_2(x, \cdot) \rangle \). We break \( V_0 \) into two parts: \( V_0(x, z) = v_0(x, z) + U_0(x) \), where \( U_0(x) = \langle \phi_0(x, \cdot) \rangle \) contains the macroscopic part of the Coulomb potential which depends on \( \langle \rho_2(x, \cdot) \rangle \), while \( v_0(x, z) \) consists of the remaining microscopic part. \( U_0 \) satisfies
\[ -L_2 U_0(x) = 4\pi(\langle \rho_2(x, \cdot) \rangle - \langle m_2(x, \cdot) \rangle). \]
(9.41)
Rewrite (9.39) using $v_0$ and $U_0$ as

$$
\rho_0(x, z) = \frac{1}{2\pi i} \int_{\mathcal{C}} \frac{1}{\lambda + a_{ij}(x)\partial_{\zeta_i}\partial_{\zeta_j} - v_0(x, \zeta) - U_0(x)} \mathrm{d}\lambda(z, z)
$$

(9.42)

$$
= \frac{1}{2\pi i} \int_{\mathcal{C}_x} \frac{1}{\lambda + a_{ij}(x)\partial_{\zeta_i}\partial_{\zeta_j} - v_0(x, \zeta)} \mathrm{d}\lambda(z, z),
$$

where the shifted contour $\mathcal{C}_x$ is defined as $\mathcal{C}_x = \{ \lambda - U_0(x) \mid \lambda \in \mathcal{C} \}$. By Cauchy’s theorem, if

$$
U_0(x) < \text{dist}(\mathcal{C}, \text{spec}(\mathcal{H}_0(x))),
$$

the contour integral will remain the same even though the contour is shifted. Therefore, we will have

$$
\rho_0(x, z) = \frac{1}{2\pi i} \int_{\mathcal{C}_x} \frac{1}{\lambda + a_{ij}(x)\partial_{\zeta_i}\partial_{\zeta_j} - v_0(x, \zeta)} \mathrm{d}\lambda(z, z).
$$

(9.44)

Recall that $v_0(x, z)$ satisfies

$$
\begin{align*}
\rho_0(x, z) &= \phi_0(x, z) - \langle \phi_0(x, \cdot) \rangle + \eta(J(x)^{-1}\rho_0(x, z)); \\
-L_0\phi_0(x, z) &= 4\pi(\rho_0(x, z) - m_0(x, z)),
\end{align*}
$$

(9.45)

with periodic boundary condition on the second variable of $\phi_0$ and $\langle \phi_0(x, \cdot) \rangle = 0$. We obtain a closed set of equations in $\rho_0$ and $v_0$. The solution to the system (9.44)-(9.45) is given by the Cauchy-Born solution corresponding to the system with homogeneous deformation with gradient $\nabla u(x)$:

$$
\rho_0(x, z) = \rho_{\text{CB}}(z; \nabla u(x)), \quad v_0(x, z) = V_{\text{CB}}(z; \nabla u(x)).
$$

(9.46)

By Theorem 4.1, we know that $\rho_0(x, z) \in C^\infty(\Gamma, H^6_{\text{per}}(\Gamma)) \subset C^\infty(\Gamma, W^{4, \infty}_{\text{per}}(\Gamma))$. Hence $v_0(x, z) \in C^\infty(\Gamma, W^{4, \infty}_{\text{per}}(\Gamma))$.

9.3.2. The next order term. The next set of equations from the $O(\varepsilon)$ terms are

$$
\rho_1(x, z) = \frac{1}{2\pi i} \int_{\mathcal{C}} \frac{1}{\lambda - \mathcal{H}_0(x)} \frac{1}{\lambda - \mathcal{H}_0(x)} \mathrm{d}\lambda(z, z);
$$

(9.47)

$$
\begin{align*}
V_1(x, z) &= \phi_1(x, z) + \eta_1(x, z); \\
-L_0\phi_1(x, z) &= 4\pi(\rho_1(x, z) - m_1(x, z)) + L_1\phi_0(x, z); \\
-L_2(\phi_1(x, \cdot)) &= 4\pi((\rho_3(x, \cdot)) - \langle m_3(x, \cdot) \rangle); \\
\eta_1(x, z) &= \eta'(J(x)^{-1}\rho_0(x, z))J(x)^{-1}\rho_1(x, z).
\end{align*}
$$

(9.48)

Here, we may take

$$
\mathcal{H}_0(x) = -a_{ij}(x)\partial_{\zeta_i}\partial_{\zeta_j} + v_0(x, \zeta),
$$

as long as (9.43) holds, by the same argument as before. The set of equations (9.47)-(9.48) is not closed, for two reasons: $\langle \phi_1 \rangle$ and hence $V_1$ depend on $\langle \rho_3(x, \cdot) \rangle$; the right-hand side of (9.47) depends on $U_0$, which is not determined yet (since it depends on $\langle \rho_2(x, \cdot) \rangle$).
To deal with the first problem, again let us break $V_1$ into a macroscopic part and a microscopic part:

(9.49) \[ U_1(x) = \langle \phi_1(x, \cdot) \rangle, \quad \text{and} \quad v_1(x) = V_1(x, z) - U_1(x). \]

Observe that the dependence of $\rho_1$ on $U_1$ is given by

(9.50) \[
\frac{1}{2\pi i} \int_{\mathcal{C}} \frac{1}{\lambda - H_0(x)} U_1(x) \frac{1}{\lambda - H_0(x)} \, d\lambda(z, z)
\]
\[
= \frac{1}{2\pi i} U_1(x) \int_{\mathcal{C}} \left( \frac{1}{\lambda - H_0(x)} \right)^2 \, d\lambda(z, z),
\]

since $U_1(x)$ does not depend on $z$. By the spectral representation of $H_0(x)$ and the Cauchy theorem, the right-hand side of (9.50) vanishes. Therefore, $U_1$ does not contribute to $\rho_1$, and we may rewrite (9.47) as

(9.51) \[
\rho_1(x, z) = \frac{1}{2\pi i} \int_{\mathcal{C}} \frac{1}{\lambda - H_0(x)} (-\zeta - z) \cdot \partial_\zeta a_{ij}(x) \partial_\zeta \partial_j - b_i(x) \partial_\zeta
\]
\[
+ (\zeta - z) \cdot \partial_\zeta V_0(x, \zeta) + v_1(x, \zeta)) \frac{1}{\lambda - H_0(x)} \, d\lambda(z, z),
\]

with $v_1$ given by

(9.52) \[
\begin{aligned}
v_1(x, z) &= \phi_1(x, z) - \langle \phi_1(x, \cdot) \rangle + \eta_1(x, z); \\
-L_0 \phi_1(x, z) &= 4\pi (p_1(x, z) - m_1(x, z)) + L_1 \phi_0(x, z); \\
\eta_1(x, z) &= \eta'(J(x)^{-1} \rho_0(x, z)) J(x)^{-1} \rho_1(x, z).
\end{aligned}
\]

We next decompose $v_1$ further into two parts $v_1 = v_{1,1} + v_{1,2}$, with $v_{1,1}$ depending on $\rho_1$ and $v_{1,2}$ independent of $\rho_1$:

(9.53) \[
-L_0 v_{1,2}(x, z) = -4\pi m_1(x, z) + L_1 \phi_0(x, z).
\]

The above equation for $v_{1,2}$ is solvable since $\langle m_1(x, \cdot) \rangle = 0$. For later use, let us denote the dependence of $v_{1,1}$ on $\rho_1$ by an operator $\mathcal{V}_x$, $v_{1,1}(x, z) = \mathcal{V}_x p_1(x, z)$:

(9.54) \[
\begin{aligned}
\mathcal{V}_x w(x, z) &= \phi(x, z) + \eta(x, z); \\
-L_0 \phi(x, z) &= 4\pi w(x, z), \quad \text{with} \quad \langle \phi(x, \cdot) \rangle = 0; \\
\eta(x, z) &= \eta'(J(x)^{-1} \rho_0(x, z)) J(x)^{-1} w(x, z).
\end{aligned}
\]

Recall that $L_0 = a_{ij}(x) \partial_\zeta \partial_j$, also depends on $x$ through $a_{ij}(x)$.

Using the linearized Kohn-Sham operator for a system with homogeneous deformation gradient $\nabla u(x)$: $\mathcal{L}_x = \mathcal{L}_{\nabla u(x)}$, we may then rewrite the set of equations
Lemma 9.2. For $f$ and $g$, where the functions $f$ and $g$ are given by

$$f_1(x,z) = \frac{1}{2\pi i} \int_{\gamma} \frac{1}{\lambda - \mathcal{H}_0(x)} \cdots$$

and

$$g_1(x,z) = \frac{1}{2\pi i} \int_{\gamma} \frac{1}{\lambda - \mathcal{H}_0(x)} \cdots$$

For $f_1$ and $g_1$, we have the following lemma.

**Lemma 9.2.** $f_1 \in C^\infty(\Gamma, H^4(\Gamma))$ and $g_1 \in C^\infty(\Gamma, H^4(\Gamma))$. Moreover, $\langle f_1(x, \cdot) \rangle = 0$ and $\langle g_1(x, \cdot) \rangle = 0$.

**Proof.** Using the symmetry of the operator $\mathcal{H}_0(x)$, we have

$$g_1(x, -z) = \frac{1}{2\pi i} \int_{\gamma} \frac{1}{\lambda - \mathcal{H}_0(x)}(-\zeta + z) \cdots$$

It follows that $\langle g_1(x, \cdot) \rangle = 0$.

The calculations for $f_1$ is similar:

$$f_1(x, -z) = \frac{1}{2\pi i} \int_{\gamma} \frac{1}{\lambda - \mathcal{H}_0(x)}(-\zeta + z) \cdots$$

The second equality holds since $\partial_x v_0(x,z)$ is an even function of $z$ and $v_{1,2}(x,z)$ is odd in $z$. Taking average of $f_1$, we conclude that $\langle f_1(x, \cdot) \rangle = 0$.
For the regularity property, by definition,

$$ f_1(x, z) = \frac{1}{2\pi i} \int_{\mathcal{C}} \frac{1}{\lambda - \mathcal{H}_0(x)} \left( - (\xi - z) \cdot \partial_x a_{ij}(x) \partial_{\xi_j} \partial_{\xi_i} - b_i(x) \partial_{\xi_i} + (\xi - z) \cdot \partial_z v_0(x, \xi) + v_{1, 2}(x, \xi) \right) \frac{1}{\lambda - \mathcal{H}_0(x)} \, d\lambda(z, z). $$

For the four terms in the bracket, let us consider only the first term, the argument for the other terms is analogous and actually simpler. Let

$$ f_{1,1}(x, z) = -\frac{1}{2\pi i} \int_{\mathcal{C}} \frac{1}{\lambda - \mathcal{H}_0(x)} (\xi - z) \cdot \partial_x a_{ij}(x) \partial_{\xi_j} \partial_{\xi_i} \frac{1}{\lambda - \mathcal{H}_0(x)} \, d\lambda(z, z). $$

The boundedness of $f_{1,1}(x, z)$ follows from Proposition 8.5. Taking derivative with respect to $z$, we have

$$ \nabla_z f_{1,1}(x, z) = -\frac{1}{2\pi i} \int_{\mathcal{C}} \nabla_\xi \left[ \frac{1}{\lambda - \mathcal{H}_0(x)} \right] (\xi - z) \cdot \partial_x a_{ij}(x) \partial_{\xi_j} \partial_{\xi_i} \frac{1}{\lambda - \mathcal{H}_0(x)} \, d\lambda(z, z) $$

$$ + \frac{1}{2\pi i} \int_{\mathcal{C}} \frac{1}{\lambda - \mathcal{H}_0(x)} (\xi - z) \cdot \partial_x a_{ij}(x) \frac{1}{\lambda - \mathcal{H}_0(x)} \, d\lambda(z, z). $$

Here we have simplified the expression using the obvious fact that

$$ (\nabla_\xi + \nabla_z) ((\xi - z) \cdot \partial_x a_{ij}(x)) = 0. $$

Let us consider the second term in the expression of $\nabla_z f_{1,1}$, the first term follows from a similar argument after integration by parts. Notice that

$$ \left[ \nabla_\xi, \frac{1}{\lambda - \mathcal{H}_0(x)} \right] = \frac{1}{\lambda - \mathcal{H}_0(x)} \partial_z v_0(x, z) \frac{1}{\lambda - \mathcal{H}_0(x)}. $$

Thus, considered as a function in $\xi$, we have

$$ \left\| \partial_{\xi_i} \partial_{\xi_j} \left[ \nabla_\xi, \frac{1}{\lambda - \mathcal{H}_0(x)} \right](\xi, z) \right\|_{L^2_\xi} \lesssim \| v_0(x, \cdot) \|_{W^{1, \infty}}. $$

By compactness of the contour $\mathcal{C}$, and the Schwartz inequality, we have

$$ \left| -\frac{1}{2\pi i} \int_{\mathcal{C}} \frac{1}{\lambda - \mathcal{H}_0(x)} (\xi - z) \cdot \partial_x a_{ij}(x) \partial_{\xi_j} \partial_{\xi_i} \left[ \nabla_\xi, \frac{1}{\lambda - \mathcal{H}_0(x)} \right] \, d\lambda(z, z) \right| $$

$$ \lesssim \| \partial_x a_{ij} \|_{L^\infty} \left\| \partial_{\xi_i} \partial_{\xi_j} \left[ \nabla_\xi, \frac{1}{\lambda - \mathcal{H}_0(x)} \right](\xi, z) \right\|_{L^2_\xi} \left\| (\xi - z) \frac{1}{\lambda - \mathcal{H}_0(x)}(z, \xi) \right\|_{L^2_\xi}. $$

Therefore, for any $x$, $\nabla_z f_{1,1}(x, \cdot) \in L^\infty_\xi(\Gamma)$. It is not hard to see that similar arguments can be used for higher order derivatives with respect to $z$. 

The Kohn-Sham Equation for Deformed Crystals
Taking derivative of $f_{1,1}$ with respect to $x$, we get
\[
\nabla_x f_{1,1}(x, z) = -\frac{1}{2\pi i} \int_{\mathbb{C}} \nabla_x \left( \frac{1}{\lambda - \mathcal{H}_0(x)} \right) (\zeta - z) \cdot \partial_x a_{ij}(x) \\
\times \partial_{\zeta_i} \partial_{\zeta_j} \frac{1}{\lambda - \mathcal{H}_0(x)} \, d\lambda(z, z) \\
- \frac{1}{2\pi i} \int_{\mathbb{C}} \frac{1}{\lambda - \mathcal{H}_0(x)} (\zeta - z) \cdot \partial_x \partial_{\zeta_i} a_{ij}(x) \\
\times \partial_{\zeta_i} \partial_{\zeta_j} \frac{1}{\lambda - \mathcal{H}_0(x)} \, d\lambda(z, z) \\
- \frac{1}{2\pi i} \int_{\mathbb{C}} \frac{1}{\lambda - \mathcal{H}_0(x)} (\zeta - z) \cdot \partial_{\zeta_i} a_{ij}(x) \\
\times \partial_{\zeta_i} \partial_{\zeta_j} \nabla_x \left( \frac{1}{\lambda - \mathcal{H}_0(x)} \right) \, d\lambda(z, z).
\]

The second term is bounded by Proposition 8.5. For the first and third terms, notice that
\[
\nabla_x \left( \frac{1}{\lambda - \mathcal{H}_0(x)} \right) = \frac{1}{\lambda - \mathcal{H}_0(x)} \nabla_x (\mathcal{H}_0(x)) \frac{1}{\lambda - \mathcal{H}_0(x)} \\
= \frac{1}{\lambda - \mathcal{H}_0(x)} (\nabla_x a_{ij}(x) \partial_{\zeta_i} \partial_{\zeta_j} + \partial_x v_0(x, \zeta)) \frac{1}{\lambda - \mathcal{H}_0(x)},
\]

using Proposition 8.6, they are bounded.

By a similar argument, using Propositions 8.5, 8.6 and 8.7, one can also prove the boundedness of higher order derivatives. Therefore, we conclude that $f_{1,1} \in C^\infty(\Gamma, H^4(\Gamma))$.

The argument for $g(x, z)$ is similar and we omit it here.

\[\square\]

Inverting $(\mathcal{I} - \mathcal{L}_x)$, we get
\[
(9.55) \quad \rho_1(x, z) = (\mathcal{I} - \mathcal{L}_x)^{-1} f_1(x, z) + \partial_x U_0(x) \cdot (\mathcal{I} - \mathcal{L}_x)^{-1} g_1(x, z).
\]

\[
(9.56) \quad v_{1,1}(x, z) = V_x (\mathcal{I} - \mathcal{L}_x)^{-1} f_1(x, z) + \partial_x U_0(x) \cdot V_x (\mathcal{I} - \mathcal{L}_x)^{-1} g_1(x, z)
= V_{f_1}(x, z) + \partial_x U_0(x) \cdot V_{g_1}(x, z),
\]

with $V_{f_1}(x, \cdot) = V_x (\mathcal{I} - \mathcal{L}_x)^{-1} f_1(x, \cdot)$ and $V_{g_1}(x, \cdot) = V_x (\mathcal{I} - \mathcal{L}_x)^{-1} g_1(x, \cdot)$. Therefore
\[
(9.57) \quad V_1(x, z) = U_1(x) + v_{1,2}(x, z) + V_{f_1}(x, z) + \partial_x U_0(x) \cdot V_{g_1}(x, z).
\]

By the regularity of $f_1$ and $g_1$ and the property of the operators $V_x$ and $(\mathcal{I} - \mathcal{L}_x)^{-1}$ (Proposition 6.15 and 7.5), we have $V_{f_1} \in C^\infty(\Gamma, H^4(\Gamma))$ and $V_{g_1} \in C^\infty(\Gamma, H^4(\Gamma))$.

So far, $\rho_1$ is not yet determined since we do not know $U_0(x)$. To obtain $U_0(x)$, let us look at the equation for $\rho_2$. Taking the average of both sides of (9.37) (and
replace \( w_2 \) by \( \rho_2 \), we get
\[
\langle \rho_2(x, \cdot) \rangle = \frac{1}{2\pi i} \left\langle \int_{\mathfrak{g}} \frac{1}{\lambda - \mathcal{H}_0(x)} \left( -\frac{1}{2}((\zeta - z) \cdot \partial_z)^2 a_{ij}(x) \partial_{\xi_i} \partial_{\xi_j} \\
+ (\zeta - z) \cdot \partial_z b_1(x) \partial_{\xi_i} - c(x) + \frac{1}{2}((\zeta - z) \cdot \partial_z)^2 V_0(x, \zeta) \right) \right\rangle
\]
\[
\left( \frac{1}{\lambda - \mathcal{H}_0(x)} \frac{1}{\lambda - \mathcal{H}_0(x)} \right) \left( \frac{1}{\lambda - \mathcal{H}_0(x)} \frac{1}{\lambda - \mathcal{H}_0(x)} \right) \left( \frac{1}{\lambda - \mathcal{H}_0(x)} \frac{1}{\lambda - \mathcal{H}_0(x)} \right)
\]
(9.58)
\[
\left( \frac{1}{\lambda - \mathcal{H}_0(x)} \frac{1}{\lambda - \mathcal{H}_0(x)} \right) \left( \frac{1}{\lambda - \mathcal{H}_0(x)} \frac{1}{\lambda - \mathcal{H}_0(x)} \right) \left( \frac{1}{\lambda - \mathcal{H}_0(x)} \frac{1}{\lambda - \mathcal{H}_0(x)} \right)
\]
\[
\left( \frac{1}{\lambda - \mathcal{H}_0(x)} \frac{1}{\lambda - \mathcal{H}_0(x)} \right) \left( \frac{1}{\lambda - \mathcal{H}_0(x)} \frac{1}{\lambda - \mathcal{H}_0(x)} \right) \left( \frac{1}{\lambda - \mathcal{H}_0(x)} \frac{1}{\lambda - \mathcal{H}_0(x)} \right)
\]
\[
\left( \frac{1}{\lambda - \mathcal{H}_0(x)} \frac{1}{\lambda - \mathcal{H}_0(x)} \right) \left( \frac{1}{\lambda - \mathcal{H}_0(x)} \frac{1}{\lambda - \mathcal{H}_0(x)} \right) \left( \frac{1}{\lambda - \mathcal{H}_0(x)} \frac{1}{\lambda - \mathcal{H}_0(x)} \right)
\]
Notice that compared to (9.37), we have dropped the terms depending on \( U_1 \) or \( V_2 \), since the contributions from these terms are zero. Indeed, for the term depending on \( V_2 \), we have
\[
\langle \int_{\mathfrak{g}} \frac{1}{\lambda - \mathcal{H}_0(x)} V_2(x, \zeta) \frac{1}{\lambda - \mathcal{H}_0(x)} d\lambda(z, z) \rangle
\]
\[
\sum_{n \leq 2} \sum_{m > 2} \int_{\mathbb{R}} \frac{d\xi}{\mathcal{E}_{x,m}(\xi) - \mathcal{E}_{x,n}(\xi)} \times
\]
\[
\times \left( \langle \overline{\psi}_{x,n,\xi} \psi_{x,n,\xi} \rangle \langle \overline{\psi}_{x,m,\xi} \psi_{x,m,\xi} \rangle V_2(x, \cdot) \rangle + c.c. \right)
\]
\[
= 0.
\]
For terms depending on \( U_1 \), we have
\[
\langle \int_{\mathfrak{g}} \frac{1}{\lambda - \mathcal{H}_0(x)} (\zeta - z) \cdot \partial_z U_1(x) \frac{1}{\lambda - \mathcal{H}_0(x)} d\lambda(z, z) \rangle
\]
\[
= \langle \int_{\mathfrak{g}} \frac{1}{\lambda - \mathcal{H}_0(x)} (\zeta - z) \frac{1}{\lambda - \mathcal{H}_0(x)} d\lambda(z, z) \rangle \cdot \partial_z U_1(x) = 0,
\]
by Lemma 9.2. Moreover,
\[
\langle \int_{\mathfrak{g}} \frac{1}{\lambda - \mathcal{H}_0(x)} U_1(x) \frac{1}{\lambda - \mathcal{H}_0(x)} (- (\zeta - z) \cdot \partial_z a_{ij}(x) \partial_{\xi_i} \partial_{\xi_j} - b_1(x) \partial_{\xi_i} \\
+ (\zeta - z) \cdot \partial_z V_0(x, \zeta) + v_1(x, \zeta) \frac{1}{\lambda - \mathcal{H}_0(x)} d\lambda(z, z) \rangle = 0,
\]
since the term under the average is an odd function of \( z \). Finally, we have
\[
\langle \int_{\mathfrak{g}} \frac{1}{\lambda - \mathcal{H}_0(x)} U_1(x) \frac{1}{\lambda - \mathcal{H}_0(x)} U_1(x) \frac{1}{\lambda - \mathcal{H}_0(x)} d\lambda(z, z) \rangle
\]
\[
= |U_1(x)|^2 \langle \int_{\mathfrak{g}} \left( \frac{1}{\lambda - \mathcal{H}_0(x)} \right)^3 d\lambda(z, z) \rangle = 0
\]
using the spectral representation of $\mathcal{H}_0(x)$ and Cauchy’s theorem.

Now, observe that the right-hand side of (9.58) depends only on $V_0$ and $v_1$, and hence on $\langle \rho_2(x, \cdot) \rangle$. Therefore, (9.58) together with (9.52) and (9.55) form a closed system for $\langle \rho_2(x, \cdot) \rangle$ and $U_0$. Reorganizing the terms, we obtain the following equation for $\langle \rho_2(x, \cdot) \rangle$:

(9.59) \quad \langle \rho_2(x, \cdot) \rangle = A_{\alpha\beta}(x)\partial_{x\alpha}\partial_{x\beta}U_0(x) + B_{\alpha}(x)\partial_{x\alpha}U_0(x) + D(x).

The coefficients are given by

(9.60) \quad A_{\alpha\beta}(x) = \frac{1}{2\pi i} \left( \int \frac{1}{\lambda - \mathcal{H}_0(x)} \left( \frac{1}{2}(\zeta - z)_{\alpha}(\zeta - z)_{\beta} + (\zeta - z)_{\alpha}V_{g1,\beta}(x, \zeta) \right) \frac{1}{\lambda - \mathcal{H}_0(x)} d\lambda(z, z) \right),

where $V_{g1,\beta}$ is the $\beta$-component of $V_{g1}$.

\[
B_{\alpha}(x) = \frac{1}{2\pi i} \left( \int \frac{1}{\lambda - \mathcal{H}_0(x)} ((\zeta - z)_{\alpha} + V_{g1,\alpha}(x, \zeta)) \frac{1}{\lambda - \mathcal{H}_0(x)} d\lambda(z, z) \right) \times \delta H_1^1 \frac{1}{\lambda - \mathcal{H}_0(x)} \frac{\delta H_2^1}{\lambda - \mathcal{H}_0(x)} d\lambda(z, z),
\]

(9.61) \quad + \frac{1}{2\pi i} \left( \int \frac{1}{\lambda - \mathcal{H}_0(x)} ((\zeta - z)_{\alpha} + V_{g1,\alpha}(x, \zeta)) \frac{1}{\lambda - \mathcal{H}_0(x)} \times \delta H_1^1 \frac{1}{\lambda - \mathcal{H}_0(x)} \frac{\delta H_2^1}{\lambda - \mathcal{H}_0(x)} d\lambda(z, z) \right),

and,

(9.62) \quad D(x) = \frac{1}{2\pi i} \left( \int \frac{1}{\lambda - \mathcal{H}_0(x)} \delta H_1^1 \frac{1}{\lambda - \mathcal{H}_0(x)} \frac{\delta H_2^1}{\lambda - \mathcal{H}_0(x)} d\lambda(z, z) \right) \times \delta H_1^1 \frac{1}{\lambda - \mathcal{H}_0(x)} \frac{\delta H_2^1}{\lambda - \mathcal{H}_0(x)} d\lambda(z, z),

where the short hand notation $\delta H_1^1$ and $\delta H_2^1$ is used:

$\delta H_1^1 = -(\zeta - z) \cdot \partial_x a_{ij}(x) \partial_{\xi_i} \partial_{\xi_j} - b_i(x) \partial_{\xi_i}$,

$\delta H_2^1 = -\frac{1}{2}(\zeta - z) \cdot \partial_x^2 a_{ij}(x) \partial_{\xi_i} \partial_{\xi_j} - (\zeta - z) \cdot \partial_x b_i(x) \partial_{\xi_i} + (\zeta - z) \cdot \partial_x v_0(x, \zeta) + (\zeta - z) \cdot \partial_x (v_{1,2}(x, \zeta) + V_{f_1}(x, \zeta)),$

and

$\delta H_2^1 = -\frac{1}{2}((\zeta - z) \cdot \partial_x)^2 a_{ij}(x) \partial_{\xi_i} \partial_{\xi_j} - (\zeta - z) \cdot \partial_x b_i(x) \partial_{\xi_i} + \frac{1}{2}((\zeta - z) \cdot \partial_x)^2 v_0(x, \zeta) + (\zeta - z) \cdot \partial_x (v_{1,2}(x, \zeta) + V_{f_1}(x, \zeta)).$
In deriving (9.59), we have used the fact that the quadratic term in \( \partial_x U_0(x) \) in (9.58) vanishes:

\[
\frac{1}{2\pi i} \left\langle \int \frac{1}{\lambda - \mathcal{H}_0(x)} \left( (\zeta - z)_\alpha + V_{g_1,\alpha}(x, \zeta) \right) \frac{1}{\lambda - \mathcal{H}_0(x)} \right. \\
\times \left( (\zeta - z)_\beta + V_{g_1,\beta}(x, \zeta) \right) \frac{1}{\lambda - \mathcal{H}_0(x)} d\lambda(z, z) \left\rangle \partial_{x,\alpha} U_0(x) \partial_{x,\beta} U_0(x) = 0. \right.
\]

This is an immediate corollary of the following lemma, whose proof is deferred to Appendix A. Denote the coefficient in front of the term \( \partial_{x,\alpha} U_0(x) \partial_{x,\beta} U_0(x) \) by \( C_{\alpha\beta} \).

**Lemma 9.3.** \( C_{\alpha\beta} = -C_{\beta\alpha} \).

Replacing \( \langle \rho_2(x, \cdot) \rangle \) on the left hand side of (9.59) using (9.41), we obtain the equation for \( U_0 \) as

\[
(9.63) \quad A_{\alpha\beta} \partial_{x,\alpha} \partial_{x,\beta} U_0(x) + \frac{1}{4L_x^2} L_2 U_0(x) + B_\alpha \partial_{x,\alpha} U_0(x) + D - \langle m_2(x, \cdot) \rangle = 0
\]

with the constraint that \( \int U_0 dx = 0 \) to fix the arbitrary constant.

**Proposition 9.4.** (9.63) has a unique solution. The solution \( U_0 \) satisfies

\[ \|U_0\|_{L^\infty} = O(M_A). \]

In particular, \( U_0 \) satisfies (9.43) if \( M_A \) is sufficiently small.

**Remark.** \( U_0 \) is the macroscopic potential generated as a result of the crystal distortion, a manifestation of the piezoelectric effect of the material. (9.63) can be regarded as being the homogenized equation for the system under consideration.

Before proving this proposition, we need some preliminary results for the properties of the coefficients in (9.63).

**Lemma 9.5.** The coefficient \( A_{\alpha\beta} \in C^\infty(\Gamma) \) and is given by

\[
A_{\alpha\beta}(x) = -2\pi i \sum_{n \leq \mathbb{Z}, m > Z} \int_{\Gamma} \frac{d\xi}{E_{x,n}(\xi) - E_{x,m}(\xi)} \\
\times \langle u_{x,m,\xi}, \partial_{x,n,\xi} \rangle \langle u_{x,m,\xi}, \partial_{x,n,\xi} \rangle \langle g_{\xi}(x, \cdot), V_x(\mathcal{I} - L_x)^{-1} g_{\xi}(x, \cdot) \rangle.
\]

**Proof.** By definition,

\[
(9.65) \quad A_{\alpha\beta}(x) = \frac{1}{2\pi i} \left\langle \int \frac{1}{\lambda - \mathcal{H}_0(x)} \left( \frac{1}{\lambda - \mathcal{H}_0(x)} \left( (\zeta - z)_\alpha (\zeta - z)_\beta \\
+ (\zeta - z)_\alpha V_{g_1,\beta}(x, \zeta) \right) \frac{1}{\lambda - \mathcal{H}_0(x)} d\lambda(z, z) \right) \right. \\
\left\rangle \partial_{x,\alpha} U_0(x) \partial_{x,\beta} U_0(x) = 0. \right.
\]
For the first term in the bracket, we have (for simplicity of notation, the dependence on \(x\) is suppressed),

\[
A_{\alpha,1} = \frac{1}{2\pi i} \left\langle \int_{\mathcal{C}} \frac{1}{\lambda - \mathcal{H}_0} \frac{1}{2}(\zeta - z)_\alpha (\zeta - z)_\beta \frac{1}{\lambda - \mathcal{H}_0} \, d\lambda(z, z) \right\rangle
\]

(9.66)

\[
= \text{Re} \sum_{n \leq Z} \sum_{m > Z} \int_{[\Gamma]^2} d\xi d\eta \frac{1}{E_n(\xi) - E_m(\eta)}
\]

\[
\times \left\langle \psi^*_n(\xi) \psi_{m,\eta}(\xi) F_{n, \xi, m, \eta}^{\alpha, \beta}(\xi) \right\rangle,
\]

where

\[
F_{n, \xi, m, \eta}^{\alpha, \beta}(\xi) = \int_{\mathbb{R}^3} (\zeta - z)_\alpha (\zeta - z)_\beta \psi^*_n(\xi)(\zeta) \psi_{m,\eta}(\xi) \, d\zeta.
\]

Direct evaluation using the Poisson summation formula and orthogonality of the Bloch functions yields

\[
F_{n, \xi, m, \eta}^{\alpha, \beta}(\xi) = -\left\langle u_{m,\xi,\eta}, \partial_{\xi, \eta} u_{m,\xi,\eta} \right\rangle (\eta - \xi)|\Gamma^*| + \left\langle u_{m,\xi,\eta}, \partial_{\xi} u_{m,\xi,\eta} \right\rangle (\eta - \xi)|\Gamma^*|
\]

(9.67)

\[
+ \left\langle u_{m,\xi,\eta}, \partial_{\eta} u_{m,\xi,\eta} \right\rangle (\eta - \xi)|\Gamma^*|.
\]

in the weak sense. Therefore, by substituting the expression of \(F\) into (9.66), one obtains

\[
A_{\alpha,1} = -2\pi \sum_{n \leq Z} \sum_{m > Z} \int_{[\Gamma]^2} \frac{d\xi}{E_n(\xi) - E_m(\xi)}
\]

\[
\times \left\langle u_{m,\xi,\eta}, \partial_{\xi, \eta} u_{m,\xi,\eta} \right\rangle z \left\langle u_{m,\xi,\eta}, \partial_{\xi, \eta} u_{m,\xi,\eta} \right\rangle \xi.
\]

(9.68)

It is easy to see that the matrix \(A_1 = (A_{\alpha,1})_{1 \leq \alpha, \beta \leq 3}\) is positive definite, since by the ordering of eigenvalues and the gap condition, we always have \(E_n(\xi) < E_m(\xi)\), if \(n \leq Z < m\).

Similarly,

\[
A_{\alpha,2} = \frac{1}{2\pi i} \left\langle \int_{\mathcal{C}} \frac{1}{\lambda - \mathcal{H}_0} (\zeta - z)_\alpha V_{g_{1,\beta}}(\zeta) \frac{1}{\lambda - \mathcal{H}_0} \, d\lambda(z, z) \right\rangle
\]

(9.69)

\[
= -2\pi \sum_{n \leq Z} \sum_{m > Z} \int_{[\Gamma]^2} \frac{d\xi}{E_n(\xi) - E_m(\xi)}
\]

\[
\times \left\langle u_{m,\xi,\eta}, i\partial_{\xi, \eta} u_{m,\xi,\eta} \right\rangle z \left\langle u_{m,\xi,\eta}, V_{g_{1,\beta}} u_{m,\xi,\eta} \right\rangle \xi.
\]

On the other hand, we have

\[
g_{1,\alpha}(x, z) = \frac{1}{2\pi i} \int_{\mathcal{C}} \frac{1}{\lambda - \mathcal{H}_0(x)} (\zeta - z)_\alpha \frac{1}{\lambda - \mathcal{H}_0(x)} \, d\lambda(z, z)
\]

(9.70)

\[
= 2\pi \sum_{n \leq Z} \sum_{m > Z} \int_{[\Gamma]^2} \frac{d\xi}{E_n(\xi) - E_m(\xi)}
\]

\[
\times u^*_n(\xi) u_{m,\xi,\eta}(\xi) \left\langle u_{m,\xi,\eta}, i\partial_{\xi, \eta} u_{m,\xi,\eta} \right\rangle.
\]
Therefore
\begin{equation}
\mathbf{A}_{\alpha,\beta,2} = -(g_{1,\alpha}, V_{g_1,\beta}) z = -(g_{1,\alpha}, V_{\mathcal{I} - \mathcal{L} z}^{-1} g_{1,\beta}) z.
\end{equation}

The last equality follows from the definition of \( V_{g_1} \).

We conclude by combining the expression of \( \mathbf{A}_{\alpha,\beta,1} \) and \( \mathbf{A}_{\alpha,\beta,2} \).

\begin{proof}
\begin{equation}
\mathbf{A}_{e,\alpha,\beta} = \frac{1}{2\pi i} \left\langle \int_{\mathcal{E}} \frac{1}{\mathcal{I} - \mathcal{L}_e} \frac{1}{\mathcal{I} - \mathcal{L}_g} \frac{1}{\mathcal{I} - \mathcal{L}_e} \frac{1}{\mathcal{I} - \mathcal{L}_g} d\lambda(z, z) \right\rangle
\end{equation}
\end{proof}

Let
\begin{equation}
\mathbf{A}_{e,\alpha,\beta} = \frac{1}{2\pi i} \left\langle \int_{\mathcal{E}} \frac{1}{\mathcal{I} - \mathcal{L}_e} \frac{1}{\mathcal{I} - \mathcal{L}_g} \frac{1}{\mathcal{I} - \mathcal{L}_e} \frac{1}{\mathcal{I} - \mathcal{L}_g} d\lambda(z, z) \right\rangle
\end{equation}

where \( \mathbf{g}_e = V_e (\mathcal{I} - \mathcal{L}_e)^{-1} g_e \) and
\begin{equation}
ge_e(\xi) = \frac{1}{2\pi i} \int_{\mathcal{E}} \frac{1}{\mathcal{I} - \mathcal{L}_e} \frac{1}{\mathcal{I} - \mathcal{L}_g} \frac{1}{\mathcal{I} - \mathcal{L}_e} \frac{1}{\mathcal{I} - \mathcal{L}_g} d\lambda(z, z).
\end{equation}

Recall \( M_A = \sup_j \| \nabla^j u \|_{L^\infty} \), we have

Lemma 9.6. \( \| \mathbf{A} - \mathbf{A}_e \|_{L^\infty} = \mathcal{O}(M_A) \).

\begin{proof}
First note that \( \mathbf{A}_{\alpha,\beta}(x) \) depends on \( x \) only through \( A(x) = \nabla u(x) \). Indeed, let
\begin{equation}
\mathbf{A}_{A,\alpha,\beta} = \frac{1}{2\pi i} \left\langle \int_{\mathcal{E}} \frac{1}{\mathcal{I} - \mathcal{L}_e} \frac{1}{\mathcal{I} - \mathcal{L}_g} \frac{1}{\mathcal{I} - \mathcal{L}_e} \frac{1}{\mathcal{I} - \mathcal{L}_g} d\lambda(z, z) \right\rangle
\end{equation}
\end{proof}

We then have \( A(x) = A_{\nabla u(x)} \). Therefore, it suffices to show that
\begin{equation}
|A - A_e| \lesssim |A|.
\end{equation}

Consider the two parts of \( A \) separately, we have
\begin{equation}
|A_{A,\alpha,\beta,1} - A_{e,\alpha,\beta,1}| = \frac{1}{2\pi i} \left\langle \int_{\mathcal{E}} \frac{1}{\mathcal{I} - \mathcal{L}_e} \frac{1}{\mathcal{I} - \mathcal{L}_g} \frac{1}{\mathcal{I} - \mathcal{L}_e} \frac{1}{\mathcal{I} - \mathcal{L}_g} d\lambda(z, z) \right\rangle
\end{equation}

Consider the first term on the right hand side, let
\begin{equation}
h_e(\xi) = \frac{1}{2}(\xi - z)_a(\xi - z)_b(\mathcal{I} - \mathcal{L}_e)^{-1}(\xi, z).
\end{equation}
By Corollary 8.3, for any $z$, $h_z$ is a $L^2$ function in $\zeta$. Observe that
\[
\left| \frac{1}{\lambda - \mathcal{H}_e} (\mathcal{H}_A - \mathcal{H}_e) \right| \frac{1}{\lambda - \mathcal{H}_A} \frac{\hat{z}(z)}{(\zeta - z)^\alpha (\zeta - z)^\beta} \frac{1}{\lambda - \mathcal{H}_A} (z, z)
\]
\[
= \left| \left( \frac{1}{\lambda - \mathcal{H}_e} (\mathcal{H}_A - \mathcal{H}_e) \right) \frac{1}{\lambda - \mathcal{H}_A} h_z(z) \right|
\]
\[
\leq \left\| \frac{1}{\lambda - \mathcal{H}_e} (\mathcal{H}_A - \mathcal{H}_e) \right\|_{\mathcal{L}(L^2)} \left\| \frac{1}{\lambda - \mathcal{H}_A} \right\|_{\mathcal{L}(L^2, L^2)} \|h_z\|_{L^2}
\]
\[
\lesssim MA,
\]
where the last inequality follows from (7.1). Now consider the difference between $A_\alpha \beta$ and $A e_\alpha \beta$, by a similar argument as above, it suffices to bound $\|e g A; e g e;\|_{L^1(\Gamma)}$. This follows from the estimates of $\|V A; V e;\|_{\mathcal{L}(L^2)}$, $\|g g A; g g e;\|_{H^2}$, and $\|\mathcal{I} - \mathcal{L}_A\|_{\mathcal{L}(H^2; L^2)}$, and $\|g A, g e;\|_{H^2}$. The estimate of the difference of $\mathcal{V}$ is straightforward. The argument for the difference of $g$ follows from a similar argument as before for $A_\alpha \beta$ and hence will be omitted. Let us consider the difference of $(\mathcal{I} - \mathcal{L})^{-1}$. We have
\[
(\mathcal{I} - \mathcal{L}_A)^{-1} - (\mathcal{I} - \mathcal{L}_e)^{-1} = (\mathcal{I} - \mathcal{L}_A)^{-1} (\mathcal{L}_A - \mathcal{L}_e) (\mathcal{I} - \mathcal{L}_e)^{-1}.
\]
Therefore, the desired estimate follows from the boundedness of $(\mathcal{I} - \mathcal{L}_e)^{-1}$ and $(\mathcal{I} - \mathcal{L}_A)^{-1}$ by Proposition 7.5 and the estimate
\[
\|\mathcal{L}_A - \mathcal{L}_e\|_{\mathcal{L}(H^2; L^2)} \lesssim MA,
\]
which is an easy consequence of Proposition 6.16.

We next give the estimate of the terms $B$ and $D$.

**Lemma 9.7.** $\|B_\alpha\|_{L^\infty(\Gamma)}, \|D\|_{L^\infty(\Gamma)} = O(M_A)$.

**Proof.** We will only consider $D$, since the argument for both terms are very similar. By definition, we have
\[
D(x) = \frac{1}{2\pi i} \left( \int_{\mathcal{C}} \frac{1}{\lambda - \mathcal{H}_0(x)} \frac{1}{\delta \mathcal{H}_1} \frac{1}{\lambda - \mathcal{H}_0(x)} \frac{1}{\lambda - \mathcal{H}_0(x)} d\lambda(z, z) \right)
\]
\[
+ \frac{1}{2\pi i} \left( \int_{\mathcal{C}} \frac{1}{\lambda - \mathcal{H}_0(x)} \left( \delta \mathcal{H}_1 \frac{1}{\lambda - \mathcal{H}_0(x)} \right)^2 d\lambda(z, z) \right),
\]
Let us consider the second term on the right hand side, the argument for the first term is similar. It suffices to bound
\[
I(x, z) = \frac{1}{2\pi i} \int_{\mathcal{C}} \frac{1}{\lambda - \mathcal{H}_0(x)} \left( \delta \mathcal{H}_1 \frac{1}{\lambda - \mathcal{H}_0(x)} \right)^2 d\lambda(z, z)
\]
in $L^\infty(\Gamma \times \Gamma)$. Recall that
\[
\delta \mathcal{H}_1 = - (\zeta - z) \cdot \partial_\alpha a_{ij}(x) \partial_\alpha \partial_\beta - b_i(x) \partial_\alpha
\]
\[
+ (\zeta - z) \cdot \partial_\alpha v_0(x, \zeta) + v_{1,2}(x, \zeta) + V_f(x, \zeta).
\]
Notice that by the definition of $a_{ij}$ and $b_i$, we have
\[ \| \partial_x a_{ij} \|_{L^\infty(G)} \cdot \| b_i \|_{L^\infty(G)} = O(M_A). \]

Let us assume for a moment that
\[ \| \partial_x v_0 \|_{L^\infty(G \times \Gamma)} \cdot \| v_{1,2} \|_{L^\infty(G \times \Gamma)} \cdot \| V_{f_1} \|_{L^\infty(G \times \Gamma)} = O(M_A), \]
then using Propositions 8.5 and 8.6, we have
\[ |I(x, z)| = O(M_A). \]

Therefore, it suffices to prove (9.74), which we state as Lemma 9.8.

\[ \square \]

**Lemma 9.8.**
\[ \| \partial_x v_0 \|_{L^\infty(G \times \Gamma)} \cdot \| v_{1,2} \|_{L^\infty(G \times \Gamma)} \cdot \| V_{f_1} \|_{L^\infty(G \times \Gamma)} = O(M_A). \]

**Proof.** First observe that $v_0$ is given by the Cauchy-Born construction:
\[ v_0(x, z) = V_{CB}(z; \nabla u(x)). \]

Taking the derivative, it is easy to see that
\[ \| \partial_x v_0 \|_{L^\infty(G \times \Gamma)} = O(M_A). \]

Similarly, we also have the estimate
\[ \| L_1 \phi_0 \| \lesssim M_A. \]

We also have Lemma 9.1, so that the right hand side of (9.53) is $O(M_A)$ in $L^\infty$ norm. By standard elliptic theory (notice that the constraint that $\langle v_{1,2} \rangle_z = 0$ fixes the arbitrary constant), we have
\[ \| v_{1,2} \|_{L^\infty(G \times \Gamma)} = O(M_A). \]

For $f_1(x, z)$, by definition, it is given by
\[ f_1(x, z) = \frac{1}{2\pi i} \int_{\mathcal{C}} \frac{1}{\lambda - \mathcal{H}_0(x)} (-\zeta - z) \cdot \partial_x a_{ij}(x) \partial_i \zeta \partial_{\zeta^j} \
- b_i(x) \partial_i \zeta \cdot \frac{1}{\lambda - \mathcal{H}_0(x)} d\lambda(z, z) + \frac{1}{2\pi i} \int_{\mathcal{C}} \frac{1}{\lambda - \mathcal{H}_0(x)} (\langle \zeta - z \rangle \cdot \partial_x v_0(x, \zeta) \\n+ v_{1,2}(x, \zeta) \cdot \frac{1}{\lambda - \mathcal{H}_0(x)} d\lambda(z, z). \]

The estimate for the second term comes from the boundedness of $v_{1,2}$ from above with the control that
\[ |(\zeta - z) \cdot \partial_x v_0(x, \zeta)| \leq |\zeta - z| |\partial_x v_0(x, \zeta)| \lesssim M_A |\zeta - z|, \]
and the exponential decay of the Green’s function. For the first term on the right hand side, the term $\partial_x a_{ij}(x)$ and $b_i(x)$ can be taken out of the integral as they do not depend on $\lambda$ or $\xi$. We can then write the first term as

$$\partial_x a_{ij}(x) \cdot \frac{1}{2\pi i} \int_C \frac{1}{\lambda - H_0(x)} (-\zeta - z) \partial_\zeta \partial_\zeta) \frac{1}{\lambda - H_0(x)} (z, z).$$

The term $\partial_x a_{ij}(x)$ is $O(M_A)$, since $a_{ij}(x) = a_{ij}(\nabla u(x))$ (with a slight abuse of notation) and the other term in the product is bounded due to localization. Therefore, the whole term is $O(M_A)$. The treatment for the term that depends on $b$ is similar. To conclude, we have obtained

$$\|f_1\|_{L^\infty(\Gamma \times \Gamma)} = O(M_A).$$

It follows immediately that

$$\|Vf_1\|_{L^\infty(\Gamma \times \Gamma)} = O(M_A).$$

We also need the following lemma about the normalization of $\rho_2$. The proof is given in Appendix A.

**Lemma 9.9.** For any $U_0 \in C^2(\Gamma)$, $\langle \rho_2(x, \cdot) \rangle$ given by (9.58) satisfies

$$\int_\Gamma \langle \rho_2(x, \cdot) \rangle \, dx = 0.$$

Now we are ready to prove Proposition 9.4:

**Proof of Proposition 9.4.** In (9.63), let

$$L = A_{\alpha \beta} \partial_\alpha \partial_\beta + \frac{1}{4\pi} L_2 + B_\alpha \partial_\alpha.$$

Its adjoint operator is given by

$$L^* f = \partial_\alpha \partial_\beta (A_{\alpha \beta} f) + \frac{1}{4\pi} L_2^* f - \partial_\alpha (B_\alpha f).$$

Equation (9.63) can be rewritten as

(9.77) \quad LU_0(x) = \langle m_2(x, \cdot) \rangle - D.$

By Assumption C and Lemma 9.6, $L$ is a uniformly elliptic operator if the deformation is sufficiently small. Therefore, using Fredholm alternative, to prove the solvability, it suffices to prove that for any $f \in \ker L^*$,

$$\int_\Gamma f(\langle m_2(x, \cdot) \rangle - D) \, dx = 0.$$

Integrating (9.59) with respect to $x$ over $\Gamma$, we obtain

$$\int_\Gamma \left( A_{\alpha \beta} \partial_\alpha \partial_\beta U_0(x) + B_\alpha \partial_\alpha U_0(x) + D \right) \, dx = \int_\Gamma \int_\Gamma \rho_2(x, z) \, dz \, dx.$$
By Lemma 9.9, for any smooth \( U_0(x) \), we have
\[
\int_{\Gamma} \int_{\Gamma} \rho_2(x, z) \, dz \, dx = 0.
\]
Hence,
\[
\int_{\Gamma} (A_{\alpha\beta} \partial_\alpha \partial_\beta U_0(x) + B_{\alpha} \partial_\alpha U_0(x) + D) \, dx = 0.
\]
In particular, taking \( U_0(x) \) to be a constant leads to
\begin{equation}
(9.78) \quad \int_{\Gamma} D \, dx = 0.
\end{equation}
Then by the arbitrariness of \( U_0 \), we have
\[
\partial_\alpha \partial_\beta (A_{\alpha\beta} f) - \partial_\alpha (B_{\alpha} f) = 0,
\]
for \( f \) being any constant. On the other hand, we know constant functions lie in the kernel of \( L^*_2 \). Therefore, \( L^* \) vanishes on constant functions.

Using the uniform ellipticity and the control of the low order terms given by Lemma 9.7, it is easy to see that if
\[
L^* f = 0
\]
than \( f \) must be a constant. Hence, the kernel of \( L^* \) consists only of constant functions. Hence, the solvability of (9.77) reduces to
\[
\int (\langle m_2(x, \cdot) \rangle - D) \, dx = 0.
\]
Moreover, by Lemmas 9.1 and 9.7, the right hand side of (9.77) is \( O(M_A) \). Standard elliptic estimates and the Sobolev inequality yield
\[
\| U_0 \|_{L^\infty} = O(M_A).
\]
\[\square\]
So far, we have obtained \( \rho_0(x, z) \), \( \rho_1(x, z) \) and \( \langle \rho_2(x, \cdot) \rangle \) on the density side, \( V_0(x, z) \) and \( v_1(x, z) \) on the potential side.

9.3.3. The third order term. As we have seen in the last two subsections, the equations for \( \rho_0 \), \( \rho_1 \) and \( \langle \rho_2(x, \cdot) \rangle \) form a closed system. To prove that the solutions we obtained provides a good approximate solution for the Kohn-Sham equation, however, we need to go one step further to obtain \( \rho_2(x, z) \) and \( \langle \rho_3(x, \cdot) \rangle \). We will discuss how to get the third order term in this subsection. From the discussion, it will be clear that we may proceed to even higher orders to obtain the pairs \( \rho_k(x, z) \) and \( \langle \rho_{k+1}(x, \cdot) \rangle \).

First, let us consider the equation that involves \( \rho_2 \). Follow the same steps as in the last subsection, decompose \( V_2(x, z) \) into \( v_2(x, z) + U_2(x) \),
\begin{equation}
(9.79) \quad -L_2 U_2(x) = 4\pi (\langle \rho_4(x, \cdot) \rangle - \langle m_4(x, \cdot) \rangle),
\end{equation}
and,

\begin{equation}
\begin{aligned}
\nu_2(x, z) &= \phi_2(x, z) - \langle \phi_2(x, \cdot) \rangle + \eta_2(x, z); \\
-L_0 \phi_2(x, z) &= 4\pi (\rho_2(x, z) - m_2(x, z)) + L_1 \phi_1(x, z) + L_2 \phi_0(x, z); \\
\eta_2(x, z) &= \eta' (J(x)^{-1} \rho_0(x, z)) J(x)^{-1} \rho_2(x, z) \\
&\quad + \frac{1}{2} \eta'' (J(x)^{-1} \rho_0(x, z)) (J(x)^{-1} \rho_1(x, z))^2.
\end{aligned}
\end{equation}

(9.80)

Again, we further decompose \( \nu_2 \) into two parts \( \nu_2 = \nu_{2,1} + \nu_{2,2} \), with \( \nu_{2,1} \) depending on \( \rho_2(x, z) - \langle \rho_2(x, \cdot) \rangle \) and \( \nu_{2,2} \) independent of \( \rho_2(x, z) - \langle \rho_2(x, \cdot) \rangle \) (but it depends on \( \langle \rho_2(x, \cdot) \rangle \)):

\begin{equation}
\nu_{2,1} = \mathcal{V}_2(\rho_2(x, z) - \langle \rho_2(x, \cdot) \rangle) = \phi_{2,1} + \eta_{2,1},
\end{equation}

where

\begin{align*}
-L_0 \phi_{2,1}(x, z) &= 4\pi (\rho_2(x, z) - \langle \rho_2(x, \cdot) \rangle); \\
\eta_{2,1}(x, z) &= \eta' (J(x)^{-1} \rho_0(x, z)) J(x)^{-1} (\rho_2(x, z) - \langle \rho_2(x, \cdot) \rangle).
\end{align*}

And

\[ \nu_{2,2} = \phi_{2,2} + \eta_{2,2}, \]

with

\begin{align*}
-L_0 \phi_{2,2}(x, z) &= 4\pi (\langle \rho_2(x, \cdot) \rangle - m_2(x, z)) + L_1 \phi_1(x, z) + L_2 \phi_0(x, z); \\
\eta_{2,2}(x, z) &= \eta' (J(x)^{-1} \rho_0(x, z)) J(x)^{-1} (\rho_2(x, \cdot)) \\
&\quad + \frac{1}{2} \eta'' (J(x)^{-1} \rho_0(x, z)) (J(x)^{-1} \rho_1(x, z))^2.
\end{align*}

We may write the equations of \( \rho_2 \) as follows

\begin{equation}
\rho_2(x, z) - \langle \rho_2(x, \cdot) \rangle = (\mathcal{I} - \mathcal{L}_x)^{-1} (f_2(x, z) - \langle f_2(x, \cdot) \rangle) \\
+ \partial_z U_1(x) \cdot (\mathcal{I} - \mathcal{L}_x)^{-1} g_1(x, z) + U_1(x) (\mathcal{I} - \mathcal{L}_x)^{-1} g_2(x, z).
\end{equation}

(9.82)

and,

\begin{align*}
\nu_{2,1}(x, z) &= \mathcal{V}_2 (\mathcal{I} - \mathcal{L}_x)^{-1} (f_2(x, z) - \langle f_2(x, \cdot) \rangle) \\
&\quad + \partial_z U_1(x) \cdot \mathcal{V}_2 (\mathcal{I} - \mathcal{L}_x)^{-1} g_1(x, z) + U_1(x) \mathcal{V}_2 (\mathcal{I} - \mathcal{L}_x)^{-1} g_2(x, z) \\
&= \mathcal{V}_2 f_2(x, z) + \partial_z U_1(x) \cdot \mathcal{V}_2 g_1(x, z) + U_1(x) \mathcal{V}_2 g_2(x, z).
\end{align*}

Here \( g_1(x, z) \) and \( \mathcal{V}_2 g_1(x, z) \) are defined by

\begin{align*}
g_2(x, z) &= \frac{1}{2\pi i} \int_{\mathcal{C}} \left( \frac{1}{\lambda - \mathcal{H}_0(x)} \right)^2 (-\langle \zeta - z \rangle \cdot \partial_z a_{ij}(x) \partial_{\zeta_i} \partial_{\zeta_j} - b_i(x) \partial_{\zeta_i} \\
&\quad + \langle \zeta - z \rangle \cdot \partial_z \mathcal{V}_0(x, \zeta) + v_1(x, \zeta)) \frac{1}{\lambda - \mathcal{H}_0(x)} \, d\lambda(z, z) \\
&\quad + \frac{1}{2\pi i} \int_{\mathcal{C}} \frac{1}{\lambda - \mathcal{H}_0(x)} (-\langle \zeta - z \rangle \cdot \partial_z a_{ij}(x) \partial_{\zeta_i} \partial_{\zeta_j} - b_i(x) \partial_{\zeta_i} \\
&\quad + \langle \zeta - z \rangle \cdot \partial_z \mathcal{V}_0(x, \zeta) + v_1(x, \zeta)) \left( \frac{1}{\lambda - \mathcal{H}_0(x)} \right)^2 \, d\lambda(z, z)
\end{align*}
and

\[ f_2(x, z) = \frac{1}{2\pi i} \int_{\mathcal{C}} \frac{1}{\lambda - H_0(x)} \left( \left(-\frac{1}{2}((\zeta - z) \cdot \partial_x)^2 a_{ij}(x) \partial_{\zeta_i} \partial_{\zeta_j} \right) 
- (\zeta - z) \cdot \partial_x b_i(x) \partial_{\zeta_i} + \frac{1}{2}((\zeta - z) \cdot \partial_x)^2 V_0(x, \zeta) 
+ (\zeta - z) \cdot \partial_x v_1(x, \zeta) + v_{2,2}(x, \zeta) \right) \frac{1}{\lambda - H_0(x)} d\lambda(z, z) 
+ \frac{1}{2\pi i} \int_{\mathcal{C}} \frac{1}{\lambda - H_0(x)} \left( (-(\zeta - z) \cdot \partial_x a_{ij}(x) \partial_{\zeta_i} \partial_{\zeta_j} - b_i(x) \partial_{\zeta_i}) 
+ (\zeta - z) \cdot \partial_x V_0(x, \zeta) + v_1(x, \zeta) \right) \frac{1}{\lambda - H_0(x)} d\lambda(z, z). \]

**Lemma 9.10.** \( f_2(x, \cdot), g_2(x, \cdot), V_{f_2}(x, \cdot), \) and \( V_{g_2}(x, \cdot) \in C^\infty(\Gamma, H^4(\Gamma)) \). Moreover, \( \langle g_2(x, \cdot) \rangle = 0 \).

**Proof.** The regularity is proved by similar arguments as those in the proof of Lemma 9.2, using Propositions 8.5, 8.6 and 8.7. The conclusion that \( \langle g_2(x, \cdot) \rangle = 0 \) follows from a similar symmetry argument as the one used in the proof of Lemma 9.2.

We conclude that (9.82) is well-defined and

\[ V_2(x, z) = U_2(x) + v_{2,2}(x, z) + V_{f_2}(x, z) + \partial_x U_1(x) \cdot V_{g_1}(x, z) + U_1(x) V_{g_2}(x, z). \]  

As before, \( \rho_2(x, z) \) depends linearly on \( U_1(x) \). To determine \( U_1(x) \), we take average of the equation for \( \rho_3 \) (9.38). We will obtain after straightforward calculations,

\[ \langle \rho_3(x, \cdot) \rangle = A_{\alpha, \beta} \partial_{x_\alpha} \partial_{x_\beta} U_1(x) + B' \partial_{x_\alpha} U_1(x) + C' U_1(x) + D'. \]

Here the coefficients \( A \) is the same as before, the other coefficients are given by

\[ B' = \frac{1}{2\pi i} \int_{\mathcal{C}} \frac{1}{\lambda - H_0(x)} \left( (\zeta - z) \cdot \partial_x V_{g_1,\alpha}(x, \zeta) 
+ (\zeta - z) \partial_x V_{g_2}(x, \zeta) \right) \frac{1}{\lambda - H_0(x)} d\lambda(z, z) \]

\[ + \frac{1}{2\pi i} \int_{\mathcal{C}} \frac{1}{\lambda - H_0(x)} \left( \delta H_1^2 \frac{1}{\lambda - H_0(x)} 
\times ((\zeta - z) \partial_x V_{g_1,\alpha}(x, \zeta) + V_{g_1,\alpha}(x, \zeta)) \frac{1}{\lambda - H_0(x)} d\lambda(z, z) \right); \]
Proposition 9.12.  \( (9.88) \) has a unique solution.
Let us summarize the results of the asymptotic analysis in this section. We have obtained the density functions $\rho_0(x, z), \rho_1(x, z), \rho_2(x, z), \langle \rho_3(x, \cdot) \rangle$ and the potential functions $V_0(x, z), V_1(x, z)$ and $v_2(x, z)$, which satisfy the following relations.

The potentials are determined by the densities from:

\begin{align}
V_0(x, z) &= \phi_0(x, z) + \eta(J(x)^{-1}\rho_0(x, z)); \\
V_1(x, z) &= \phi_1(x, z) + \eta_1(x, z); \\
V_2(x, z) &= \phi_2(x, z) - \langle \phi_2(x, \cdot) \rangle + \eta_2(x, z); \\
\eta_1(x, z) &= \eta'(J(x)^{-1}\rho_0(x, z))J(x)^{-1}\rho_1(x, z).
\end{align}

Note that $U_0(x) = \langle \phi_0(x, \cdot) \rangle$.

\begin{align}
v_2(x, z) &= \phi_2(x, z) - \langle \phi_2(x, \cdot) \rangle + \eta_2(x, z); \\
- L_0\phi_2(x, z) &= 4\pi(\rho_2(x, z) - m_2(x, z)) + L_1\phi_0(x, z); \\
- L_2\phi_1(x, z) &= 4\pi(\eta_2(x, z)) - \langle m_3(x, z) \rangle; \\
\eta_2(x, z) &= \eta'(J(x)^{-1}\rho_0(x, z))J(x)^{-1}\rho_2(x, z) \\
&+ \frac{1}{2}\eta''(J(x)^{-1}\rho_0(x, z))(J(x)^{-1}\rho_1(x, z))^2.
\end{align}

The densities are consistent with those given by the potentials:

\begin{align}
\rho_0(x, z) &= \frac{1}{2\pi i} \int_{\gamma^*} \frac{1}{\lambda - \mathcal{H}_0(x)} d\lambda(z, z) \\
\rho_1(x, z) &= \frac{1}{2\pi i} \int_{\gamma^*} \frac{1}{\lambda - \mathcal{H}_0(x)} \mathcal{H}_1(x, z) \frac{1}{\lambda - \mathcal{H}_0(x)} d\lambda(z, z) \\
\rho_2(x, z) &= \frac{1}{2\pi i} \int_{\gamma^*} \frac{1}{\lambda - \mathcal{H}_0(x)} \mathcal{H}_2(x, z) \frac{1}{\lambda - \mathcal{H}_0(x)} d\lambda(z, z) \\
&+ \frac{1}{2\pi i} \int_{\gamma^*} \frac{1}{\lambda - \mathcal{H}_0(x)} \left( \delta\mathcal{H}_1(x, z) \frac{1}{\lambda - \mathcal{H}_0(x)} \right)^2 d\lambda(z, z)
\end{align}
Here we have used the notations
\[ \langle \rho_i(x, \cdot) \rangle = \frac{1}{2\pi i} \left\langle \int_{\mathbb{C}} \frac{1}{\lambda - H_0(x)} \delta H_3(x, z) \frac{1}{\lambda - H_0(x)} d\lambda(z, z) \right\rangle \]
\[ + \frac{1}{2\pi i} \left\langle \int_{\mathbb{C}} \frac{1}{\lambda - H_0(x)} \delta H_1(x, z) \frac{1}{\lambda - H_0(x)} \times \delta H_2(x, z) \frac{1}{\lambda - H_0(x)} d\lambda(z, z) \right\rangle \]
\[ + \frac{1}{2\pi i} \left\langle \int_{\mathbb{C}} \frac{1}{\lambda - H_0(x)} \delta H_2(x, z) \frac{1}{\lambda - H_0(x)} \times \delta H_1(x, z) \frac{1}{\lambda - H_0(x)} d\lambda(z, z) \right\rangle \]
\[ + \frac{1}{2\pi i} \left\langle \int_{\mathbb{C}} \frac{1}{\lambda - H_0(x)} \delta H_1(x, z) \frac{1}{\lambda - H_0(x)} \times \delta H_3(x, z) \frac{1}{\lambda - H_0(x)} d\lambda(z, z) \right\rangle. \]
(9.95)

Here we have used the notations
\[ H_0(x) = -a_{ij}(x) \partial_{\zeta_i} \partial_{\zeta_j} + V_0(x, \zeta); \]
\[ \delta H_1(x, z) = - (\zeta - z) \cdot \partial_x a_{ij}(x) \partial_{\zeta_i} \partial_{\zeta_j} - b_i(x) \partial_{\zeta_i}; \]
\[ + (\zeta - z) \cdot \partial_x V_0(x, \zeta) + V_1(x, \zeta); \]
\[ \delta H_2(x, z) = - \frac{1}{2} ((\zeta - z) \cdot \partial_x)^2 a_{ij}(x) \partial_{\zeta_i} \partial_{\zeta_j} - (\zeta - z) \cdot \partial_x b_i(x) \partial_{\zeta_i} - c(x) \]
\[ + \frac{1}{2} ((\zeta - z) \cdot \partial_x)^2 V_0(x, \zeta) + (\zeta - z) \cdot \partial_x V_1(x, \zeta) + v_2(x, \zeta); \]
\[ \delta H_3(x, z) = - \frac{1}{2} ((\zeta - z) \cdot \partial_x)^3 a_{ij}(x) \partial_{\zeta_i} \partial_{\zeta_j} - \frac{1}{2} ((\zeta - z) \cdot \partial_x)^2 b_i(x) \partial_{\zeta_i} \]
\[ - (\zeta - z) \cdot \partial_x c(x) + \frac{1}{3} ((\zeta - z) \cdot \partial_x)^3 V_0(x, \zeta) \]
\[ + \frac{1}{3} ((\zeta - z) \cdot \partial_x)^2 V_1(x, \zeta) + (\zeta - z) \cdot \partial_x v_2(x, \zeta). \]
(9.96)

10. **Higher order approximate solution to the Kohn-Sham equation**

The asymptotic analysis of the previous section provides an approximate solutions of the Kohn-Sham equation in the following form:

(10.1) \[ \bar{\rho}^\varepsilon(x) = \varepsilon^{-3} \rho_0(x, x/\varepsilon) + \varepsilon^{-2} \rho_1(x, x/\varepsilon) + \varepsilon^{-1} \rho_2(x, x/\varepsilon) + \langle \rho_3(x, \cdot) \rangle + \varepsilon n_\varepsilon. \]

Here the functions \( \rho_i \) are constructed in the last section, see (9.92)-(9.95). \( n_\varepsilon \) is a constant (depending on \( \varepsilon \)) chosen such that the normalization constraint for \( \bar{\rho}^\varepsilon \) is satisfied:

\[ \int_G \bar{\rho}^\varepsilon(x) dx = Z \varepsilon^{-3}. \]

\( \bar{\rho}^\varepsilon \) serves as the initial condition \( \rho^0 \) in the iteration scheme introduced in Section 5.

In this section, we will prove that the density given by (10.1) is a good approximate solution to the Kohn-Sham equation in the sense stated in the following theorem, and therefore (5.15) is satisfied.

**Theorem 10.1.** Under the same assumptions as Theorem 5.1, we have

\[ \| \bar{\rho}^\varepsilon - \mathcal{F}_\varepsilon^\varepsilon(\bar{\rho}^\varepsilon) \|_{\mathcal{H}^{-1}\cap \mathcal{H}^1} \lesssim \varepsilon^{1/2}. \]
We will prove this theorem in three steps: First, we show that \( n_{\varepsilon} \) is \( O(1) \); then we characterize the effective potential given by \( \bar{\rho} \); finally, we consider the image of the Kohn-Sham map of \( \bar{\rho} \) and estimate its difference with \( \rho^* \) in the space \( H_2 \). These three steps are accomplished in Propositions 10.3, 10.4 and 10.5 respectively.

Before going into the proofs of Theorem 10.1, let us first make sure that the system under consideration has a spectral gap and the Kohn-Sham map is well defined. Consider the Hamiltonian given by

\[
H_\varepsilon^\tau = -\varepsilon^2 a_{ij}(x) \partial_i \partial_j - \varepsilon^2 b_i(x) \partial_i - \varepsilon^2 c(x) + V(x),
\]

where the coefficients \( a, b, c \) are given in (5.9), we have

\[\text{Lemma 10.2.} \quad \text{There exist constants } a, \delta > 0, \text{ such that if } M_A = \sup_j \|\nabla^j u\|_{L^\infty} \leq a \text{ and } \|V - V_0\|_{L^\infty} \leq \delta \text{ with } V_0 \text{ given in } (9.89), \text{ we have} \]

\[
\text{dist}(\mathcal{C}, \text{spec}(H_\varepsilon^\tau)) \geq E_g/4.
\]

\[\text{Proof.} \quad \text{Let us compare the Hamiltonian } H_\varepsilon^\tau \text{ with that for the undeformed system} \]

\[
H_\varepsilon^c = -\varepsilon^2 \Delta + V_\varepsilon^c = -\varepsilon^2 \Delta + V_{\text{KB}}(x/\varepsilon; 0).
\]

Note that the difference in potential is bounded by

\[
\|V - V_\varepsilon^c\|_{L^\infty} \leq \|V - V_0\|_{L^\infty} + \|V_{\text{KB}}(x/\varepsilon; \nabla u(x)) - V_{\text{KB}}(x/\varepsilon; 0)\|_{L^\infty} \lesssim \delta + M_A \leq \delta + a.
\]

Straightforward calculations yield

\[
|a_{ij}(x) - \delta_{ij}|, |b_i(x)|, |c(x)| \leq M_A,
\]

for \( i, j = 1, 2, 3 \) and all \( x \in \Gamma \). Hence, for \( f \in \mathcal{D}(\Delta) \), we have

\[
\|(a_{ij}(x) - \delta_{ij}) \partial_i \partial_j - b_i(x) \partial_i - c(x)) f\|_{L^2} \lesssim M_A \|\Delta f\|_{L^2}.
\]

Therefore, for \( \lambda \in \mathcal{C} \), we obtain

\[
\|(H_\varepsilon^\tau - H_\varepsilon^c)(\lambda - H_\varepsilon^c)^{-1}\|_{\mathcal{L}(L^2)} \lesssim a + \delta.
\]

Note that

\[
(\lambda - H_\varepsilon^c)^{-1} = (\lambda - H_\varepsilon^c)^{-1}(I - (H_\varepsilon^\tau - H_\varepsilon^c)(\lambda - H_\varepsilon^c)^{-1})^{-1}.
\]

By choosing \( a \) and \( \delta \) sufficiently small, \( \|(H_\varepsilon^\tau - H_\varepsilon^c)(\lambda - H_\varepsilon^c)^{-1}\|_{\mathcal{L}(L^2)} \) is bounded by 1/2 uniformly with respect to \( \lambda \in \mathcal{C} \), then \( I - (H_\varepsilon^\tau - H_\varepsilon^c)(\lambda - H_\varepsilon^c)^{-1} \) is invertible, and

\[
\left\| (I - (H_\varepsilon^\tau - H_\varepsilon^c)(\lambda - H_\varepsilon^c)^{-1})^{-1} \right\| \leq 2.
\]

Therefore, we obtain

\[
\|(\lambda - H_\varepsilon^c)^{-1}\|_{\mathcal{L}(L^2)} \leq 2\|(\lambda - H_\varepsilon^c)^{-1}\|_{\mathcal{L}(L^2)} \leq 4/E_g,
\]

for any \( \lambda \in \mathcal{C} \), and hence \( \text{dist}(\mathcal{C}, \text{spec}(H_\varepsilon^\tau)) \geq E_g/4. \)

\[\Box\]
The following propositions are proved under the assumptions of Theorem 5.1.

**Proposition 10.3.** We have $|n_\varepsilon| \lesssim 1$ as $\varepsilon \to 0$.

**Proof.** Let

$$V(x) = V_0(x, x/\varepsilon) + \varepsilon V_1(x, x/\varepsilon) + \varepsilon^2 v_2(x, x/\varepsilon)$$

where $V_0$, $V_1$ and $v_2$ are given in (9.89), (9.90), (9.91) respectively. Define

$$w(x) = \frac{1}{2\pi i} \int_{\gamma} \frac{1}{\lambda - \mathcal{H}} \, d\lambda(x, x),$$

where

$$\mathcal{H} = -\varepsilon^2 a_{ij}(x) \partial_i \partial_j - \varepsilon^2 b_i(x) \partial_i - \varepsilon c(x) + V(x).$$

Assume for the moment that

$$w(x) = \varepsilon^{-3} \rho_0(x, x/\varepsilon) + \varepsilon^{-2} \rho_1(x, x/\varepsilon) + \varepsilon^{-1} \rho_2(x, x/\varepsilon) + \{\rho_3(x, \cdot) + \tilde{w}_3(x, x/\varepsilon) + \varepsilon w_4(x),$$

where $\tilde{w}_3$ and $w_4$ satisfy the following estimates

$$\langle \tilde{w}_3(x, \cdot) \rangle = 0, \quad \|\partial_x \tilde{w}_3\|_{L^\infty(\Gamma \times \Gamma)} \lesssim 1, \quad \|w_4\|_{L^\infty(\Gamma)} \lesssim 1.$$

By the normalization of $\tilde{w}^3$ and $w$, we have

$$Z/\varepsilon^3 = \int_{\Gamma} \tilde{w}^3(x) \, dx$$

$$= \int_{\Gamma} \left( \varepsilon^{-3} \rho_0(x, x/\varepsilon) + \varepsilon^{-2} \rho_1(x, x/\varepsilon) + \varepsilon^{-1} \rho_2(x, x/\varepsilon) + \{\rho_3(x, \cdot) + \varepsilon \tilde{w}_3(x, x/\varepsilon) + \varepsilon w_4(x) \right) \, dx$$

$$= \int_{\Gamma} w(x) - \tilde{w}_3(x, x/\varepsilon) - \varepsilon w_4(x) \, dx + \varepsilon n_\varepsilon |\Gamma|$$

$$= Z/\varepsilon^3 + \varepsilon n_\varepsilon |\Gamma| - \int_{\Gamma} \tilde{w}_3(x, x/\varepsilon) \, dx - \varepsilon \int_{\Gamma} w_4(x) \, dx.$$

Hence

$$n_\varepsilon = \varepsilon^{-1} \int_{\Gamma} \tilde{w}_3(x, x/\varepsilon) \, dx + \int_{\Gamma} w_4(x) \, dx.$$ 

Since

$$\left| \int_{\Gamma} \tilde{w}_3(x, x/\varepsilon) \, dx \right| = \left| \int_{\Gamma} \sum_{X_i \in L \cap \Gamma} \int_{X_i + \varepsilon \Gamma} \tilde{w}_3(x, x/\varepsilon) - \tilde{w}_3(X_i, x/\varepsilon) \, dx \right|$$

$$\lesssim \sum_{X_i \in L \cap \Gamma} \int_{X_i + \varepsilon \Gamma} |x - X_i| \|\partial_x \tilde{w}_3\|_{L^\infty(\Gamma \times \Gamma)} \, dx$$

$$\lesssim \varepsilon \|\partial_x \tilde{w}_3\|_{L^\infty(\Gamma \times \Gamma)},$$

and

$$\left| \int_{\Gamma} w_4(x) \, dx \right| \leq \|w_4\|_{L^\infty(\Gamma)}.$$

We conclude that $n_\varepsilon = O(1)$ as $\varepsilon \to 0$. 

Let us come back to the proof of (10.3) and (10.4). For the Hamiltonian given in (10.2), using a similar expansion as in section 9.2, we obtain (10.3) with
\begin{equation}
\begin{aligned}
w_3(x, z) &= \langle \rho_3(x, \cdot) \rangle + \tilde{w}_3(x, z) \\
&= \frac{1}{2\pi i} \int_{\mathcal{C}} \frac{1}{\lambda - \mathcal{H}_0(x)} \delta \mathcal{H}_3(x, z) \frac{1}{\lambda - \mathcal{H}_0(x)} \, d\lambda(z, z) \\
&+ \frac{1}{2\pi i} \int_{\mathcal{C}} \frac{1}{\lambda - \mathcal{H}_0(x)} \delta \mathcal{H}_1(x, z) \frac{1}{\lambda - \mathcal{H}_0(x)} \\
&\times \delta \mathcal{H}_2(x, z) \frac{1}{\lambda - \mathcal{H}_0(x)} \, d\lambda(z, z) \\
&+ \frac{1}{2\pi i} \int_{\mathcal{C}} \frac{1}{\lambda - \mathcal{H}_0(x)} \delta \mathcal{H}_1(x, z) \frac{1}{\lambda - \mathcal{H}_0(x)} \\
&\times \delta \mathcal{H}_2(x, z) \frac{1}{\lambda - \mathcal{H}_0(x)} \, d\lambda(z, z) \\
&+ \frac{1}{2\pi i} \int_{\mathcal{C}} \frac{1}{\lambda - \mathcal{H}_0(x)} \left( \delta \mathcal{H}_1(x, z) \frac{1}{\lambda - \mathcal{H}_0(x)} \right)^3 \, d\lambda(z, z).
\end{aligned}
\end{equation}

where \( \mathcal{H}_0, \delta \mathcal{H}_i \) are given by (9.96). Compare (10.5) with (9.95), it is clear that

\[ \langle \tilde{w}_3(x, \cdot) \rangle = \langle w_3(x, \cdot) \rangle. \]

Hence,

\[ \langle \tilde{w}_3(x, \cdot) \rangle = \langle w_3(x, \cdot) \rangle - \langle \rho_3(x, \cdot) \rangle = 0. \]

To prove

\[ \| \partial_x \tilde{w}_3(x, z) \|_{L^\infty(\Gamma \times \Gamma)} \lesssim 1, \]

it suffices to show

\[ \| \partial_x w_3(x, z) \|_{L^\infty(\Gamma \times \Gamma)} \lesssim 1, \]

since

\[ \| \partial_x \tilde{w}_3(x, z) \|_{L^\infty(\Gamma \times \Gamma)} = \| \partial_x w_3(x, z) - \langle \partial_x w_3(x, z) \rangle \|_{L^\infty(\Gamma \times \Gamma)} \]

\[ \leq \| \partial_x w_3(x, z) \|_{L^\infty(\Gamma \times \Gamma)} + \| \langle \partial_x w_3(x, z) \rangle \|_{L^\infty(\Gamma \times \Gamma)} \]

\[ \leq \| \partial_x w_3(x, z) \|_{L^\infty(\Gamma \times \Gamma)} + \| \partial_x w_3(x, z) \|_{L^\infty(\Gamma \times \Gamma)} \]

\[ \leq 2\| \partial_x w_3(x, z) \|_{L^\infty(\Gamma \times \Gamma)}. \]

The treatment for the four terms on the right hand side of (10.5) is similar. Therefore we will focus on the first term:

\[ w_{3,1}(x, z) = \frac{1}{2\pi i} \int_{\mathcal{C}} \frac{1}{\lambda - \mathcal{H}_0(x)} \delta \mathcal{H}_3(x, z) \frac{1}{\lambda - \mathcal{H}_0(x)} \, d\lambda(z, z). \]
Taking derivative with respect to $x$, we have

(10.6)

$$
\partial_x w_{3,1}(x, z) = \frac{1}{2\pi i} \int_{\mathcal{C}} \frac{1}{\lambda - H_0(x)} \partial_x \delta H_3(x, z) \frac{1}{\lambda - H_0(x)} d\lambda(z, z) \\
+ \frac{1}{2\pi i} \int_{\mathcal{C}} \frac{1}{\lambda - H_0(x)} \partial_x H_0(x) \frac{1}{\lambda - H_0(x)} \delta H_3(x, z) \frac{1}{\lambda - H_0(x)} d\lambda(z, z) \\
+ \frac{1}{2\pi i} \int_{\mathcal{C}} \frac{1}{\lambda - H_0(x)} \delta H_3(x, z) \frac{1}{\lambda - H_0(x)} \partial_x H_0(x) \frac{1}{\lambda - H_0(x)} d\lambda(z, z),
$$

since

$$
\partial_x \frac{1}{\lambda - H_0(x)} = \frac{1}{\lambda - H_0(x)} \partial_x H_0(x) \frac{1}{\lambda - H_0(x)}.
$$

Consider the first term on the right hand side of (10.6). By the definition of $\delta H_3(x, z)$, we have

$$
\partial_x \delta H_3(x, z) = -\frac{i}{4} (\xi - z) \cdot \partial_x a_{ij}(x) \partial_x \xi \cdot \partial_x \xi_i - \frac{1}{2} (\xi - z) \cdot \partial_x b_i(x) \partial_x \xi_i \\
- (\xi - z) \cdot \partial_x c(x) + \frac{i}{2} (\xi - z) \cdot \partial_x V_0(x, \xi) \\
+ \frac{1}{2} (\xi - z) \cdot \partial_x V_1(x, \xi) + (\xi - z) \cdot \partial_x \nu_2(x, \xi).
$$

Substituting into the expression of $\partial_x w_{3,1}(x, z)$ (10.6), we see that the representative terms are of the form:

$$
\frac{1}{2\pi i} \int_{\mathcal{C}} \frac{1}{\lambda - H_0(x)} ((\xi - z) \cdot \partial_x \xi) \cdot \partial_x V_0(x, \xi) \frac{1}{\lambda - H_0(x)} d\lambda(z, z); \\
\frac{1}{2\pi i} \int_{\mathcal{C}} \frac{1}{\lambda - H_0(x)} ((\xi - z) \cdot \partial_x \xi) \cdot \partial_x a_{ij}(x) \partial_x \xi \cdot \partial_x \xi_i \frac{1}{\lambda - H_0(x)} d\lambda(z, z).
$$

The boundedness of these terms follow from the regularity of $V_0$, Propositions 8.4 and 8.5. Hence, we obtain the desired estimate for the first term in (10.6).

The analysis of the second and third terms in (10.6) is the same. Let us consider the second term. Notice that

$$
\partial_x H_0(x) = -\partial_x a_{ij}(x) \partial_x \xi \cdot \partial_x \xi_i + \partial_x V_0(x, \xi),
$$

and use the definition of $\delta H_3$, we see that a typical term takes the form:

$$
\frac{1}{2\pi i} \int_{\mathcal{C}} \frac{1}{\lambda - H_0(x)} (-\partial_x a_{ij}(x) \partial_x \xi \cdot \partial_x \xi_i) \frac{1}{\lambda - H_0(x)} d\lambda(z, z) \\
\times (-\frac{1}{6} (\xi - z) \cdot \partial_x a_{kl}(x) \partial_x \xi \cdot \partial_x \xi_i) \frac{1}{\lambda - H_0(x)} d\lambda(z, z).
$$

Using Proposition 8.6, we see that this term is bounded. The other terms can be estimated similarly. Therefore, we have

$$
\|\partial_x w_{3,1}\|_{L^\infty(\Gamma \times \Gamma)} \lesssim 1.
$$

Similarly for $\partial_x w_3(x, z)$ by applying the same argument to the remaining terms in (10.5).

The treatment of $w_4$ is similar and will be omitted.
Proposition 10.4. Denote the potential generated by $\tilde{\rho}^\varepsilon$ as $V^\varepsilon$. $V^\varepsilon$ can be expressed as

$$V^\varepsilon(x) = V_0(x, x/\varepsilon) + \varepsilon V_1(x, x/\varepsilon) + \varepsilon^2 v_2(x, x/\varepsilon) + V_r(x)$$

where $V_0$, $V_1$ and $v_2 \in C^\infty(\Gamma, W^{2,\infty}_0(\Gamma))$ and given by (9.89), (9.90) and (9.91) respectively. In addition, $V_r$ satisfies

$$\|V_r\|_{W^{1,\infty}(\Gamma)} = O(\varepsilon^2), \quad \|\nabla V_r\|_{W^{1,\infty}(\Gamma)} = O(\varepsilon), \quad \text{and} \quad \|\nabla^2 V_r\|_{W^{1,\infty}(\Gamma)} = O(1).$$

Proof. By definition, we have

$$V^\varepsilon = \phi_0^\varepsilon[\rho] + \eta(J(x)^{-1} \varepsilon^3 \tilde{\rho}^\varepsilon(x)).$$

Let us first consider the Coulomb part (denoted as $\phi$ for simplicity), which solves

$$(-a_{ij} \partial_i \partial_j - b_i \partial_i) \phi = 4\pi \varepsilon (\rho^\varepsilon - m^\varepsilon).$$

Note that

$$m^\varepsilon(x) = \varepsilon^{-3} m_0(x, x/\varepsilon) + \varepsilon^{-2} m_1(x, x/\varepsilon) + \varepsilon^{-1} m_2(x, x/\varepsilon) + \varepsilon m_r(x).$$

Write $\phi$ as

$$\phi(x) = \phi_0(x, x/\varepsilon) + \varepsilon \phi_1(x, x/\varepsilon) + \varepsilon^2 \phi_2(x, x/\varepsilon) + \varepsilon^3 \phi_3(x, x/\varepsilon) + \phi_r(x),$$

where $\phi_i$, $0 \leq i \leq 3$ satisfy

$$-L_0 \phi_0(x, z) = 4\pi (\rho_0(x, z) - m_0(x, z)), \quad -L_0 \phi_1(x, z) = 4\pi (\rho_1(x, z) - m_1(x, z)) + L_1 \phi_0(x, z), \quad -L_0 \phi_2(x, z) = 4\pi (\rho_2(x, z) - m_2(x, z)) + L_1 \phi_1(x, z) + L_2 \phi_0(x, z), \quad -L_0 \phi_3(x, z) = 4\pi (\rho_3(x, z) - m_3(x, z)) + L_1 \phi_2(x, z) + L_2 \phi_1(x, z),$$

with $\langle \phi_0(x, \cdot) \rangle$, $\langle \phi_1(x, \cdot) \rangle$ given by the solvability condition of the equations for $\phi_2$ and $\phi_3$, and $\langle \phi_2(x, \cdot) \rangle = \langle \phi_3(x, \cdot) \rangle = 0$. The remainder $\phi_r$ satisfies

$$(10.7) \quad (-a_{ij} \partial_i \partial_j - b_i \partial_i) \phi_r(x) = 4\pi \varepsilon^2 (n_r - m_r(x)) + \varepsilon^2 L_2 \phi_2(x, x/\varepsilon) + \varepsilon^3 L_2 \phi_3(x, x/\varepsilon).$$

Let us denote the right hand side of the above equation as $\varepsilon^2 f(x)$ with

$$f(x) = 4\pi (n_r - m_r(x)) + L_2 \phi_2(x, x/\varepsilon) + L_1 \phi_3(x, x/\varepsilon) + \varepsilon L_2 \phi_3(x, x/\varepsilon).$$

It is easy to see from the equations of $\phi_2$ and $\phi_3$ that we have,

$$\|f\|_{L^\infty} \lesssim 1, \quad \|\nabla f\|_{L^\infty} \lesssim \varepsilon^{-1}, \quad \text{and} \quad \|\nabla^2 f\|_{L^\infty} \lesssim \varepsilon^{-2}.$$ 

Applying standard elliptic regularity estimate to (10.7), we obtain

$$\|\phi_r(x)\|_{W^{1,\infty}} \lesssim \|\varepsilon^2 f\|_{L^\infty} \lesssim \varepsilon^2; \quad \|\nabla \phi_r(x)\|_{W^{1,\infty}} \lesssim \|\varepsilon^2 \nabla f\|_{L^\infty} \lesssim \varepsilon; \quad \|\nabla^2 \phi_r(x)\|_{W^{1,\infty}} \lesssim \|\varepsilon^2 \nabla^2 f\|_{L^\infty} \lesssim 1.$$
Using Taylor expansion, we can express the exchange-correlation part as
\[
\eta(J(x)^{-1}\varepsilon^3 \bar{\rho}^c(x)) = \eta(J(x)^{-1}(\rho_0(x, x/\varepsilon) + \varepsilon \rho_1(x, x/\varepsilon) + \varepsilon^2 \rho_2(x, x/\varepsilon) + O(\varepsilon^3)))
\]
\[
= \eta(J(x)^{-1}\rho_0(x, x/\varepsilon)) + \varepsilon J(x)^{-1}\rho_1(x, x/\varepsilon)\eta' + \varepsilon^2 J(x)^{-1}\rho_2(x, x/\varepsilon)\eta'' + \frac{1}{2} \varepsilon^2 (J(x)^{-1}\rho_1(x, x/\varepsilon))^2 \eta'' + O(\varepsilon^3),
\]
where \(\eta'\) and \(\eta''\) are evaluated at \(J(x)^{-1}\rho_0(x, x/\varepsilon)\). Set
\[
\eta_0(x, z) = \eta(J(x)^{-1}\rho_0(x, z));
\]
\[
\eta_1(x, z) = J(x)^{-1}\rho_1(x, z)\eta';
\]
\[
\eta_2(x, z) = J(x)^{-1}\rho_2(x, z)\eta' + \frac{1}{2} (J(x)^{-1}\rho_1(x, z))^2 \eta'',
\]
with \(\eta'\) and \(\eta''\) evaluated at \(J(x)^{-1}\rho_0(x, z)\), and
\[
\eta_r(x) = \eta(J(x)^{-1}\varepsilon^3 \bar{\rho}^c(x)) - \eta_0(x, x/\varepsilon) - \varepsilon \eta_1(x, x/\varepsilon) - \varepsilon^2 \eta_2(x, x/\varepsilon).
\]
Let
\[
V_0(x, z) = \phi_0(x, z) + \eta_0(x, z);
\]
\[
V_1(x, z) = \phi_1(x, z) + \eta_1(x, z);
\]
\[
v_2(x, z) = \phi_2(x, z) + \eta_2(x, z);
\]
\[
V_r(x) = \varepsilon^3 \phi_3(x, x/\varepsilon) + \phi_r(x) + \eta_r(x).
\]
We conclude with the desired estimates.

\[\square\]

We are now ready to study the difference between \(\bar{\rho}^c\) and the image of the Kohn-Sham map acting on \(\bar{\rho}^c\).

**Proposition 10.5.** Let \(w\) be the density given by the Hamiltonian operator
\[
\mathcal{H}^\varepsilon = -\varepsilon^2 a_{ij}(x) \partial_i \partial_j - \varepsilon^2 b_i(x) \partial_i - \varepsilon^2 c(x) + V^\varepsilon(x),
\]
then
\[
\|\bar{\rho}^c - w\|_{L^2} \lesssim \varepsilon^{1/2}.
\]

**Proof.** By definition, \(w\) is given by
\[
w(x) = \frac{1}{2\pi i} \int_{\mathcal{C}} \frac{1}{\lambda - \mathcal{H}^\varepsilon} \, d\lambda(x, x).
\]
The wellposedness follows from Lemma 10.2. As before, we can write \(w\) in the form
\[
w(x) = \varepsilon^{-3} w_0(x, x/\varepsilon) + \varepsilon^{-2} w_1(x, x/\varepsilon) + \varepsilon^{-1} w_2(x, x/\varepsilon) + w_r(x),
\]
where
\[
w_0(x, z) = \frac{1}{2\pi i} \int_{\mathcal{C}} \frac{1}{\lambda - \mathcal{H}_0(x)} \, d\lambda(z, z),
\]
\[
w_1(x, z) = \frac{1}{2\pi i} \int_{\mathcal{C}} \frac{1}{\lambda - \mathcal{H}_0(x)} \delta \mathcal{H}_1(x, z) \frac{1}{\lambda - \mathcal{H}_0(x)} \, d\lambda(z, z),
\]
(10.9)
\[ w_2(x, z) = \frac{1}{2\pi i} \int \frac{1}{\lambda - \mathcal{H}_0(x)} \delta \mathcal{H}_2(x, z) \frac{1}{\lambda - \mathcal{H}_0(x)} \, d\lambda(z, z) \]

\[ + \frac{1}{2\pi i} \int \frac{1}{\lambda - \mathcal{H}_0(x)} \left( \delta \mathcal{H}_1(x, z) \frac{1}{\lambda - \mathcal{H}_0(x)} \right)^2 \, d\lambda(z, z) \]

with

\[ \mathcal{H}_0(x) = -a_{ij}(x)\partial_{x_i} \partial_{x_j} + V_0(x, \zeta); \]

\[ \delta \mathcal{H}_1(x, z) = -(\zeta - z) \cdot \partial_x a_{ij}(x) \partial_{x_i} \partial_{x_j} - b_i(x) \partial_{x_i} \]

\[ + (\zeta - z) \cdot \partial_x V_0(x, \zeta) + V_1(x, \zeta); \]

\[ \delta \mathcal{H}_2(x, z) = -\frac{1}{2} ((\zeta - z) \cdot \partial_x)^2 a_{ij}(x) \partial_{x_i} \partial_{x_j} - (\zeta - z) \cdot \partial_x b_i(x) \partial_{x_i} - c(x) \]

\[ + \frac{1}{2} ((\zeta - z) \cdot \partial_x)^2 V_0(x, \zeta) + (\zeta - z) \cdot \partial_x V_1(x, \zeta) \]

\[ + v_2(x, \zeta) + \varepsilon^{-2} V_0(x). \]

The remainder term \( w_r \) is given by

\[ w_r(x) = \frac{1}{2\pi i} \int \frac{1}{\lambda - \mathcal{H}_0^c(x)} \delta \mathcal{H}_r^c(x) \frac{1}{\lambda - \mathcal{H}_0^c(x)} \, d\lambda(x, x) \]

\[ + \frac{1}{2\pi i} \int \frac{1}{\lambda - \mathcal{H}_0^c(x)} \left( \delta \mathcal{H}_r^c(x) \frac{1}{\lambda - \mathcal{H}_0^c(x)} \right)^2 \, d\lambda(x, x) \]

\[ - \frac{1}{2\pi i} \int \frac{1}{\lambda - \mathcal{H}_0^c(x)} \left( \delta \mathcal{H}_r^c(x) \frac{1}{\lambda - \mathcal{H}_0^c(x)} \right)^3 \, d\lambda(x, x), \]

with the short-hand notations

\[ \mathcal{H}_0^c(x) = -\varepsilon^2 a_{ij}(x)\partial_{y_i} \partial_{y_j} + V_0(x, y/\varepsilon), \]

\[ \delta \mathcal{H}_r^c(x) = \mathcal{H}_r^c - \mathcal{H}_0^c(x) = \delta \mathcal{H}_1^c(x) + \delta \mathcal{H}_2^c(x) + \delta \mathcal{H}_r^c(x), \]

where

\[ \delta \mathcal{H}_1^c(x) = -\varepsilon^2 (y - x) \cdot \partial_x a_{ij}(x) \partial_{y_i} \partial_{y_j} - \varepsilon^2 b_i(x) \partial_{y_i} \]

\[ + (y - x) \cdot \partial_x V_0(x, y/\varepsilon) + \varepsilon V_1(x, y/\varepsilon); \]

\[ \delta \mathcal{H}_2^c(x) = -\frac{1}{2} \varepsilon^2 ((y - x) \cdot \partial_x)^2 a_{ij}(x) \partial_{y_i} \partial_{y_j} - \varepsilon^2 (y - x) \cdot \partial_x b_i(x) \partial_{y_i} \]

\[ - \varepsilon^2 c(x) + \frac{1}{2} ((y - x) \cdot \partial_x)^2 V_0(x, y/\varepsilon) \]

\[ + \varepsilon (y - x) \cdot \partial_x V_1(x, y/\varepsilon) + \varepsilon^2 v_2(x, y/\varepsilon) + V_0(x). \]

By Proposition 10.4, it is easy to see that

\[ w_0(x, z) = \rho_0(x, z), \quad w_1(x, z) = \rho_1(x, z), \quad \text{and} \quad \langle w_2(x, \cdot) \rangle = \langle \rho_2(x, \cdot) \rangle. \]

Therefore

\[ w(x) - \bar{\rho}^c(x) = \varepsilon^{-1} (w_2(x, x/\varepsilon) - \rho_2(x, x/\varepsilon)) + w_r(x) - \langle \rho_3(x, \cdot) \rangle - \varepsilon n_e. \]
By definition, we have
\[
\|f\|_{H^2(\Gamma)} = \|\varepsilon^3 f(x)\|_{H^2(\Gamma/\varepsilon)}
\leq \varepsilon^3(\|f(x)\|_{L^2(\Gamma/\varepsilon)} + \|\Delta_x f(x)\|_{L^2(\Gamma/\varepsilon)})
\leq \varepsilon^{3/2}(\|f(x)\|_{L^\infty(\Gamma/\varepsilon)} + \|\Delta_x f(x)\|_{L^\infty(\Gamma/\varepsilon)})
= \varepsilon^{3/2}(\|f\|_{L^\infty(\Gamma)} + \|\varepsilon^2 \Delta f\|_{L^\infty(\Gamma)}).
\]

Therefore, it suffices to bound
\[
\|w - \tilde{r}\|_{L^\infty(\Gamma)}, \quad \text{and} \quad \|\varepsilon^2 \Delta (w - \tilde{r})\|_{L^\infty(\Gamma)} \lesssim \varepsilon^{-1}.
\]

By Proposition 10.3, \(n \varepsilon = \mathcal{O}(1)\), so that the term \(n \varepsilon\) clearly satisfies the needed bound. In addition, it is easy to see from the construction that the term \(\langle \rho_3(x, \cdot) \rangle\) is bounded. It suffices now to consider the terms \(w_2\) and \(w_r\).

For the term \(w_2(x, x/\varepsilon) - \langle w_2(x, \cdot) \rangle\), using similar arguments as in the proof of Proposition 10.3, we obtain
\[
\|w_2\|_{L^\infty(\Gamma \times \Gamma)} = \mathcal{O}(1).
\]

Taking the derivative, we have
\[
\varepsilon^2 \Delta w_2(x, x/\varepsilon) = \varepsilon^2 \Delta_x w_2(x, x/\varepsilon) + 2\varepsilon \nabla_x \cdot \nabla_z w_2(x, x/\varepsilon) + \Delta_z w_2(x, x/\varepsilon).
\]

Let us focus on the first term in the expression of \(w_2(x, z)\), the argument for the other term is similar. Denote
\[
w_{2,1}(x, z) = \frac{1}{2\pi i} \int_{\mathbb{C}} \frac{1}{\lambda - \mathcal{H}_0(x)} \delta \mathcal{H}_2(x, z) \frac{1}{\lambda - \mathcal{H}_0(x)} \, d\lambda(z, z).
\]

Taking derivative with respect to \(z\), we get
\[
\nabla_z w_{2,1}(x, z) = \frac{1}{2\pi i} \int_{\mathbb{C}} \nabla_\zeta \frac{1}{\lambda - \mathcal{H}_0(x)} \delta \mathcal{H}_2(x, z) \frac{1}{\lambda - \mathcal{H}_0(x)} \, d\lambda(z, z)
- \frac{1}{2\pi i} \int_{\mathbb{C}} \frac{1}{\lambda - \mathcal{H}_0(x)} \delta \mathcal{H}_2(x, z) \frac{1}{\lambda - \mathcal{H}_0(x)} \nabla_\zeta \, d\lambda(z, z)
+ \frac{1}{2\pi i} \int_{\mathbb{C}} \frac{1}{\lambda - \mathcal{H}_0(x)} \nabla_z (\delta \mathcal{H}_2(x, z)) \frac{1}{\lambda - \mathcal{H}_0(x)} \, d\lambda(z, z).
\]

Rewriting the equation using the short-hand notation \(R_\lambda(x) = (\lambda - \mathcal{H}_0(x))^{-1}\), we have
\[
\nabla_z w_{2,1}(x, z) = \frac{1}{2\pi i} \int_{\mathbb{C}} \left[ \nabla_\zeta, R_\lambda(x) \right] \delta \mathcal{H}_2(x, z) R_\lambda(x) \, d\lambda(z, z)
+ \frac{1}{2\pi i} \int_{\mathbb{C}} R_\lambda(x) \left[ \nabla_\zeta, \delta \mathcal{H}_2(x, z) \right] R_\lambda(x) \, d\lambda(z, z)
+ \frac{1}{2\pi i} \int_{\mathbb{C}} R_\lambda(x) \nabla_z (\delta \mathcal{H}_2(x, z)) R_\lambda(x) \, d\lambda(z, z).
\]

(10.12)
First, let us consider the second and last terms on the right hand side of (10.12) together. By definition, we have

\[ \nabla_z \delta H_2(x, z) = (\zeta - z) \cdot \partial_{\Sigma}^2 \delta H_0(x, z) + \partial_{\Sigma} V_1(x, \zeta), \]

and

\[ [\nabla_\zeta, \delta H_2(x, z)] = -(\zeta - z) \cdot \partial_{\Sigma}^2 \delta H_0(x, \zeta) + \partial_{\Sigma} V_1(x, \zeta) \]

Therefore, the contribution of these two terms to \( \nabla_z w_{2,1}(x, z) \) is

\[ \frac{1}{2 \pi i} \int_{\mathcal{C}} R_\lambda(x) \left( \frac{1}{\lambda - \mathcal{H}_0} \right) \frac{1}{\lambda - \mathcal{H}_0} \]

It is bounded due to Proposition 8.4 and the regularity of \( V_0, V_1 \) and \( v_2 \).

The first and third terms in (10.12) can be treated in the same way. Notice that

\[ \left[ \nabla_\zeta, \frac{1}{\lambda - \mathcal{H}_0} \right] = \frac{1}{\lambda - \mathcal{H}_0} \left[ \nabla_\zeta, \mathcal{H}_0 \right] \frac{1}{\lambda - \mathcal{H}_0} \]

the first term becomes

\[ \frac{1}{2 \pi i} \int_{\mathcal{C}} R_\lambda(x) \partial_{\Sigma} V_0(x, \zeta) R_\lambda(x) \delta H_2(x, z) R_\lambda(x) \, d\lambda(z, z). \]

We conclude using similar arguments as in Proposition 8.6 that

\[ ||\nabla_z w_{2,1}||_{L^\infty(\Gamma \times \Gamma)} = O(1). \]

Differentiating (10.12) once more with respect to \( z \), we get an expression whose representative terms are of the form:

\[ \Delta_z w_{2,1}(x, z) = \frac{1}{2 \pi i} \int_{\mathcal{C}} R_\lambda(x) \nabla_z (\delta H_2(x, z)) \cdot [\nabla_\zeta, R_\lambda(x)] \, d\lambda(z, z) \]

\[ + \frac{1}{2 \pi i} \int_{\mathcal{C}} R_\lambda(x) \Delta_z \delta H_2(x, z) R_\lambda(x) \, d\lambda(z, z) \]

\[ + \frac{1}{2 \pi i} \int_{\mathcal{C}} R_\lambda(x) [\nabla_\zeta, \nabla_\zeta (\delta H_2(x, z))] \, d\lambda(z, z) + \text{t.s.f.,} \]

where t.s.f. represents the terms in similar forms. Using (10.13), the first term is equal to

\[ \frac{1}{2 \pi i} \int_{\mathcal{C}} \sum_j R_\lambda(x) \nabla_{\Sigma j} (\delta H_2(x, z)) R_\lambda(x) \nabla_{\Sigma j} V_0(x, \zeta) R_\lambda(x) \, d\lambda(z, z). \]
Using the similar argument as in Propositions 8.5 and 8.6, we see that this term is bounded.

For the second and third terms, note that
\[
\Delta_z \delta H_2(x, z) = -\Delta_z a_{ij}(x) \partial_{\zeta_i} \partial_{\zeta_j} + \Delta_z V_0(x, \zeta);
\]

\[
[\nabla_{\zeta_i}, \nabla_{\zeta_j}(\delta H_2(x, z))] = \Delta_z a_{ij}(x) \partial_{\zeta_i} \partial_{\zeta_j} - \Delta_z V_0(x, \zeta)
\]

hence the two terms give
\[
\frac{1}{2\pi i} \int_{\Gamma} R_\lambda(x) \left( (\zeta - z) \cdot \partial_z \partial_x \cdot \partial_2 V_0(x, \zeta) - \partial_x \partial_2 V_1(x, \zeta) \right) R_\lambda(x) d\lambda(z, z)
\]

Again, the estimate follows from the regularity of \(V_0\) and \(V_1\), and Proposition 8.4. We arrive at the estimate
\[
\|\Delta_z w_{2,1}|_{L^\infty(\Gamma \times \Gamma)} = O(1).
\]

The derivative with respect to \(x\) can be analyzed in the same way, starting from
\[
\frac{1}{2\pi i} \int_{\Gamma} \delta H_2(x, z) \frac{1}{\lambda - \delta H_0(x)} \frac{1}{\lambda - \delta H_0(x)} d\lambda(z, z)
\]

\[
+ \frac{1}{2\pi i} \int_{\Gamma} \delta H_2(x, z) \frac{1}{\lambda - \delta H_0(x)} \frac{1}{\lambda - \delta H_0(x)} d\lambda(z, z)
\]

\[
+ \frac{1}{2\pi i} \int_{\Gamma} \delta H_2(x, z) \frac{1}{\lambda - \delta H_0(x)} \frac{1}{\lambda - \delta H_0(x)} d\lambda(z, z).
\]

The other term in the expression of \(w_2\) can be treated similarly and we omit the details. To sum up, we have shown
\[
\|\varepsilon^2 \nabla_x w_2(x, x/\varepsilon)\|_{L^\infty(\Gamma)} = O(1).
\]

The estimate for \(\rho_2\) is completely parallel, and we conclude that
\[
\|\varepsilon^{-1}(w_2(x, x/\varepsilon) - \rho_2(x, x/\varepsilon))\|_{H^2(\Gamma)} = O(\varepsilon^{1/2}).
\]

For the remainder \(w_r\), let us look at the first term on the right hand side of (10.11), the arguments for other terms are similar:
\[
w_{r,1}(x) = \frac{1}{2\pi i} \int_{\Gamma} \delta H^\varepsilon(x, y) \frac{1}{\lambda - \delta H_0(x)} d\lambda(x, x).
\]

By definition, we have
\[
\delta H^\varepsilon(x) = -\varepsilon^2 a_{ij}(y) \partial_{y_i} \partial_{y_j} + \varepsilon^2 a_{ij}(x) \partial_{y_i} \partial_{y_j}
\]

\[
+ \varepsilon^2 (y - x) \cdot \partial_x a_{ij}(x) \partial_{y_i} \partial_{y_j} + \frac{1}{2} \varepsilon^2 ((y - x) \cdot \partial_x)^2 a_{ij}(x) \partial_{y_i} \partial_{y_j}
\]

\[
+ \varepsilon V_1(y, y/\varepsilon) - \varepsilon V_1(x, y/\varepsilon) - \varepsilon (y - x) \cdot \partial_x V_1(x, y/\varepsilon)
\]

\[
+ V_r(y) - V_r(x) + t.s.f.,
\]
Here, for simplicity and clarity, we have omitted terms coming from \( b_i, c, V_0 \) and \( v_2 \), which can be analyzed using similar arguments. Let

\[
A_{ij}(y, x) = -a_{ij}(y) + a_{ij}(x) + (y - x) \cdot \partial_x a_{ij}(x) + \frac{1}{2} ((y - x) \cdot \partial_x)^2 a_{ij}(x).
\]

By the smoothness of \( a \), we have

\[
|A_{ij}(y, x)| \lesssim |y - x|^3.
\]

Similarly, denote

\[
\delta V_1(y, x) = V_1(y, y/\varepsilon) - V_1(x, y/\varepsilon) - (y - x) \cdot \partial_x V_1(x, y/\varepsilon),
\]

we then have

\[
|\delta V_1(y, x)| \lesssim |y - x|^2 \|\partial^2_x V_1(x, z)\|_{L^\infty(G \times \Gamma)} \lesssim |y - x|^2.
\]

By Proposition 10.4, we further have

\[
|\delta V_r(y) - V_r(x)| \lesssim |y - x| \|\partial_x V_r\|_{L^\infty} \lesssim \varepsilon^2 |y - x|.
\]

Rewrite \( w_{r,1} \) as

\[
w_{r,1}(x) = \frac{1}{2\pi i} \int_{\mathcal{E}} \frac{1}{\lambda - \mathcal{H}_0(x)} \varepsilon^2 A_{ij}(y, x) \partial_{y_j} \partial_{y_j} \frac{1}{\lambda - \mathcal{H}_0(x)} \, d\lambda(x, x)
+ \frac{1}{2\pi i} \int_{\mathcal{E}} \frac{1}{\lambda - \mathcal{H}_0(x)} \varepsilon \delta V_1(y, x) \frac{1}{\lambda - \mathcal{H}_0(x)} \, d\lambda(x, x)
+ \frac{1}{2\pi i} \int_{\mathcal{E}} \frac{1}{\lambda - \mathcal{H}_0(x)} (V_r(y) - V_r(x)) \frac{1}{\lambda - \mathcal{H}_0(x)} \, d\lambda(x, x) + \text{t.s.f.}
\]

Define \( \tilde{w}_{r,1}(x) = \varepsilon^3 w_{r,1}(\varepsilon x) \), then it is easy to see that

\[
\tilde{w}_{r,1}(x) = \frac{1}{2\pi i} \int_{\mathcal{E}} \frac{1}{\lambda - \mathcal{H}_0(\varepsilon x)} A_{ij}(ey, ex) \partial_{y_j} \partial_{y_j} \frac{1}{\lambda - \mathcal{H}_0(\varepsilon x)} \, d\lambda(x, x)
+ \frac{\varepsilon}{2\pi i} \int_{\mathcal{E}} \frac{1}{\lambda - \mathcal{H}_0(\varepsilon x)} \delta V_1(ey, ex) \frac{1}{\lambda - \mathcal{H}_0(\varepsilon x)} \, d\lambda(x, x)
+ \frac{1}{2\pi i} \int_{\mathcal{E}} \frac{1}{\lambda - \mathcal{H}_0(\varepsilon x)} (V_r(ey) - V_r(ex)) \frac{1}{\lambda - \mathcal{H}_0(\varepsilon x)} \, d\lambda(x, x)
+ \text{t.s.f.}
\]

Using the estimates of \( A_{ij}(y, x), \delta V_1(y, x) \) and \( V_r(y) - V_r(x) \), combined with Propositions 8.4 and 8.5, we have the estimate \( \|\tilde{w}_{r,1}\|_{L^\infty} = \mathcal{O}(\varepsilon^3) \). Hence \( \|w_{r,1}\|_{L^\infty} = \mathcal{O}(1) \). Similar arguments applied to the other terms in the expression of \( w_r \) yields

\[
\|w_r\|_{L^\infty(G)} = \mathcal{O}(1).
\]
Therefore, we have the estimates

\[ \nabla w_{r,1}(x) = \frac{1}{2\pi i} \int_{\mathbb{C}} \left[ \nabla_y \frac{1}{\lambda - \mathcal{H}_0^r(x)} \delta \mathcal{H}_r^c(x_0) \frac{1}{\lambda - \mathcal{H}_0^r(x_0)} \right] d\lambda(x, x) \]

\[ + \frac{1}{2\pi i} \int_{\mathbb{C}} \frac{1}{\lambda - \mathcal{H}_0^r(x)} \left[ \nabla_y, \delta \mathcal{H}_r^c(x) \frac{1}{\lambda - \mathcal{H}_0^r(x)} \right] d\lambda(x, x) \]

\[ + \frac{1}{2\pi i} \int_{\mathbb{C}} \nabla_y \left( \frac{1}{\lambda - \mathcal{H}_0^r(x)} \delta \mathcal{H}_r^c(x) \frac{1}{\lambda - \mathcal{H}_0^r(x)} \right) d\lambda(x, x) \]

(10.14)

First we consider the sum of the second and fifth terms on the right hand side:

\[ \frac{1}{2\pi i} \int_{\mathbb{C}} \frac{1}{\lambda - \mathcal{H}_0^r(x)} \left[ (\nabla_y, \delta \mathcal{H}_r^c(x)] + \nabla_y (\delta \mathcal{H}_r^c(x)) \right] \frac{1}{\lambda - \mathcal{H}_0^r(x)} d\lambda(x, x). \]

Recall the notation introduced before

\[ \delta \mathcal{H}_r^c(x) = \varepsilon^2 A_{ij}(y, x) \partial_y \partial_{y_j} + \varepsilon \delta V_1(y, x) + V_r(y) - V_r(x) + \text{t.s.f.} \]

Direct calculation yields

\[ [\nabla_y, \delta \mathcal{H}_r^c(x)] + \nabla_y (\delta \mathcal{H}_r^c(x)) = \varepsilon^2 (\partial_{y_i} + \partial_{y_j}) A_{ij}(y, x) \partial_y \partial_{y_j} \]

\[ + \varepsilon (\partial_{y_i} + \partial_{y_j}) \delta V_1(y, x) \]

\[ + (\partial_{y_i} + \partial_{y_j}) (V_r(y) - V_r(x)) + \text{t.s.f.} \]

By definition, we have

\[ \partial_y A_{ij}(y, x) = -\partial_x a_{ij}(y) + \partial_x a_{ij}(x) + (y - x) \cdot \partial_x^2 a_{ij}(x); \]

\[ \partial_x A_{ij}(y, x) = \frac{1}{2} ((y - x) \cdot \partial_x)^2 \partial_y a_{ij}(x); \]

\[ \partial_y \delta V_1(y, x) = \partial_x V_1(y, x, y/\varepsilon) - \partial_x V_1(x, y/\varepsilon) \]

\[ + \varepsilon^{-1} (\partial_y^2 V_1(y, x, y/\varepsilon) - \partial_x V_1(x, y/\varepsilon)) \]

\[ - \varepsilon^{-1} (y - x) \cdot \partial_x \partial_y V_1(x, y/\varepsilon); \]

\[ \partial_x \delta V_1(y, x) = -(y - x) \cdot \partial_x^2 V_1(x, y/\varepsilon). \]

Therefore, we have the estimates

\[ |(\partial_y + \partial_x) A_{ij}(y, x)| \lesssim |y - x|^3, \]

\[ |(\partial_y + \partial_x) \delta V_1(y, x)| \lesssim |y - x|^2 \|\partial_x^2 V_1\|_{L^\infty} + \varepsilon^{-1} |y - x|^2 \|\partial_x^2 V_1\|_{L^\infty} \]

\[ \lesssim \varepsilon^{-1} |y - x|^2, \]

and,

\[ |(\partial_y + \partial_x)(V_r(y) - V_r(x))| \lesssim |y - x| \|\partial_x^2 V_r(x)\|_{L^\infty} \lesssim \varepsilon |y - x|. \]
Using these estimates and similar arguments as before with the decay property of the Green’s function, we obtain
\[
\left| \frac{1}{2\pi i} \int_{\Gamma} \frac{1}{\lambda - \mathcal{H}_0^e(x)} \left( \nabla_y, \delta \mathcal{H}_e^0(x) \right) \nabla_x (\delta \mathcal{H}_e^0(x)) \frac{1}{\lambda - \mathcal{H}_0^e(x)} \, d\lambda(x, x) \right| \lesssim \varepsilon^{-1}.
\]

For the other terms in (10.14), notice that
\[
\left[ \nabla_y, \frac{1}{\lambda - \mathcal{H}_0^e(x)} \right] = \frac{1}{\lambda - \mathcal{H}_0^e(x)} \nabla_y (\mathcal{H}_0^e(x)) \frac{1}{\lambda - \mathcal{H}_0^e(x)} = \varepsilon^{-1} \frac{1}{\lambda - \mathcal{H}_0^e(x)} \partial_x V_0(x, y/\varepsilon) \frac{1}{\lambda - \mathcal{H}_0^e(x)}.
\]
\[
\nabla_x \left( \frac{1}{\lambda - \mathcal{H}_0^e(x)} \right) = \frac{1}{\lambda - \mathcal{H}_0^e(x)} \nabla_x (\mathcal{H}_0^e(x)) \frac{1}{\lambda - \mathcal{H}_0^e(x)}
\]
\[
= \frac{1}{\lambda - \mathcal{H}_0^e(x)} (-\varepsilon^2 \partial_x a_{ij}(x) \partial_y \partial_y + \partial_x V_0(x, y/\varepsilon)) \frac{1}{\lambda - \mathcal{H}_0^e(x)}.
\]

Proceed as before, we conclude that \(\| \varepsilon \nabla w_r \|_{L^\infty} = \mathcal{O}(1)\). Therefore, treating the other terms in \(w_r\) similarly, we arrive at the desired estimate \(\| \varepsilon \nabla w_r \|_{L^\infty} = \mathcal{O}(1)\) and \(\| \varepsilon^2 \Delta w_r \|_{L^\infty} = \mathcal{O}(1)\). We omit the details here.

Now, let us turn to the \(H_x^{-1}\) norm. By definition, we have
\[
(10.15) \quad \| w(x) - \bar{\rho}(x) \|^2_{H_x^{-1}} = \int_{\Gamma} \phi(x) (w(x) - \bar{\rho}(x)) \, dx,
\]
where \(\phi\) is the Coulomb potential generated by \(w - \bar{\rho}\), which satisfies
\[
-\Delta \phi(x) = 4\pi \varepsilon(w - \bar{\rho}),
\]
with periodic boundary condition on \(\Gamma\). Similarly as the argument in the proof of Proposition 10.4, using \(\langle w_2(x, \cdot) \rangle = \langle \rho_2(x, \cdot) \rangle\) and standard elliptic regularity estimates, we have
\[
\| \phi(x) \|_{L^\infty(\Gamma)}, \| \nabla_x \phi(x) \|_{L^\infty(\Gamma)} \lesssim \varepsilon.
\]
Consider the right hand side of (10.15), we have
\[
\int_{\Gamma} \phi(x) (w(x) - \bar{\rho}(x)) \, dx = \int_{\Gamma} \phi(x) \varepsilon^{-1} (w_2(x, x/\varepsilon) - \rho_2(x, x/\varepsilon)) \, dx
\]
\[
+ \int_{\Gamma} \phi(x) (w_r(x) - \langle \rho_3(x, \cdot) \rangle - \varepsilon n_x) \, dx.
\]
The second term is clearly $O(\varepsilon)$. Denote $f(x, x/\varepsilon) = w_2(x, x/\varepsilon) - \rho_2(x, x/\varepsilon)$, since $\langle f(x, \cdot) \rangle = 0$, we have
\[
\left| \int_{\Gamma} \phi(x) f(x, x/\varepsilon) \, dx \right| \leq \sum_{X_i \in \varepsilon L \cap \Gamma} \int_{X_i + \varepsilon \Gamma} |\phi(x) f(x, x/\varepsilon) - \phi(X_i) f(X_i, x/\varepsilon)| \, dx
\]
\[
\leq \sum_{X_i \in \varepsilon L \cap \Gamma} \int_{X_i + \varepsilon \Gamma} |\phi(x) - \phi(X_i)||f(x, x/\varepsilon)| \, dx
\]
\[
+ \sum_{X_i \in \varepsilon L \cap \Gamma} \int_{X_i + \varepsilon \Gamma} |\phi(X_i)||f(x, x/\varepsilon) - f(X_i, x/\varepsilon)| \, dx
\]
\[
\lesssim \varepsilon^2.
\]
Therefore, we conclude that
\[
\|w - \tilde{\rho}\|_{H^{-1}} \lesssim \varepsilon^{1/2}.
\]

Before ending this section, let us state the well-posedness of the Kohn-Sham map, for density near $\varepsilon$.

**Proposition 10.6.** There exist constants $a, \delta > 0$, such that if the displacement field $u$ satisfies $M_A = \sup_j \|\nabla^j u\|_{L^\infty} \leq a$, the Kohn-Sham map $F_\varepsilon(\rho)$ is well defined for $\rho$ that $\|\rho - \tilde{\rho}\|_{H^{-1} \cap H^2} \leq \delta$.

**Proof.** The Proposition is an easy corollary of Lemma 6.4, Lemma 10.2 and Proposition 10.4, similar to the proof of Proposition 7.3. We omit the details here. \qed

11. **Proof of Lemma 5.3 and 5.4**

**Proof of Lemma 5.3.** Note that $L_{\tau, \rho}^\varepsilon = \chi_{\tau, \rho}^\varepsilon \delta_{\tau, \rho} V_\varepsilon^\tau$ and $L_{\varepsilon, \rho_e}^\varepsilon = \chi_{\varepsilon, \rho_e}^\varepsilon \delta_{\varepsilon, \rho_e} V_\varepsilon^\varepsilon$, we have
\[
L_{\tau, \rho}^\varepsilon w - L_{\varepsilon, \rho_e}^\varepsilon w = \chi_{\tau, \rho}^\varepsilon (\delta_{\tau, \rho} V_\varepsilon^\tau w - \delta_{\rho_e} V_\varepsilon^\varepsilon w) + (\chi_{\tau, \rho}^\varepsilon - \chi_{\varepsilon, \rho_e}^\varepsilon) \delta_{\rho_e} V_\varepsilon^\varepsilon w
\]

Let us first compare $\delta_{\tau, \rho} V_\varepsilon^\tau w$ and $\delta_{\rho_e} V_\varepsilon^\varepsilon w$. By definition
\[
\begin{aligned}
\delta_{\tau, \rho} V_\varepsilon^\tau (w) &= \delta \phi_e + \delta \eta_e; \\
-(a_{ij} \partial_i \partial_j + b_i \partial_i) \delta \phi_e &= 4 \pi \varepsilon w; \\
\delta \eta_e &= \eta'(J(x)^{-1} \varepsilon^3 \rho^0) J(x)^{-1} \varepsilon^3 w,
\end{aligned}
\]

and
\[
\begin{aligned}
\delta_{\rho_e} V_\varepsilon^\varepsilon (w) &= \delta \phi_e + \delta \eta_e; \\
-\Delta \delta \phi_e &= 4 \pi \varepsilon w; \\
\delta \eta_e &= \eta'(\varepsilon^3 \rho_e) \varepsilon^3 w.
\end{aligned}
\]

Consider first the difference of the exchange-correlation part:
\[
\delta \eta_e - \delta \eta_e = (\eta'(J(x)^{-1} \varepsilon^3 \rho^0) J(x)^{-1} - \eta'(\varepsilon^3 \rho_e)) \varepsilon^3 w.
\]
By the construction of $\rho^0$, we have
\[ \|\rho^0 - \rho_\varepsilon\|_{W^{2,\infty}} \lesssim M_A + \varepsilon. \]
Therefore, by the smoothness of $\eta$, we get
\[ \|\delta\eta_{\varepsilon}(x) - \delta\eta_0(x)\|_{H^2_0} \lesssim (M_A + \varepsilon)\|w\|_{H^2}. \]
For the Coulomb part, let us perform a rescaling of the variables:
\[ \delta\phi_{\varepsilon,x}(x) = \delta\phi_{rt}(ex), \quad \delta\phi_{\varepsilon,c}(x) = \delta\phi_{c}(ex), \quad \text{and} \quad w_\varepsilon(x) = \varepsilon^3 w(ex). \]
Then, we have
\[
\begin{align*}
- (a_{ij}(ex)\partial_i\partial_j + \varepsilon b_i(\varepsilon x)\partial_i)\delta\phi_{\varepsilon,x} &= 4\pi w_\varepsilon; \\
- \Delta \delta\phi_{\varepsilon,c} &= 4\pi w_\varepsilon.
\end{align*}
\]
Hence
\[
-\Delta(\delta\phi_{\varepsilon,c} - \delta\phi_{\varepsilon,x}) = (\Delta - (a_{ij}(ex)\partial_i\partial_j + \varepsilon b_i(\varepsilon x)\partial_i))\delta\phi_{\varepsilon,r}.
\]
Therefore, to prove that
\[ \|\delta\phi_{\varepsilon,c} - \delta\phi_{\varepsilon,x}\|_{H^2_0} \lesssim (M_A + \varepsilon)\|w_\varepsilon\|_{H^2}, \]
it suffices to show
\[ \|\left(\Delta - (a_{ij}(ex)\partial_i\partial_j + \varepsilon b_i(\varepsilon x)\partial_i)\right)f\|_{H^{-1}} \lesssim (M_A + \varepsilon)\|f\|_{H^2}. \]
Using the property of $a$ and $b$, it is easy to see that
\[ \|\left(\Delta - (a_{ij}(ex)\partial_i\partial_j + \varepsilon b_i(\varepsilon x)\partial_i)\right)f\|_{H^2} \lesssim (M_A + \varepsilon)\|f\|_{H^2}. \]
By duality, we have
\begin{equation}
(11.1) \quad \|\left(\Delta - (a_{ij}(ex)\partial_i\partial_j + \varepsilon b_i(\varepsilon x)\partial_i)\right)f\|_{H^{-2}} \leq \int_{\Gamma} W(\Delta - (a_{ij}(ex)\partial_i\partial_j + \varepsilon b_i(\varepsilon x)\partial_i)) f \, dx
\end{equation}
for $\|W\|_{H^1} \leq 1$. Using the notation introduced in the proof of Lemma 6.2, and changing to the Eulerian coordinates, we have
\[
\int_{\Gamma} W(a_{ij}(ex)\partial_i\partial_j + \varepsilon b_i(\varepsilon x)\partial_i) f \, dx = \int_{\Gamma} W J(\varepsilon x) \tau_x^* \Delta(\tau_x) f \, dx
\]
\[
= \int_{\tau_x(\Gamma)} ((\tau_x)_* W) \Delta((\tau_x)_* f) \, dy
\]
\[
= - \int_{\tau_x(\Gamma)} \nabla((\tau_x)_* W) \cdot \nabla((\tau_x)_* f) \, dy
\]
\[
= - \int_{\Gamma} (\tau_x^* \nabla(\tau_x)_* W) \cdot (\tau_x^* \nabla(\tau_x)_* f) J(\varepsilon x) \, dx
\]
Hence, the left hand side of (11.1) is bounded by
\[ \left| \int_{\Gamma} (-\nabla W \cdot \nabla f + (\tau_x^* \nabla(\tau_x)_* W) \cdot (\tau_x^* \nabla(\tau_x)_* f) J(\varepsilon x)) \, dx \right|. \]
It is easy to see that for \( f \in \dot{H}^1 \), we have
\[
\| \nabla f - \tau_\varepsilon \nabla (\tau_\varepsilon) f \|_{L^2} \lesssim M_A \| \nabla f \|_{L^2}.
\]
Hence, we obtain the desired estimate. Let \( \delta V_\varepsilon (x) = (\delta r_\varepsilon V_\varepsilon^r w)(\varepsilon x) \) and \( \delta V_\varepsilon (x) = (\delta r_\varepsilon V_\varepsilon^r w)(\varepsilon x) \), we then have
\[
\| \delta V_\varepsilon - V_\varepsilon \|_{H^1 + H^2} \lesssim (M_A + \varepsilon) \| w \|_{H^{-1} \cap H^2}.
\]
Using Theorem 6.3 and a simple rescaling, we obtain
\[
\| \chi_{\varepsilon, \delta, \rho}^\varepsilon \|_{H^{-1} \cap H^2} \lesssim (M_A + \varepsilon) \| w \|_{H^{-1} \cap H^2}.
\]
From Proposition 10.4, we have
\[
V_\varepsilon^r (\rho^0) - V_\varepsilon^r (\rho_\varepsilon) = V_\varepsilon^r (x; \varepsilon) - V_{\text{CB}}^r (x; \varepsilon) + \varepsilon V_1^r (x, x; \varepsilon) + \varepsilon^2 V_2^r (x, x; \varepsilon) + V_r (x)
\]
\[
= V_{\text{CB}}^r (x; \varepsilon; \nabla u (x)) - V_{\text{CB}}^r (x; \varepsilon; 0) + U_0 (x)
\]
\[
+ \varepsilon V_1^r (x, x; \varepsilon) + \varepsilon^2 V_2^r (x, x; \varepsilon) + V_r (x).
\]
Hence, using Proposition 9.4 and 10.4, we have
\[
\| V_\varepsilon^r (\rho^0) (\varepsilon) - V_\varepsilon^r (\rho_\varepsilon) (\varepsilon) \|_{W^2_{\infty}} \lesssim M_A + \varepsilon.
\]
Then, by Proposition 6.16, we obtain
\[
\| (\chi_{\varepsilon, \delta, \rho}^\varepsilon - \chi_{\varepsilon, \delta, \rho_\varepsilon}^\varepsilon) \|_{H^{-1} \cap H^2} \lesssim (M_A + \varepsilon) \| w \|_{H^{-1} \cap H^2}.
\]
The Lemma is proved by combining the above estimates.

\[\square\]

Proof of Lemma 5.4. Let us first prove a lemma comparing two linearized Kohn-Sham operators:

**Lemma 11.1.** Under the same assumptions of Lemma 5.4, we have
\[
\| \mathcal{L}_{\tau, \rho}^\varepsilon w - \mathcal{L}_{\tau, \rho}^\varepsilon w \|_{H^{-1} \cap H^2} \lesssim \| \tilde{\rho} - \tilde{\rho} \|_{H^{-1} \cap H^2} \| w \|_{H^{-1} \cap H^2}.
\]

**Proof.** Let us first compare the potentials corresponding to \( \tilde{\rho} \) and \( \tilde{\rho} \), we have
\[
V_\varepsilon^r (\tilde{\rho}) - V_\varepsilon^r (\tilde{\rho}) = \delta \phi + \eta (J(x) \varepsilon^3 \tilde{\rho}) - \eta (J(x) \varepsilon^3 \tilde{\rho}),
\]
where \( \delta \phi \) solves
\[
-\alpha_{ij} \partial_i \partial_j \partial_j = -b_i \partial_i \delta \phi = 4 \pi \varepsilon (\tilde{\rho} - \tilde{\rho}),
\]
with periodic boundary condition on \( \Gamma \) and \( \int_{\Gamma} \delta \phi = 0 \). Let \( \tilde{V} (x) = (V_\varepsilon^r (\tilde{\rho}))(\varepsilon x) \) and \( \tilde{V} (x) = (V_\varepsilon^r (\tilde{\rho}))(\varepsilon x) \), it is easy to see that
\[
\| \tilde{V} - \tilde{V} \|_{H^1 + H^2} \lesssim \| \tilde{\rho} - \tilde{\rho} \|_{H^{-1} \cap H^2}.
\]
By Sobolev inequality, it follows that
\[
\| \tilde{V} - \tilde{V} \|_{L^2} \lesssim \| \tilde{\rho} - \tilde{\rho} \|_{H^{-1} \cap H^2}.
\]
In particular, we have
\[ \| V^z_\varepsilon(\tilde{\rho}) - V^z_\varepsilon(\rho_0) \|_{L^\infty} \lesssim \| \tilde{\rho} - \rho_0 \|_{H^{-1}\cap H^2}, \]
and similarly for \( \tilde{\rho} \). Therefore, by Lemma 10.2 and Proposition 10.4, the Hamiltonian \( H^z_\varepsilon(\tilde{\rho}) \) and \( H^z_\varepsilon(\tilde{\rho}) \) have a spectral gap larger than \( E_g/4 \) for \( \delta_0 \) sufficiently small.

For simplicity of notations, let us denote
\[ \tilde{L} = \mathcal{L}^z_\tau, \quad \tilde{H} = \mathcal{H}^z_\tau(\tilde{\rho}); \]
\[ \tilde{R}_\lambda = (\lambda - \tilde{H})^{-1}, \quad \tilde{R}_\lambda = (\lambda - \tilde{H})^{-1}; \]
\[ \delta \tilde{V}(w) = \delta \tilde{\rho} V^z_\varepsilon(w), \quad \delta \tilde{V}(w) = \delta \tilde{\rho} V^z_\varepsilon(w). \]

By definition, we have
\[ (\tilde{L}w)(x) = \frac{1}{2\pi i} \int \tilde{R}_\lambda \delta \tilde{V}(w) \tilde{R}_\lambda \, d\lambda(x,x), \]
\[ (\tilde{L}w)(x) = \frac{1}{2\pi i} \int \tilde{R}_\lambda \delta \tilde{V}(w) \tilde{R}_\lambda \, d\lambda(x,x). \]

Subtracting the two, we have
\[ (\tilde{L} - \tilde{L})(w)(x) = \frac{1}{2\pi i} \int \tilde{R}_\lambda (\delta \tilde{V}(w) - \delta \tilde{V}(w)) \tilde{R}_\lambda \, d\lambda(x,x) \]
\[ + \frac{1}{2\pi i} \int \tilde{R}_\lambda \delta \tilde{V}(w) \tilde{R}_\lambda - \tilde{R}_\lambda \delta \tilde{V}(w) \tilde{R}_\lambda \, d\lambda(x,x) \]
\[ = I_1 + I_2. \]

Let us consider the first term on the right hand side. We have
\[ \delta \tilde{V}(w) - \delta \tilde{V}(w) = \left( \eta'(J(x)^{-1}e^3\tilde{\rho}(x)) - \eta'(J(x)^{-1}e^3\tilde{\rho}(x)) \right) J(x)^{-1}e^3w(x). \]

Hence, using the smoothness of \( \eta \),
\[ \| (\delta \tilde{V}(w))(\varepsilon) - (\delta \tilde{V}(w))(\varepsilon) \|_{H^2} \lesssim e^3 \| \tilde{\rho} - \rho \|_{H^2} \| w \|_{H^2}. \]

By a simple rescaling argument, Proposition 6.8 and Corollary 6.12, we obtain
\[ \| I_1 \|_{H^{-1}\cap H^2} \lesssim \| \tilde{\rho} - \rho \|_{H^{-1}\cap H^2} \| w \|_{H^{-1}\cap H^2}. \]

For \( I_2 \), note that
\[ \tilde{R}_\lambda - \tilde{R}_\lambda = \tilde{R}_\lambda(\tilde{H} - \tilde{H}) = \tilde{R}_\lambda(V^z_\varepsilon(\tilde{\rho}) - V^z_\varepsilon(\tilde{\rho})) = \tilde{R}_\lambda, \]

since the kinetic part (Laplacian) of the two Hamiltonians are the same. Therefore, using the estimate (11.3), Proposition 6.16 and a scaling argument, we have
\[ \| I_2 \|_{H^{-1}\cap H^2} \lesssim \| \tilde{\rho} - \rho \|_{H^{-1}\cap H^2} \| w \|_{H^{-1}\cap H^2}. \]

The lemma is proved. \( \square \)
Now come back to the proof of Lemma 5.4. If \( \| \tilde{\rho} - \rho^0 \|_{H^{-1} \cap H^2} \leq \delta_0 \) and \( \| \tilde{\rho} - \rho^0 \|_{H^{-1} \cap H^2} \leq \delta_0 \) for \( \delta_0 \) sufficiently small, we know that the Kohn-Sham map \( F_\tau(\tilde{\rho}) \) and \( F_\tau(\tilde{\rho}) \) are well defined by Proposition 10.6, and also
\[
F_\tau(\tilde{\rho}) - F_\tau(\tilde{\rho}) = L_\tau(\tilde{\rho} - \tilde{\rho}) + R(\tilde{\rho}, \tilde{\rho}),
\]
where the remainder \( R \) satisfies
\[
\| R(\tilde{\rho}, \tilde{\rho}) \|_{H^{-1} \cap H^2} \lesssim \| \tilde{\rho} - \rho \|_{H^{-1} \cap H^2} \lesssim \delta_0 \| \tilde{\rho} - \tilde{\rho} \|_{H^{-1} \cap H^2},
\]

since
\[
\| \tilde{\rho} - \tilde{\rho} \|_{H^{-1} \cap H^2} \lesssim \| \tilde{\rho} - \rho^0 \|_{H^{-1} \cap H^2} + \| \tilde{\rho} - \rho^0 \|_{H^{-1} \cap H^2} \lesssim 2\delta_0.
\]
By Lemma 11.1, we have
\[
\| L_{\tau, \rho}^\varepsilon - L_{\tau, \rho^0}^\varepsilon \|_{L(\vec{H}^{-1} \cap H^2)} \lesssim \| \rho - \rho^0 \|_{H^{-1} \cap H^2} \lesssim \delta_0.
\]
Therefore, combining these estimates, we obtain
\[
\| F_\tau^\varepsilon(\tilde{\rho}) - F_\tau^\varepsilon(\tilde{\rho}) - L_{\tau, \rho}^\varepsilon(\tilde{\rho} - \tilde{\rho}) \|_{H^{-1} \cap H^2} \lesssim \delta_0 \| \tilde{\rho} - \tilde{\rho} \|_{H^{-1} \cap H^2}.
\]

\[\square\]

**Appendix A. Proof of Lemmas 9.3 and 9.9**

**Proof of Lemma 9.3.** For given \( x \in \Gamma \), we will show that \( C_{\alpha \beta}(x) = -C_{\beta \alpha}(x) \). For simplicity of notations, we will suppress the dependence on \( x \) in the proof.

Using the spectral representation of \((\lambda - H_0)^{-1}\), we have \(^2\)
\[
C_{\alpha \beta} = \frac{1}{2\pi i} \sum_{n<m} \int_{p \in \Gamma} \int_{\gamma \gamma'} \frac{1}{\lambda - E_n(k)} \frac{1}{\lambda - E_m(p)} \frac{1}{\lambda - E_I(q)} \times \left\langle \psi_{n, k}(\zeta) \psi_{l, q}^*(\zeta) F_{n, k, m, p}^{\alpha} F_{m, p, l, q}^{\beta} \right\rangle_d \frac{dk dp dq d\lambda}{\lambda - E_n(k)} \frac{1}{\lambda - E_m(p)} \frac{1}{\lambda - E_I(q)}
\]

with the notation
\[
F_{n, k, m, p}^{\alpha}(\zeta) = \langle \psi_{n, k} | \zeta_\alpha - z_\alpha + \tilde{g}_1(\zeta) | \psi_{m, p} \rangle z,
\]
\[
F_{m, p, l, q}^{\beta}(\zeta) = \langle \psi_{m, p} | \zeta_\beta - z_\beta + \tilde{g}_1(\zeta) | \psi_{l, q} \rangle z.
\]

Note that
\[
\frac{1}{\lambda - E_n(k)} \frac{1}{\lambda - E_m(p)} \frac{1}{\lambda - E_I(q)} = \frac{1}{\lambda - E_n(k)} \frac{1}{\lambda - E_m(p)} \frac{1}{\lambda - E_I(q)} + \frac{1}{\lambda - E_m(p)} \frac{1}{\lambda - E_n(k)} \frac{1}{\lambda - E_I(q)} + \frac{1}{\lambda - E_I(q)} \frac{1}{\lambda - E_m(p)} \frac{1}{\lambda - E_n(k)}
\]

Therefore, by the contour integration formula, we have
\[
C_{\alpha \beta} = I_{\alpha \beta}^{++} - I_{\alpha \beta}^{+-} + I_{\alpha \beta}^{-+} - I_{\alpha \beta}^{--} + I_{\alpha \beta}^{++} - I_{\alpha \beta}^{-+} - I_{\alpha \beta}^{++} - I_{\alpha \beta}^{--}.
\]

\(^2\)Instead of using variables \( \xi \) and \( \eta \) for the Bloch decomposition, here we have used \( k, p \) and \( q \).
Here the terms are given by

\[ I_{\alpha\beta}^{++} = \sum_{n>\mathbb{Z}} \sum_{m>\mathbb{Z}} \sum_{l>\mathbb{Z}} \int_{[\Gamma_\gamma]} \frac{1}{E_l(q) - E_m(p)} \frac{1}{E_n(k) - E_n(k)} \times \left\langle \psi_n, \psi_l, \alpha \right\rangle F_{n,k,m,p}^\alpha F_{m,p,l,q}^\beta \right\rangle \text{d}k \text{d}p \text{d}q \]

\[ I_{\alpha\beta}^{-+-} = \sum_{n\leq\mathbb{Z}} \sum_{m\leq\mathbb{Z}} \sum_{l>\mathbb{Z}} \int_{[\Gamma_\gamma]} \frac{1}{E_l(q) - E_m(p)} \frac{1}{E_n(k) - E_n(k)} \times \left\langle \psi_n, \psi_l, \alpha \right\rangle F_{n,k,m,p}^\alpha F_{m,p,l,q}^\beta \right\rangle \text{d}k \text{d}p \text{d}q \]

\[ I_{\alpha\beta}^{+-+} = \sum_{n>\mathbb{Z}} \sum_{m\leq\mathbb{Z}} \sum_{l>\mathbb{Z}} \int_{[\Gamma_\gamma]} \frac{1}{E_l(q) - E_m(p)} \frac{1}{E_n(k) - E_n(k)} \times \left\langle \psi_n, \psi_l, \alpha \right\rangle F_{n,k,m,p}^\alpha F_{m,p,l,q}^\beta \right\rangle \text{d}k \text{d}p \text{d}q \]

\[ I_{\alpha\beta}^{++-} = \sum_{n\leq\mathbb{Z}} \sum_{m\leq\mathbb{Z}} \sum_{l\leq\mathbb{Z}} \int_{[\Gamma_\gamma]} \frac{1}{E_l(q) - E_m(p)} \frac{1}{E_n(k) - E_n(k)} \times \left\langle \psi_n, \psi_l, \alpha \right\rangle F_{n,k,m,p}^\alpha F_{m,p,l,q}^\beta \right\rangle \text{d}k \text{d}p \text{d}q \]

By interchanging \((n,k)\) with \((l,q)\), it is easy to see that

\[ I_{\alpha\beta}^{++} = I_{\beta\alpha}^{++}, \quad I_{\alpha\beta}^{-+-} = I_{\beta\alpha}^{-+-}, \quad I_{\alpha\beta}^{+-+} = I_{\beta\alpha}^{+-+}, \quad I_{\alpha\beta}^{++-} = I_{\beta\alpha}^{++-}. \]

Hence, we have

\[ C_{\alpha\beta} = C_{\beta\alpha}. \]

We will further show that

\[ I_{\alpha\beta}^{++} = I_{\beta\alpha}^{-+-}, \quad I_{\alpha\beta}^{+-+} = I_{\beta\alpha}^{++-}, \quad I_{\alpha\beta}^{++-} = I_{\beta\alpha}^{+-+}, \]

and hence \( C_{\alpha\beta} = -C_{\alpha\beta} \), together with (A.1), we obtain the conclusion

\[ C_{\alpha\beta} = -C_{\beta\alpha}. \]

Let us show (A.2) and (A.3) now. We first notice that \( F_{n,k,m,p}^\alpha \) can be explicitly evaluated using the Poisson summation formula and integration by parts:

\[ F_{n,k,m,p}^\alpha = \left( \langle u_{n,k}, \tilde{g}_{1,\alpha} u_{m,k} \rangle - \varepsilon_n \delta_{nm} - i \delta_{nm} \partial_{p_\alpha} + \langle u_{n,k}, i \partial_{k_\alpha} u_{m,k} \rangle \right) \delta(p - k), \]
where \( u_{n,k}(z) = e^{-ikz} \psi_{n,k}(z) \). Similarly,

\[
F_{m,p,l,q}^{\alpha} = \left((u_{m,p}, \tilde{g}_{1,\beta}u_{l,p}) - z_{\beta} \delta_{m,l} - i \delta_{m,l} \partial_{q,\beta} + \langle u_{m,p}, i \partial_{q,\beta} u_{l,p} \rangle \right) \delta(q-p).
\]

Substituting in the expressions of \( I^{++} \), after a tedious but straightforward calculation, we have

\[
I_{\alpha\beta}^{++} = - \sum_{n \in \mathbb{Z}} \sum_{l \in \mathbb{Z}} \int_{\Gamma^*} \frac{dk}{(E_{l}(k) - E_{n}(k))^{2}} \langle u_{n,k}, i \partial_{k,n} u_{l,k} \rangle \times \left( \langle u_{n,k}, \tilde{g}_{1,\beta} u_{l,k} \rangle + \langle u_{n,k}, i \partial_{k,\beta} u_{l,k} \rangle \right),
\]

and also for \( I^{--} \):

\[
I_{\alpha\beta}^{--} = - \sum_{n \leq \mathbb{Z}} \sum_{l \in \mathbb{Z}} \int_{\Gamma^*} \frac{dk}{(E_{l}(k) - E_{n}(k))^{2}} \langle u_{n,k}, i \partial_{k,n} u_{l,k} \rangle \times \left( \langle u_{n,k}, \tilde{g}_{1,\beta} u_{l,k} \rangle + \langle u_{n,k}, i \partial_{k,\beta} u_{l,k} \rangle \right).
\]

Interchanging \( n \) and \( l \) and using

\[
\langle u_{l,k}, i \partial_{k,n} u_{n,k} \rangle = \langle u_{n,k}, i \partial_{k,n} u_{l,k} \rangle,
\]

we can rewrite \( I^{--} \) as

\[
I_{\alpha\beta}^{--} = - \sum_{n \in \mathbb{Z}} \sum_{l \leq \mathbb{Z}} \int_{\Gamma^*} \frac{dk}{(E_{l}(k) - E_{n}(k))^{2}} \langle u_{n,k}, i \partial_{k,n} u_{l,k} \rangle \times \left( \langle u_{n,k}, \tilde{g}_{1,\beta} u_{l,k} \rangle + \langle u_{n,k}, i \partial_{k,\beta} u_{l,k} \rangle \right).
\]

We have shown (A.2).

Next, let us consider \( I^{++} \) and \( I^{--} \), using the expression for \( F_{n,k;m,p}^{\alpha} \) and \( F_{m,p,l,q}^{\beta} \), we have

\[
I_{\alpha\beta}^{++} = \sum_{n \geq \mathbb{Z}} \sum_{m \leq \mathbb{Z}} \int_{\Gamma^*} \frac{dk}{(E_{m}(k) - E_{n}(k))^{2}} \left( \langle u_{n,k}, \tilde{g}_{1,\alpha} u_{m,k} \rangle + \langle u_{n,k}, i \partial_{k,n} u_{m,k} \rangle \right) \times \left( \langle u_{m,k}, \tilde{g}_{1,\beta} u_{n,k} \rangle + \langle u_{m,k}, i \partial_{k,\beta} u_{n,k} \rangle \right),
\]

and

\[
I_{\alpha\beta}^{--} = \sum_{n \leq \mathbb{Z}} \sum_{m \geq \mathbb{Z}} \int_{\Gamma^*} \frac{dk}{(E_{m}(k) - E_{n}(k))^{2}} \left( \langle u_{n,k}, \tilde{g}_{1,\alpha} u_{m,k} \rangle + \langle u_{n,k}, i \partial_{k,n} u_{m,k} \rangle \right) \times \left( \langle u_{m,k}, \tilde{g}_{1,\beta} u_{n,k} \rangle + \langle u_{m,k}, i \partial_{k,\beta} u_{n,k} \rangle \right).
\]

Interchanging \( n \) and \( m \), we obtain (A.3).

\]

\textbf{Proof of Lemma 9.9.} First let us assume that \( U_{0} \) satisfies (9.43). Let us consider a potential of the form

\[
V(x) = v_{0}(x, x/\varepsilon) + U_{0}(x) + v_{1}(x, x/\varepsilon)
\]

where \( v_{1} = v_{1,1} + v_{1,2} \) with \( v_{1,2} \) given by (9.53) and \( v_{1,1} \) given by (9.56).
Consider \( w \) given by
\[
w(x) = \frac{1}{2\pi i} \int_{\mathcal{C}} \frac{1}{\lambda - \mathcal{H}} \, d\lambda(x, x),
\]
where
\[
\mathcal{H} = -\varepsilon^2 a_{ij}(x) \partial_i \partial_j - \varepsilon^2 b_i(x) \partial_i - \varepsilon^2 c(x) + V(x).
\]
By a similar argument as in the proof of Proposition 10.3, we have
\[
|w(x) - \varepsilon^{-1} \rho_0(x, x/\varepsilon) + \varepsilon^{-2} \rho_1(x, x/\varepsilon) + \varepsilon^{-1} \rho_2(x, x/\varepsilon)| \lesssim 1,
\]
as \( \varepsilon \to 0 \), where \( \rho_0(x, x/\varepsilon) = \rho_{CB}(z; \nabla u(x)) \), \( \rho_1 \) given by (9.55) and the average of \( \rho_2 \) over the unit cell is given by (9.58)

From the normalization of \( \mathbf{m} \), \( \rho_0 \) and using similar argument as in Lemma 9.1, we arrive at the conclusion that
\[
\int_{\Gamma} \langle \rho_2(x, \cdot) \rangle \, dx = 0.
\]

For a general \( U_0 \), since \( U_0 \) is continuous and hence bounded, we can take \( \lambda > 0 \) sufficiently small such that \( \lambda U_0 \) satisfies (9.43). Applying the previous argument to \( \lambda U_0 \), we have
\[
\lambda \int_{\Gamma} \alpha_{\beta}(x) \partial_{x_\alpha} U_0(x) \, dx + \lambda \int_{\Gamma} \beta_{\alpha}(x) \partial_{x_\alpha} U_0(x) \, dx + \int_{\Gamma} D(x) \, dx = 0.
\]
Since this is valid for arbitrary \( \lambda \) sufficiently small, it is also valid for \( \lambda = 1 \), and the Lemma is proved.

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