Macroscopic Electrostatics at Positive Temperature from the Density Functional Theory

by

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A thesis submitted in conformity with the requirements
for the degree of Doctor of Philosophy
Graduate Department of Mathematics
University of Toronto

Abstract

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2019

The purpose of this thesis is to study local perturbations of equilibrium crystalline states of the density functional theory (DFT) at positive temperature through the Kohn-Sham equations under local-density approximation (LDA). Under suitable scaling and at low temperature, we prove an existence result for the Kohn-Sham equations and show that local macroscopic perturbations from periodic equilibrium states give rise to the Poisson equation as an effective equation.

Dedicated to Chen Zhiyuan, Sun Jingwen, and Sun Lanzhi.

Acknowledgements

I would like to thank my adviser Prof. Israel Michael Sigal for his guidance and genuine advices throughout my doctoral study. I am indebted to my graduate committee members, Prof. Almut Buchard and Prof. Robert Jerrard, for their useful discussions and expert advices. In addition, I would also like to thank Greg Fournodavlos, Antoine Levitt, and Panayotis Smyrnelis for enjoyable discussions.

My graduate study would not be possible without the close friendship and support of Andrew Juno Jung since the beginning of our freshman year. In addition, I would like to thank Krishan Rajaratnam and Dmitri Chouchkov for their kind friendship. Krishan has challenged me to be a critical thinker in all matters of life while Dmitri has been the solution tank for all my research troubles. Moreover, I would like to thank Adam Gardner and Afroditi Talidou for fighting through our graduate studies together and sitting through every Friday seminar (especially the ones that I have to give a long talk).

I thank all my friends who made my graduate experience enjoyable and productive: Xinliang An, Afiny Akdemir, Francis Bischoff, Gong Chen, Elizabeth Ching, Sunny Choi, Andrew Colinet, Travis Ens, Vivek Gandhi, Timothée Haggstrom, Jeffery Im, Jia Ji, Christopher Kennedy, Tomas Kojar, Jiaqi Liu, Joshua Kung, Mykola Matviichuk, Tristan Milne, Beatriz Navarro Lameda, Adriano Pacifico, Justin Pham, Artane Siad, David Yew, Shuangjian Zhang, Yuanyuan Zheng, Tianyu Zhou, and Steven Zhu. For those whose name I missed, I apologize and thank them once more for their contributions. I also thank Ashley Armogan, Sonja Injac, Jemima Merisca, and Patrina Seepersaud, whose hard work made all of the graduate students' life many times better.

I want to also thank Prof. Gian Michele Graf for hosting me at ETH Zürich during a part of my Ph.D study. This opportunity has greatly enriched my physical intuition. My experience in Europe was made all the more enlightening through useful discussions with Prof. Rupert Frank, Prof. Christian Hainzl, Prof. Marchello Porta, and Prof. Benjamin Schlein. At the same time, I am grateful for the friendship of Vincent Beaud, Chiara Boccato, Christian Brenneke, Martin Gebert, Lisa Hänggli, Simone Rademacher, Chiara Saffirio, Jacob Shapiro, and David Taj (without whom I could not have settled in my new flat in Zürich).

Last but not least, I would like to thank my mother Jingwen Sun and my grandmother Lanzhi Sun – two strong women who prepared me for success. I would like to thank my uncle and aunts, Daoyuan Chen and Min Wei, Jingru Sun, Jingyun Qiu, and my cousins Cha Chen and Bin Luo for their love and support. Without these people, I could not have finished my study.

The content of this thesis is supported in part by NSERC Grant No. NA7901. I would also like to acknowledge the generous support of NSERC CGS D and M graduate scholarships, the Ontario Graduate scholarship, and the Queen Elizabeth II Graduate Scholarship.

Contents

Chapter 1

Introduction

The economics of scientific theory is a delicate balance between accuracy and efficiency. This statement is particularly true for many body quantum mechanics. On one hand, quantum mechanics is a highly accurate theory. On the other hand, its practical usefulness is limited by its complexity in describing large systems of particles. This inefficiency should not be surprising as quantum mechanics is a highly comprehensive theory. Nevertheless, since it often suffices to extract certain characteristic properties and neglect other degrees of freedom, effective theory is derived. One outstanding example is the density functional theory (DFT) of quantum chemistry. Its tremendous success in revealing the electronic structure of matter warrants a rigorous investigation of its mathematical structure and its use as a starting point in the derivation of emergent macroscopic properties of quantum matter.

The first attack on the macroscopic consequences of DFT was made in pioneering works of E. Cansès, M. Lewin and G. Stolz and W. E and J. Lu and their collaborators ([12, 8, 9, 10, 11, 22, 18, 19, 22]). These works considered the zero temperature case. The first treatment of the positive temperature DFT was given by Levitt ([32], see also [16]). In this thesis we derive the effective Poisson equation of electrostatics from the microscopic DFT at positive temperatures.

This thesis paper is organized as follows. In Chapter 1, we provide background material and a formal derivation of the DFT via the general frame work of quasi-free reduction. In Chapter 2, we will provide a review of the historical development of DFT and its rigorous mathematical derivation. Then, we specify the problem of DFT that we wish to study in this thesis. The main results of this thesis (5) is stated in Chapter 3 as an accumulation of the works in [15, 16]. Before proving the main results, we will insert necessary preliminary materials on densities and Bloch-Floquet decomposition in Chapter 4. Immediately after the preliminary preparation in Chapters 5, we will provide proofs for the claimed result with detailed technical estimates delayed to Appendices B - C. Appendix A shows that the current result agrees with previous results when $T = 0$ and the exchange-correlation term is set to zero in the Kohn-Sham equation.

1.1 Fermion Many Body Theory

1.1.1 Dynamics of Quantum Many Body Systems

Many Body Hamiltonian

Unlike much literature on the DFT (for example, [27, 30, 33, 34, 35, 36]), we approximate the dynamics of many body evolution via a general frame work of quasi-free reduction (see, for example, [26, 5, 3]). This view allows us to survey a large array of effective equations simultaneously while retaining sufficient intuition for DFT. A more rigorous mathematical derivation of the DFT will be considered later in Section 2.2. We start with a description of the fermion many body system as we focus on the electronic theory of matter.

A single quantum state or particle (ignoring spin) is described by an element of the Hilbert space $\mathcal{H} = L^2(\mathbb{R}^3)$ of unit norm. A system with n fermions is therefore described by an element of

$$\mathcal{H}^{(n)} = \underbrace{\mathcal{H} \wedge \mathcal{H} \cdots \mathcal{H} \wedge \mathcal{H}}_{n \text{ copies}}, \tag{1.1}$$

where $\wedge$ is the exterior tensor product. To describe a system with an unfixed number of particles, we pass to the Fock space of states. In particular, we define

$$\mathcal{F}_{\mathcal{H}} := \bigoplus_{n=0}^{\infty} \mathcal{H}^{(n)} \tag{1.2}$$

where $\mathcal{H}^{(0)} = \mathbb{C}$ is spanned by the normalized vacuum state $|\Omega\rangle = 1$.

A Hamiltonian $\mathbb{H}$ on $\mathcal{F}_{\mathcal{H}}$ is a self-adjoint operator. Given $\mathbb{H}$, it generates a quantum dynamics for an initial state $\Psi_0 \in \mathcal{F}_{\mathcal{H}}$ via the time-dependent Schrödinger's equation

$$i\partial_t \Psi = \mathbb{H}\Psi. \tag{1.3}$$

This dynamics is equivalent to the dynamics in the Heisenberg picture:

$$i\partial_t \hat{\omega} = [\hat{\omega}, \mathbb{H}] \tag{1.4}$$

where $\hat{\omega} = |\Psi\rangle\langle\Psi|$ with initial condition $\hat{\omega}_0 = |\Psi_0\rangle\langle\Psi_0|$.

In the most general setting, let $\mathcal{B}(\mathbb{H})$ denote the C^*-algebra of bounded linear operators on $\mathbb{H}$. A state, ω, is a positive functional on $\mathcal{B}(\mathbb{H})$ such that $\omega(A) \geq 0$ for all positive operators $A \in \mathcal{B}(\mathbb{H})$ and $\omega(\mathbf{1}) = 1$ where $\mathbf{1}$ is the identity map on $\mathbb{H}$. Then, equation (1.4) becomes

$$i\partial_t \omega = \omega \circ \mathrm{ad}_{\mathbb{H}} \tag{1.5}$$

where $\mathrm{ad}_{\mathbb{H}}(A) = [\mathbb{H}, A]$ for any $A \in \mathcal{B}(\mathcal{F}_{\mathcal{H}})$ with initial condition ω_0. Often, each state ω is demanded to be continuous. Consequently,

$$\omega(A) = \mathrm{Tr}(A\hat{\omega}) \tag{1.6}$$

for some operator $\hat{\omega} \in \mathcal{B}(\mathcal{F}_{\mathcal{H}})$ ([21]). In this case, the operator $\hat{\omega}$ satisfies (1.4). Nonetheless, any practical computation is unfeasible in this generality.

To produce a tractable theory, we specialize our Hamiltonian to one involving at most particle pair interactions. In particular, let h denote

$$h = -\Delta + W \tag{1.7}$$

denote the 1-particle Hamiltonian for some external potential W on $\mathcal{H}$ and let $v(x-y)$ denote the pair interaction potential. We consider n particle Hamiltonian

$$H_n = \sum_{i=1}^{n} h_i + \sum_{1\le i<j\le n} v(x_i - x_j) \tag{1.8}$$

where each h_i is a copy of h acting on the i-th variable x_i. Note that H_n leaves $\mathcal{H}^{(n)}$ invariant in $\mathcal{F}_{\mathcal{H}}$. The many body Hamiltonian $\mathbb{H}$ is therefore

$$\mathbb{H} = \sum_{n=1}^{\infty} H_n \tag{1.9}$$

where H_n acts on $\mathcal{H}^{(m)}$ as the zero operator if $n \neq m$. In this form, the Hamiltonian $\mathbb{H}$ remains difficult to study. We introduce in the next section the creation and annihilation operators to aid further simplification in the study of $\mathbb{H}$.

Creation and Annihilation Operators [25]

Let $f \in \mathbb{H}$, we define the annihilation operator $a(f) : \mathcal{H}^{(n)} \to \mathcal{H}^{(n-1)}$ via

$$(a(f)\Psi)(x_1, ..., x_{n-1}) = \sqrt{n} \int_{\mathbb{R}^3} dx_n f(x_n)\Psi(x_1, ..., x_n). \tag{1.10}$$

By setting $a(f)|\Omega\rangle = 0$ for all f, we can extend $a(f)$ to $\mathcal{F}_{\mathcal{H}}$ by linearity. We define the creation operator $a^*(f)$ to be the adjoint of $a(f)$ on $\mathcal{F}_{\mathcal{H}}$. To invoke the language of second quantization, we define operator valued distribution a_x and a^*_x by

$$a(f) = \int_{\mathbb{R}^3} dx\, \bar{f}(x)a_x \text{ and } a^*(f) = \int_{\mathbb{R}^3} dx\, f(x)a^*_x. \tag{1.11}$$

Proposition 1 ([25]). *The operator* $\mathbb{H}$ *in* (1.9) *has the following explicit quartic (in* *creation and annihilation operators) form.*

$$\mathbb{H} = \int_{\mathbb{R}^3} dx\, a_x^* h_x a_x + \int_{\mathbb{R}^3} dx \int_{\mathbb{R}^3} dy\, a_x^* a_y^* v(x-y) a_x a_y \tag{1.12}$$

where h_x is the the operator h in (1.7) *acting on the variable x.*

As it is the case with all self-adjoint operators, the study of the spectrum of $\mathbb{H}$ (see (1.12)) is crucial to the understanding of its associated physical properties and its dynamics. From Proposition 1, $\mathbb{H}$ is quadratic and diagonalized if $v = 0$. Moreover, its evolution can be written explicitly in terms of 1-particle operator:

$$e^{-i\mathbb{H}t} = \int_{\mathbb{R}^3} dx\, a_x^* e^{-ih_x t} a_x \,. \tag{1.13}$$

(1.13) induces explicit solution to the evolution equation (1.5). That is

$$\omega_t = \omega_0 \circ \mathrm{Ad}_{-i\mathbb{H}t} \tag{1.14}$$

where $\mathrm{Ad}_X(A) = e^{-X} A e^X$.

When $v \neq 0$, such explicit expression for the evolution of $\mathbb{H}$ is not readily attainable. In this setting, the insight of Bardeen-Cooper-Schrieffer theory is to reduce $\mathbb{H}$ into an effective quadratic Hamiltonian using self-consistent principle or quasi-free states [2].

1.1.2 Quasi-Free Reduction

Quasi-Free States and the Effective Quadratic Hamiltonian

Definition 1 (Wick's Theorem)**.** A quasi-free state is a state on $\mathcal{B}(\mathcal{F}_\mathcal{H})$ with the following properties. Let $a_i^\sharp$ denote either a_{x_i} or $a_{x_i}^*$. Then for each positive integer n,

$$\omega(a_1^\sharp \cdots a_{2n}^\sharp) = \sum_{\sigma \in S'_{2n}} (-1)^\sigma \omega(a_{\sigma(1)}^\sharp a_{\sigma(2)}^\sharp) \cdots \omega(a_{\sigma(2n-1)}^\sharp a_{\sigma(2n)}^\sharp) \tag{1.15}$$

$$\omega(a_1^\sharp \cdots a_{2n-1}^\sharp) = 0 \tag{1.16}$$

where S'_{2n} is the subgroup of the permutation group S_{2n} such that $\sigma(1) < \sigma(3) < \cdots < \sigma(2n-1)$ and $\sigma(2j-1) < \sigma(2j)$ for all $1 \leq j \leq n$.

We remark that Definition 1 is also known as Wick's theorem. We make two important observations below.

Our first observation is that quasi-free state reduces $\mathbb{H}$ (see (1.12)) to an effective or self-consistent quadratic Hamiltonian. Indeed,

$$\begin{aligned}
\omega(\mathbb{H}) = \int_{\mathbb{R}^3} dx\, \omega(a_x^* h_x a_x) + \int_{\mathbb{R}^3} dx \int_{\mathbb{R}^3} dy\, v(x-y)\omega(a_x^* a_y^*)\omega(a_y a_x) && (1.17)\\
+ \int_{\mathbb{R}^3} dx \int_{\mathbb{R}^3} dy\, v(x-y)\omega(a_x^* a_x)\omega(a_y^* a_y) && (1.18)\\
+ \int_{\mathbb{R}^3} dx \int_{\mathbb{R}^3} dy\, v(x-y)\omega(a_x^* a_y)\omega(a_y^* a_x). && (1.19)
\end{aligned}$$

In an alternative view, we can write

$$\omega(\mathbb{H}) = \omega(\mathbb{H}_\omega) \tag{1.20}$$

where $\mathbb{H}_\omega$ is quadratic and

$$\begin{aligned}
\mathbb{H}_\omega = & \int_{\mathbb{R}^3} dx\, a_x^*(h_x + V_\omega(x))a_x \\
& + \int_{\mathbb{R}^3} dx \int_{\mathbb{R}^3} dy\, U_\omega(x,y) a_x a_y + \int_{\mathbb{R}^3} dx \int_{\mathbb{R}^3} dy\, \bar{U}_\omega(x,y) a_y^* a_x^* \\
& + \int_{\mathbb{R}^3} dx \int_{\mathbb{R}^3} dy\, W_\omega(x,y) a_x^* a_y + \int_{\mathbb{R}^3} dx \int_{\mathbb{R}^3} dy\, \bar{W}_\omega(x,y) a_y^* a_x
\end{aligned} \tag{1.21}$$

and

$$\begin{aligned}
U_\omega(x,y) = & \frac{1}{2} v(x-y)\omega(a_x^* a_y^*) && (1.22)\\
V_\omega(x,y) = & \int_{\mathbb{R}^3} dy\, v(x-y)\omega(a_y^* a_y) && (1.23)\\
W_\omega(x,y) = & \frac{1}{2} v(x-y)\omega(a_y^* a_x). && (1.24)
\end{aligned}$$

In this form, the quadratic Hamiltonian $\mathbb{H}_\omega$ can be diagonalized explicitly as ([24, 50])

$$\mathbb{H}_\omega = \int_{\mathbb{R}^3} dx\, c_x^* \tilde{h}_x c_x \tag{1.25}$$

for some effective 1 particle operator $\tilde{h}_x$ and a new set of creation and annihilation operators c_x and c_x^* satisfying the canonical anti-commutation relation. We remark here that $c_x, c_x^*, \tilde{h}_x$ depends on ω.

Our second observation is that definition 1 implies that any quasi-free state is uniquely determined by its quadratic expectation. We define the density operator γ and coherent operator α on $\mathcal{H}$ via their integral kernel

$$\gamma(x,y) = \omega(a_y^* a_x) \tag{1.26}$$

$$\alpha(x,y) = \omega(a_x a_y). \tag{1.27}$$

We form the generalized 1-particle operator Γ on $\mathcal{H} \times \mathcal{H}$:

$$\Gamma := \begin{pmatrix} \gamma & \alpha \\ \alpha^* & 1-\bar{\gamma} \end{pmatrix} \tag{1.28}$$

where $\bar{T} = \mathcal{C}T\mathcal{C}$ for any operator T, and $\mathcal{C}$ is the complex conjugation. The following theorem characterizes quasi-free states.

Theorem 2 ([50])**.** *A state ω is a quasi-free state on $\mathcal{F}_\mathcal{H}$ if and only if the generalized 1-particle operator Γ (1.28) constructed from ω satisfies*

$$0 \le \Gamma = \Gamma^* \le 1 \text{ and } \alpha^* = \bar{\alpha}. \tag{1.29}$$

Conversely any such Γ came from a quasi-free state on $\mathcal{F}_\mathcal{H}$.

The two observations show that if we can approximate the evolution (1.5) by quasi-free states, we will be able to obtain a more tractable effective quadratic Hamiltonian. In the mean time, all information of these states are stored in the simpler generalized 1-particle density matrix Γ. As such, we seek ways to approximate the full evolution by evolution of quasi-free states.

Dirac-Frenkel Principle

Let $\mathcal{M}$ denote a manifold embedded in a Banach space X and consider the evolution

$$i\partial_t \omega = F(\omega) \tag{1.30}$$

on X where $F : X \to X$ with initial condition $\omega_0 \in \mathcal{M}$. The Dirac-Frenkel Principle gives the best infinitesimal approximation of (1.30) on $\mathcal{M}$ by the using the evolution

$$i\partial_t \omega = P(\omega)F(\omega) \tag{1.31}$$

where $P(\omega)$ is the projection onto the tangent space at ω of $\mathcal{M}$, $T_\omega\mathcal{M}$. Applying the Dirac-Frenkel Principle to $\mathcal{M}$ =quasi-free states and (1.5), we obtain the effective equation

$$i\partial_t \omega = P(\omega)(\omega \circ \mathrm{ad}_{\mathbb{H}}) \tag{1.32}$$

with initial condition $\omega_0 \in \mathcal{M}$. Equation (1.32) can be written explicitly as

$$i\partial_t \omega = \omega \circ \mathrm{ad}_{\mathbb{H}_\omega} \tag{1.33}$$

where $\mathbb{H}_\omega$ is given in (1.21) [5, 3, 15]. The advantage of this new equation is that it has an explicit tractable form in terms of Γ. From its explicit form, we obtain an array of effective equations.

Theorem 3 ([5, 3, 15])**.** *Equation* (1.32) *is equivalent to*

$$i\partial_t \Gamma = [\Gamma, H_\Gamma] \tag{1.34}$$

where Γ *is given in Theorem 2,*

$$H_\Gamma = \begin{pmatrix} h_\gamma & v\sharp\alpha \\ v\sharp\alpha^* & -\bar{h}_\gamma \end{pmatrix} \tag{1.35}$$

$$h_\gamma = -\Delta + W + v * \rho_\gamma + ex(\gamma), \tag{1.36}$$

$\rho_\gamma(x) = \gamma(x,x)$, *and in terms of integral kernel,* $ex(\gamma)(x,y) = v(x-y)\gamma(x,y)$ *and* $(v\sharp\alpha)(x,y) = v(x-y)\alpha(x,y)$.

1.2 Effective Dynamics

Hartree-Fock-Bogoliubov Equation

Equation (1.28) is the time dependent Bogoliubov-de Gennes (BdG) equations from the BCS theory of superconductivity. Since superconductivity is naturally associated with a magnetic field, one may couple the electro-magnetic potential pair (ϕ, A) to (1.28) through minimal coupling. A more detailed review can be found in [15].

Hartree-Fock Type Equations

We can make further simplification to (1.28) if we ignore the pairing term (i.e. set $\alpha = 0$ where α is defined in (1.27)). Then (1.28) becomes

$$i\partial_t \gamma = [\gamma, h_\gamma] \tag{1.37}$$

where γ and h_γ are give in (1.26) and (1.36), respectively. We can classify (1.37) depending on its exchange term ex:

1. Reduce Hartree equation (rHF): $ex(\gamma) := 0$,
2. Hartree-Fock (HF): $ex(\gamma) := -v\sharp\,\gamma$ (c.f. Theorem 3 for definition of $\sharp$).
3. Density Functional Theory (DFT): $ex(\gamma) := \mathrm{xc}(\rho_\gamma)$ where $\rho_\gamma(x) := \gamma(x, x)$ ($A(x, y)$ is the integral kernel of the operator A) and $\mathrm{xc} : \mathbb{R}_{\geq 0} \to \mathbb{R}$.

1.3 Static Equations

To limit the scope of this thesis, we study equilibrium systems. In this case, the object of interest in an equilibrium system is the Gibbs state. This state is a static solution to the evolution (1.28). In particular, we seek a state Γ such that

$$[\Gamma, H_\Gamma] = 0. \tag{1.38}$$

The BdG Equation

The Gibbs state corresponding to temperature $T = 1/\beta$ and chemical potential μ is a state Γ solving the BdG equation

$$\Gamma = f_{\mathrm{FD}}(\beta(H_\Gamma - \mu)) \tag{1.39}$$

where

$$f_{\mathrm{FD}}(\lambda) = \frac{1}{1+e^\lambda} \tag{1.40}$$

is the Fermi-Dirac distribution. One can see that a solution to (1.39) solves (1.38). When coupled to an magnetic field, a, (1.39) is extended to precisely the Euler-Lagrange equation of the BCS free energy functional. We will focus on the simpler DFT and refer interested readers to a more detailed review in [15].

Static Hartree-Fock Equation

The next step in our progress of simplification is to consider quasi-free state without pairing. That is, $\alpha = 0$. In this case, (1.39) becomes

$$\gamma = f_{\mathrm{FD}}(\beta(h_\gamma - \mu)) \tag{1.41}$$

where f_{FD} is once again the Fermi-Dirac distribution in (1.40) and h_γ is given in (1.36). This is the static Hartree-Fock equation.

Density Functional Theory

Despite the vast reduction of the many body evolution through quasi-free reduction and the omission of the pairing term α in the HF equation, this system remains difficult to study. In the static case, a further simplification is possible if the exchange term $ex(\gamma)$ only depends on the density ρ_γ (see Item 3 in the list in 1.2). This type of exchange term makes all the difference between a practically intractable and imprecise model and the tractable and precise one. In the next chapter, we will consider in detail the density functional theory.

Chapter 2

Density Functional Theory (DFT)

2.1 Introduction

The density functional theory is based on the Kohn-Sham (KS) equation and the corresponding energy functional. It was first derived in the static zero density and zero temperature case ([29]) and extended to positive temperatures in [42, 51] (see [7] for a review).

In the case $T > 0$, let $\text{den} : A \to \rho_A$ be the map from operators, A, to functions $\rho_A(x) := A(x,x)$ (here $A(x,y)$ stands for the integral kernel of an operator A, details in Chapter 4 below). Applying den to equation (1.41), we can rewrite it as an equation of the particle density ρ alone:

$$\rho = \text{den}[f_{\text{FD}}(\beta(h_\rho - \mu))], \tag{2.1}$$

where f_{FD} is given in (1.40) and (upon a modification of the sign of v since electrons are negatively charged)

$$h_\rho := -\Delta + W + v * \rho + \text{xc}(\rho_\gamma)\,. \tag{2.2}$$

Equation (2.1) is the celebrated Kohn-Sham (KS) equation of DFT.

The function $\mathrm{xc}(\rho)(x) = \mathrm{xc}(\rho(x))$ is called the exchange-correlation term. (one would like to include terms like $\int |\nabla\rho|^2$, see [4, 36, 35]) It combines contributions from the exchange interactions, due to the Fermi-Dirac statistics, and from (non-exchange) correlations between electrons. The exchange part is given by Dirac exchange energy $-c\rho^{1/3}$ for some constant $c > 0$. The correlation part is chosen empirically. Various correlation terms are listed in [20, 52, 45, 17, 44], see [6, 28] for reviews of popular exchange-correlation terms.

For a wide class of ρ's, the operator h_ρ is self-adjoint and the r.h.s. of (2.1) is well defined. Given ρ, we can define the density operator

$$\gamma = f_{\mathrm{FD}}(\beta(h_\rho - \mu)) \tag{2.3}$$

acting on $L^2(\mathbb{R}^d)$. If ρ solves (2.1), then $\gamma = f_{\mathrm{FD}}(\beta(h_\rho - \mu))$ solves

$$\gamma = f_{\mathrm{FD}}(\beta(h_{\rho_\gamma} - \mu)), \tag{2.4}$$

where, recall, $\rho_\gamma(x) := \gamma(x, x)$. Applying the map den to equation (2.4) gives (2.1).

As was mentioned above, equation (2.1), or (2.4), is an extension of the original Kohn-Sham equation to positive temperatures and we will use for it the same name – the Kohn-Sham, or KS equation.

DFT and the electrostatic potential

The case of most significance is when the pair potential $v(r) = \frac{2\pi}{|r|}$ is the Coulomb potential, corresponding to the integral kernel of $(-\Delta)^{-1}$ in $d = 3$. In what follows, we will assume that v is this Coulomb potential.

Moreover, we specialize to the case where the external potential W is generated through a positively charged background distribution κ. That is, $W = -v * \kappa$ (the negative sign comes from the electron's negative charge). In this case, the Hamiltonian (2.2) becomes

$$h_\rho := -\Delta - v * (\kappa - \rho) + \mathrm{xc}(\rho_\gamma)\,. \tag{2.5}$$

To each ρ, we associate an electrostatic potential

$$\phi := v * (\kappa - \rho). \tag{2.6}$$

Thus, we can replace the KS equations (2.1) by the system

$$\rho = \mathrm{den}[f_{\mathrm{FD}}(\beta(h^\phi - \mu))], \tag{2.7}$$

$$-\Delta\phi = 4\pi(\kappa - \rho), \tag{2.8}$$

where

$$h^\phi = -\Delta - \phi + \mathrm{xc}(\kappa + (4\pi)^{-1}\Delta\phi). \tag{2.9}$$

We can further eliminate ρ from (2.7) - (2.8) in favor of ϕ alone to obtain

$$-\Delta\phi = 4\pi(\kappa - \mathrm{den}[f_{\mathrm{FD}}(\beta(h^\phi - \mu))]). \tag{2.10}$$

If κ and ρ are periodic with respect to a lattice $\mathcal{L} \subset \mathbb{R}^3$, then integrating (2.8), we arrive at the relation

$$\int_\Omega \rho_\gamma = \int_\Omega \kappa, \tag{2.11}$$

where Ω is a fundamental cell of $\mathcal{L}$. In this case, we have to add to the KS equation (2.1) (or (2.10)) the solvability condition (2.11) which determines the chemical potential μ. (2.11) can be interpreted as the conservation of the charge per fundamental cell of $\mathcal{L}$.

In what follows we will deal either with equation (2.1) for ρ and associate with a solution ρ the electrostatic potential

$$\phi_\rho = 4\pi(-\Delta)^{-1}(\kappa - \rho)\,, \tag{2.12}$$

or with equation (2.10) and associate with a solution ϕ the charge density ρ according to (2.7).

2.2 Mathematical Justification

In Chapter 1, we gave a formal derivation of the DFT. In this section, we review some mathematical treatment of the derivation from many body system. In the static setting, we are interested in the ground state of H_n and its energy (see (1.8)):

$$E_{\mathrm{gs}} = \inf_{\Psi \in \mathcal{H}^{(n)}} \langle \Psi, H_n \Psi \rangle. \tag{2.13}$$

The goal of DFT is to construct an energy functional $E_{\mathrm{DFT}}(\rho)$ dependent on ρ only such that

$$E_{\mathrm{gs}} = \inf_{\rho} E_{\mathrm{DFT}}(\rho). \tag{2.14}$$

One approach to construct $E_{\mathrm{DFT}}(\rho)$ is as follows. Let v denote the pair interaction potential in H_n. There are two maps

$$v \to \Psi \to \rho \tag{2.15}$$

where Ψ is the ground state of H_n with pair potential v, if it exists, and

$$\rho(x) = \int_{\mathbb{R}^{3(n-1)}} dx_2 \cdots dx_n |\Psi(x, x_2, \cdots, x_n)|^2 \tag{2.16}$$

is the 1-particle density of Ψ. If we can invert and obtain a map $\rho \to \Psi_\rho$, then we can write

$$E_{\mathrm{DFT}}(\rho) = \inf_{\rho} \langle \Psi_\rho, H_n \Psi_\rho \rangle. \tag{2.17}$$

Since $\Psi \to \rho$ is highly non-injective, such an inverse is not readily available. The helpful approach is to invert the entire chain of maps $v \to \Psi \to \rho$ instead. This way, we obtain

$$\rho \to v_\rho \to \Psi. \tag{2.18}$$

The inverse of $v \to \Psi \to \rho$ is made possible by the Hohenberg-Kohn (HK) Theorem ([30]) below.

Theorem 4 ([30])**.** *Let v and v' be two pair potentials with ground states Ψ_v and $\Psi_{v'}$. Assume that the associated densities $\rho_v = \rho_{v'}$ are equal. Then, under mild technical assumptions, $v - v'$ is a constant.*

Proof. We provide a sketch here. Let $H(v)$ denote the Hamiltonian in (1.8) with pair potential v. By minimality

$$\langle \Psi_v, H(v)\Psi_v\rangle \le \langle \Psi_{v'}, H(v)\Psi_{v'}\rangle = \langle \Psi_{v'}, H(v')\Psi_{v'}\rangle + \langle \Psi_{v'}, (v - v')\Psi_{v'}\rangle \tag{2.19}$$

$$= \langle \Psi_{v'}, H(v')\Psi_{v'}\rangle + \langle v - v', \rho_{v'}\rangle. \tag{2.20}$$

Since $\rho_v = \rho_{v'}$, we can reverse the role of v and v' in the above proof and observe that the inequality sign can be reversed. In particular, we may replace the $\le$ sign by $=$ in (2.19). Hence $\Psi_{v'}$ is also a ground state of $H(v)$, vise versa. Let E_v denotes the ground state energy $H(v)$. Then

$$(E_v - E_{v'})\Psi_v = (H(v) - H(v'))\Psi_v \tag{2.21}$$

$$= (v - v')\Psi_v. \tag{2.22}$$

If $\Psi_v \neq 0$ a.e., then we see that $v - v'$ is a constant. □

The HK theorem allows the construction of (2.18). Though theoretically sound, the functional $E_{\mathrm{DFT}}(\rho)$ cannot be computed practically. Levy improved this by introducing a new variation problem as follows ([33], also see [34]). The equality is proved by Lieb in 1982 [36].

$$E_{\mathrm{gs}} = \inf_{\rho \in I_N} E_{\mathrm{DFT}}(\rho) = \inf_{\rho \in I_N} \inf_{\Psi \to \rho} \langle \Psi, H_n \Psi\rangle \tag{2.23}$$

where the outer inf is take over the set

$$I_N := \{\rho \mid \text{there is a } \Psi \text{ whose density is } \rho \tag{2.24}$$

$$\text{and is normalized to } n \text{, denote by } \Psi \to \rho\}. \tag{2.25}$$

Luckily, The set I_N can be explicitly computed to be

$$I_N = \{\rho \mid \rho \geq 0, \int_{\mathbb{R}^3} \rho = n, \nabla \rho^{1/2} \in L^2\}. \tag{2.26}$$

Explicit expressions for $E_{\mathrm{DFT}}(\rho)$ are not attainable in practice. However, we may approximate $E_{\mathrm{DFT}}(\rho)$ by using a physically intuitive functional as a leading order approximation while delegate all left over errors into an exchange-correlation term $\mathrm{xc}(\rho)$. One of the early approximation which inspired the DFT is the Thomas-Fermi theory (see [37, 35, 39]). More modern approximations often resemble the following energy functional [15]

$$E(\gamma) := \mathrm{Tr}((-\Delta)\gamma) + \frac{1}{2}\int_{\mathbb{R}^3} (\rho_\gamma - \kappa)v * (\rho_\gamma - \kappa) + \mathrm{Xc}(\rho_\gamma). \tag{2.27}$$

It turns out that (2.1) is the Euler-Lagrange equations of the following free energy.

$$F_\beta(\gamma) := E(\gamma) - \beta^{-1}S(\gamma) - \mu N(\gamma). \tag{2.28}$$

where $\beta = T^{-1}$ is the inverse temperature, μ is the chemical potential, $S(\gamma) = -\mathrm{Tr}(\gamma \ln \gamma + (1-\gamma)\ln(1-\gamma)$ and $N(\gamma) = \mathrm{Tr}\gamma$, and $\mathrm{Xc}' = \mathrm{xc}$.

2.3 DFT in the Thermodynamical Limit

The most important quantities of interest are physical quantities in the thermodynamical limit. That is, if A_Λ is an observable depending on a subset $\Lambda \subset \mathbb{R}^3$, we are interested in

$$\lim_{\Lambda \to \mathbb{R}^3} \frac{1}{|\Lambda|} A_\Lambda(\rho) \tag{2.29}$$

for $\rho \in L^p_{\text{loc}}(\mathbb{R}^3)$ for a suitable p. So far our state space has been $\mathcal{H} = L^2(\mathbb{R}^3)$ and the set of densities are finite in the number of particles, i.e. $\rho \in L^1(\mathbb{R}^3)$. Such ρ has zero density in the thermodynamical limit:

$$\lim_{\Lambda \to \mathbb{R}^3} \frac{1}{|\Lambda|} N(\rho) = \lim_{\Lambda \to \mathbb{R}^3} \frac{1}{|\Lambda|} \int_{\mathbb{R}^3} \rho = 0. \tag{2.30}$$

Likewise, it has zero energy density (see (2.27) - (2.28)). These densities corresponds to fluctuation of the vacuum and are not of significant interest to us.

Some special cases of the positive density DFT theory has been studied, (see [13] and [14] for the reduce Hartree-Fock case at zero temperature). In general, computing (2.29) is beyond the scope of our current reach. As a result, we restrict our attention to periodic densities and local perturbation of such densities. There is also a considerable amount of literature on global perturbation of a periodic state. We refer interested readers to, for example, [18, 19, 22, 23].

Energies in the Periodic Case

As shown in [13, 14], the thermodynamical limit of a periodic system of the KS equation (2.1) can be obtained. Here we record simultaneously the resulting energies of DFT for both the $\mathbb{R}^3$ and periodic system.

Depending on whether $\kappa \in L^1(\mathbb{R}^d)$ or $L^1(\Omega)$, where Ω is a fundamental cell Ω of a Bravais lattice $\mathcal{L} \subset \mathbb{R}^3$, we let X be either $\mathbb{R}^d$ or Ω. Furthermore, let Tr_X denote the standard trace on $L^2(\mathbb{R}^d)$, if $X = \mathbb{R}^d$, and the trace per volume Ω,

$$\text{Tr}_\Omega(A) := \frac{1}{|\Omega|} \text{Tr}_{L^2(\mathbb{R}^3)}(\chi_\Omega A \chi_\Omega), \tag{2.31}$$

where χ_Ω is the indicator function on Ω, if $X = \Omega$ is a fundamental cell of a lattice $\mathcal{L}$.

As we mentioned in Section 2.2, Equation (2.4) is the Euler-Lagrange equations for the free energy functional

$$F_T(\gamma) := E_X(\gamma) - \beta^{-1} S_X(\gamma) - \mu N_X(\gamma), \tag{2.32}$$

where $\beta = T^{-1}$ is the inverse temperature, μ is the chemical potential, $S_X(\gamma) = -\mathrm{Tr}_X(\gamma \ln \gamma + (\mathbf{1} - \gamma)\ln(\mathbf{1} - \gamma))$ is the entropy, $N_X(\gamma) := \mathrm{tr}_X \gamma$ is the number of particles, and $E_X(\gamma)$ is the energy functional given by

$$E_X(\gamma) = \mathrm{Tr}_X\big((-\Delta)\gamma\big) + \frac{1}{2}\int_X \sigma_\gamma v * \sigma_\gamma + \int_X \mathrm{Xc}(\rho_\gamma), \tag{2.33}$$

where $\sigma_\gamma := \kappa - \rho_\gamma$ and $\mathrm{Xc}(\lambda)$ is an anti-derivative of $\mathrm{xc}(\lambda)$. In the case if one desires to express energies (2.32) and (2.33) in terms of ρ and ϕ, we substitute $\gamma = f_{FD}(\beta(h_\rho - \mu))$ and $\gamma = f_{FT}(\beta(h^\phi - \mu))$, respectively, into (2.33) and (2.32).

Chapter 3

Main Result

Derivation of macroscopic Maxwell's equations for the electro-magnetic fields in dielectrics from the many-body Quantum Mechanics (Schrödinger equation) is one of the key problems in theoretical and mathematical physics. In the full generality, this problem is far from our reach. Thence there is a great interest in derivation of these equations from reliable microscopic models.

With success in describing the electronic structure of matter, the DFT is presently the *leading such microscopic theory*. Hence it is an interesting proposition to derive the macroscopic Maxwell's equations from the DFT microscopic theory.

In this thesis, we derive, within the framework of DFT at $T > 0$, the dielectric response in a medium subjected to a local deformation of the crystalline structure. The main theorem of the thesis is presented in Section 3.2.

In what follows, we assume that $d = 3$ and let $\mathcal{L}$ be a (crystalline) Bravais lattice in $\mathbb{R}^3$. Let $L^2_{\text{loc}}(\mathbb{R}^3)$ denote the space of locally $L^2(\mathbb{R}^3)$ functions. We also define the Hilbert space of $\mathcal{L}$-periodic functions

$$L^2_{\text{per}}(\mathbb{R}^3) = \{ f \in L^2_{\text{loc}}(\mathbb{R}^3) : f \text{ is } \mathcal{L}\text{-periodic} \}, \tag{3.1}$$

with the inner product $\langle f, g\rangle = \int_\Omega \bar{f} g$ and the norm $\|f\|^2_{L^2_{\rm per}} = \int_\Omega |f|^2$ for some arbitrary fundamental domain Ω of $\mathcal{L}$. We denote its associated Sobolev space and its norm by $H^s(\mathbb{R}^3)$ and $\|\cdot\|_{H^s}$.

We begin introducing key notions used below.

3.1 Crystals and Dielectrics

We consider background charge distribution, $\kappa(y) \equiv \kappa_{\rm per}(y) \in L^2_{\rm per}(\mathbb{R}^3)$, periodic with respect to some lattice $\mathcal{L}$ (crystal). Here y stands for the microscopic coordinate.

We think of $\mathcal{L}$ and $\kappa_{\rm per}$ as a crystal lattice and the ionic charge distribution of $\mathcal{L}$. An example of $\kappa_{\rm per}$ is

$$\kappa_{\rm per}(y) = \sum_{l\in\mathcal{L}} \kappa_a(y-l)\,, \tag{3.2}$$

where κ_a denotes an ionic ("atomic") charge distribution.

Next, we describe a model of the (crystalline) dielectric. We say that an $\mathcal{L}$-periodic background charge density $\kappa_{\rm per} \in L^2_{\rm per}(\mathbb{R}^3)$ is a dielectric one iff the Kohn-Sham equation (2.1) with $\kappa = \kappa_{\rm per}$ has an $\mathcal{L}$-periodic solution $(\rho_{\rm per}, \mu_{\rm per})$, with the following properties

(a) the periodic one-particle Schrödinger operator

$$h_{\rm per,xc} := -\Delta - \phi_{\rm per} + {\rm xc}(\kappa_{\rm per} + 4\pi^{-1}\Delta\phi_{\rm per}), \text{ with} \tag{3.3}$$

$$\phi_{\rm per} := 4\pi(-\Delta)^{-1}(\kappa_{\rm per} - \rho_{\rm per}), \tag{3.4}$$

acting on $L^2(\mathbb{R}^3)$ is self-adjoint and has a gap in its spectrum,

(b) $\mu_{\rm per}$ is in this gap.

Existence results for the ideal crystal and dielectrics are discussed in the remarks after the main theorem.

3.2 Dielectric Response

We describe a macroscopically deformed microscopic crystal charge distribution,

$$\kappa_\delta(y) = \kappa_{\text{per}}(y) + \delta^3\kappa'(\delta y), \tag{3.5}$$

where δ is a small parameter which stands for the ratio of microscopic and macroscopic scale and $\kappa'(x) \in L^2(\mathbb{R}^3)$ is a small local perturbation living on the macroscopic scale. By y and $x = \delta y$, we denote the microscopic and macroscopic coordinates, respectively.

We formulate the conditions for our main result. We introduce our assumptions

[A1] (Periodicity)

$$\kappa_{\text{per}} \text{ is } \mathcal{L}\text{-periodic and } \kappa_{\text{per}} \in H^2_{\text{per}}(\mathbb{R}^3)$$

[A2] (Dielectricity) κ_{per} is dielectric.

Let $h_{\text{per,xc}}$ (or h_{per} when xc $= 0$) denote operator (3.3) acting on $L^2(\mathbb{R}^3)$. This operator is self-adjoint and has purely discrete spectrum. Moreover, let $h_{\text{per,xc,0}}$ (or $h_{\text{per,0}}$ when xc $= 0$) denote the 0-fiber of $h_{\text{per,xc}}$ in its Bloch-Floquet decomposition (see Section 4.2 below). It follows that the gaps of $h_{\text{per,xc}}$ are contained in gaps of $h_{\text{per,xc,0}}$. Let

$$\eta(\mathbb{R}^3) = \text{dist}(\mu_{\text{per}}, \sigma(h_{\text{per,xc}})), \tag{3.6}$$

$$\eta(\Omega) = \text{dist}(\mu_{\text{per}}, \sigma(h_{\text{per,xc,0}})). \tag{3.7}$$

With this notation, we assume the following properties.

[A3] (Spectral gap inequality)

$$\eta := \eta(\mathbb{R}^3) - \frac{5}{6}\eta(\Omega) > 0 \tag{3.8}$$

[A4] (Scaling)

$$\delta \ll 1 \text{ and } \frac{3\ln(\delta^{-1})}{\eta(\Omega)} < \beta$$

[A5] (Perturbation κ')

$$\kappa' \in (H^2 \cap H^{-2})(\mathbb{R}^3).$$

[A6] (Exchange-correlation term)

$$\begin{aligned} &\mathrm{xc} \in C^3(\mathbb{R}_+), \quad \text{and} \\ &\|\mathrm{xc}\|_{W^{3,1}} \leq c\min(1, \delta^{-2}\|V\|_{L^1_{\mathrm{per}}}^{1/2}) \end{aligned}$$

for a sufficiently small $c > 0$ constant and where

$$V(x) = -\,\mathrm{den}\left[\beta f'_{FD}(\beta(h_{\mathrm{per,xc},0} - \mu))\right] \geq 0. \tag{3.9}$$

We discuss the assumptions above in the remarks after the next theorem. Finally, we introduce the homogeneous Sobolev spaces

$$\dot{H}^s(\mathbb{R}^3) = \left\{ f \text{ measurable on } \mathbb{R}^3 : \|f\|_{\dot{H}^s(\mathbb{R}^3)} < \infty \right\} \tag{3.10}$$

for $s \geq 0$ with the associated norm

$$\|f\|^2_{\dot{H}^s(\mathbb{R}^3)} = \int |(-\Delta)^{s/2} f(k)|^2 \,. \tag{3.11}$$

Our main result is

Theorem 5. *Let Assumptions [A1] - [A6] hold and let* $(\rho_{\mathrm{per}}, \mu_{\mathrm{per}})$ *be the dielectric solution of the Kohn-Sham equation* (2.1) *with* $\kappa = \kappa_{\mathrm{per}}$ *stipulated in Assumption [A2]. Then*

1. *Kohn-Sham equation* (2.1)*, with* (3.5) *and* $\mu = \mu_{\text{per}}$*, has a unique solution* $\rho_\delta(y) \in L^2_{\text{per}}(\mathbb{R}^3) + L^2(\mathbb{R}^3) + \dot{H}^{-1}(\mathbb{R}^2) + \dot{H}^{-2}(\mathbb{R}^3)$*;*

2. *The potential* $\phi_\delta(y)$ *associated with* $\rho_\delta(y)$ *is of the form*

$$\phi_\delta(y) = \phi_{\text{per}}(y) + \delta\phi(\delta y) + \delta\phi_{\text{rem},1}(\delta y) + \delta\phi_{\text{rem},2}(\delta y) \tag{3.12}$$

where $\phi_{\text{per}} \in H^2_{\text{per}}(\mathbb{R}^3)$ *is given in* (3.4)*,* $\phi_{\text{rem},i} \in H^{i-1}(\mathbb{R}^3), i = 1, 2,$ *and obey the estimates*

$$\|\phi_{\text{rem},i}\|_{\dot{H}^{i-1}(\mathbb{R}^3)} \lesssim \delta^{1/2}, \tag{3.13}$$

and $\phi \in H^2(\mathbb{R}^3)$ *and satisfies the equation*

$$-\operatorname{div} \epsilon \nabla \phi = \kappa' \tag{3.14}$$

with a constant real, symmetric 3×3 *matrix,* $\epsilon \geq 1$*. Moreover,* ϵ *is given explicitly in* (5.63) *for* $xc = 0$*, and in* (5.288) *for* $xc \neq 0$*.*

(3.14) is the *macroscopic Poisson equation* in a dielectric medium.

The proof of Theorem 5, with xc = 0 is given in Section 5.1. In Section 5.3, we sketch an upgraded proof including the exchange term xc.

Main idea of the proof of Theorem 5. As in [32], we study (2.10) rather than (2.7) - (2.8). We rescale (2.10) to the macroscopic coordinate x as $y \to x = y/\delta$ to obtain equation

$$-\Delta\phi^\delta = 4\pi(\kappa - \text{den}[f_{\text{FD}}(\beta(h^{\phi^\delta}_\delta - \mu))]) := F(\phi^\delta), \tag{3.15}$$

where $\phi^\delta(x) := \delta\phi_\delta(\delta x)$ is related to solution ϕ_δ given in (3.12), and

$$h^{\phi^\delta}_\delta = -\delta^2\Delta - \delta\phi^\delta + \text{xc}(\delta^3(\kappa^\delta + (4\pi)^{-1}\Delta\phi^\delta)) \tag{3.16}$$

which leads to a fixed point problem for ϕ^δ. We show existence of the fixed point ϕ^δ in

(3.15). Then, we derive the existence of solution ρ^δ to (2.1) by using

$$\rho^\delta = \mathrm{den}[f_{\mathrm{FD}}(\beta(h_\delta^{\phi^\delta} - \mu))]. \tag{3.17}$$

Reversing the scaling, we recover the results for ϕ_δ and ρ_δ in Theorem 5.

Let $\phi^\delta_{\mathrm{per}}(x) := \delta^{-1}\phi_{\mathrm{per}}(\delta^{-1}x)$. Writing

$$\varphi \equiv \varphi^\delta := \phi^\delta - \phi^\delta_{\mathrm{per}}$$

and expanding the right hand side of (3.15) in φ, we write (3.15) as

$$K_\delta\varphi + N_\delta(\varphi) - F(\phi^\delta_{\mathrm{per}}) = 0 \tag{3.18}$$

where $K_\delta = -\Delta + M_\delta$, $M_\delta := -d_\phi F(\phi) \mid_{\phi=0}$, and N_δ is defined by this expression. Following [11], we treat small and large momenta differently. To this end, we use the Lyapunov-Schmidt reduction with projection $P_r = \chi_{B_r}(-i\nabla)$ where χ_S is the indicator function on the set $S \subset \mathbb{R}^3$ and B_r is the ball of radius r centered at the origin.

Let $\bar{P}_r = 1 - P_r$. We split (3.18) into

$$P_r(K_\delta\varphi + N_\delta(\varphi) - F(\phi^\delta_{\mathrm{per}})) = 0 \tag{3.19}$$

$$\bar{P}_r(K_\delta\varphi + N_\delta(\varphi) - F(\phi^\delta_{\mathrm{per}})) = 0. \tag{3.20}$$

We decompose $\varphi := \varphi_s + \varphi_l$ into small and large momenta parts, where $\varphi_s = P_r\varphi$ and $\varphi_l = \bar{P}_r\varphi$. For a given φ_s, we solve for φ_l in equation (3.20). Then, we substitute the φ_s-dependent solution $\varphi_l = \varphi_l(\varphi_s)$ into (3.19) to obtain an equation for φ_s. Then, we find the asymptote of (3.19) as $\delta \to 0$. In the case xc $= 0$, there are two properties which enable this procedure: $M_\delta = -d_\phi F(\phi) \mid_{\phi=0} \geq 0$ and if $B_r \subset \Omega^*_\delta$ for r small, then $P_r K_\delta P_r$ is purely a function of $-i\nabla$. When xc is small, it can be treated as a perturbation term.

The proof of Theorem 5 is organized as follows. After presenting in Chapter 4 preliminary materials on charge density estimates and the Bloch-Floquet decomposition, we prove Theorem 5 in Section 5.1, with technical computations delegated to Section 5.2. Section 5.1 contains the main ingredients of the proof of Theorem 5 and spans about 20 pages. Some of technical computations are carried out in the appendices.

3.3 Discussions

Existence of ideal crystals

Assumptions [A1] and [A6] ensure that an equilibrium crystalline structures exists at $T > 0$:

Theorem 6 ([15]). *Let Assumptions [A1] and [A6] hold. Then the Kohn-Sham equation* (2.1)*, with the* $\mathcal{L}-$*periodic background charge density* $\kappa_{\rm per} \in H^2_{\rm per} \cap H^{-2}_{\rm per}$*, has a periodic solution* $(\rho_{\rm per}(y), \mu_{\rm per})$*, with* $\rho_{\rm per}$ *periodic and satisfying* $\sqrt{\rho_{\rm per}} \in H^1_{\rm per}(\mathbb{R}^3)$*.*

Existence of crystalline dielectric

We say that the potential V is gapped iff the Schrödinger operator $-\Delta + V$ has a gap in its continuous spectrum.

Proposition 7. *For any* $\mathcal{L}$*-periodic, gapped potential* $V_{\rm per} \in H^2_{\rm per}(\mathbb{R}^3)$ *and any real number* $\mu_{\rm per}$ *in the gap of* $h_{\rm per} := -\Delta + V_{\rm per}$*, there is* $\mathcal{L}$*-periodic* $\kappa_{\rm per} \in L^2_{\rm per}(\mathbb{R}^3)$ *such that* $(\rho_{\rm per}, \mu_{\rm per})$ *solves the Kohn-Sham equation* (2.1) *with* $\kappa = \kappa_{\rm per}$ *and* $\mu_{\rm per}$ *is in the gap of* $h_{\rm per}$*. Moreover,* $V_{\rm per} = -\phi_{\rm per} + xc(\rho_{\rm per})$ *where* $\phi_{\rm per}$ *is the associated electrostatic potential of* $\rho_{\rm per}$ *(according to* (2.8)*).*

Proof. Let $V_{\rm per}$ be such that $h_{\rm per} := -\Delta - V_{\rm per}$ has a gap. We choose $\mu_{\rm per}$ to be in this gap and define (see (2.7)-(2.9))

$$\rho_{\rm per} := \mathrm{den}[f_{\rm FD}(\beta(h_{\rm per} - \mu_{\rm per})]. \tag{3.21}$$

Next, we define in sequence

$$\phi_{\rm per} := \mathrm{xc}(\rho_{\rm per}) - V_{\rm per} \text{ and} \tag{3.22}$$

$$\kappa_{\rm per} := -\Delta\phi_{\rm per} + \rho_{\rm per}. \tag{3.23}$$

Then, it is straightforward to check that $(\rho_{\mathrm{per}}, \mu_{\mathrm{per}})$ is a solution of the KS equation (2.1) as given in Theorem 6 with background potential κ_{per}. By construction, h_{per} has a gap and μ_{per} is in this gap. $\square$

One can extend Proposition 7 to construct pairs $(h = -\Delta + V, \mu)$ having any desired property **P**. Following Proposition 7, we construct ρ, ϕ, and κ via (3.21), (3.22), and (3.23) in this order. Then (ρ, μ) is a solution of the KS equation (2.1) with background potential κ. By construction, h has property **P**.

General dielectrics

We say that the background charge density κ is a dielectric one iff the Kohn-Sham equation (2.1) with background charge distribution κ has a solution (ρ, μ), with ρ in an appropriate space, say $(H^2_{\mathrm{loc}} \cap L^\infty)(\mathbb{R}^3)$ such that

(a) the one-particle Schrödinger operator, defined for this solution,

$$h := -\Delta - \phi + \mathrm{xc}(\kappa + 4\pi^{-1}\Delta\phi), \text{ with} \tag{3.24}$$

$$\phi := 4\pi(-\Delta)^{-1}(\kappa - \rho), \tag{3.25}$$

acting on $L^2(\mathbb{R}^3)$ is self-adjoint, and has a gap in its spectrum;

(b) μ is in this gap.

By the remark after Proposition 7, we have

Proposition 8 (Existence of crystalline dielectrics). *For any $\mathcal{L}$-periodic, gapped potential $V \in (H^2_{\mathrm{loc}} \cap L^\infty)(\mathbb{R}^3)$ and any real number μ in the gap of $h_V := -\Delta + V$, there is $\kappa \in (L^2_{\mathrm{loc}} \cap L^\infty)(\mathbb{R}^3)$ such that (ρ, μ) solves the Kohn-Sham equation (2.1) with κ and μ is in the gap of h_V. Moreover, $V = -\phi + xc(\rho)$ where ϕ is the associated electrostatic potential of ρ (according to (2.8)).*

Remarks on Assumption [A3]

(a) Let Ω^* and $h_{\text{per},k}$, $k \in \Omega^*$, denote a fundamental cell of the reciprocal lattice and the k-th fiber in the Bloch-Floquet decomposition of the operator h_{per} (see Section 4.2 below).[1] The inequality in Assumption [A3] says that the corresponding gap in the spectrum of $h_{\text{per},k}$ depends on k sufficiently little. This condition can be achieved if the lattice $\mathcal{L}$ is sparse (i.e. the minimal distance between vertices is sufficiently large), as in this case Ω^* is small.

(b) Both, $\eta(\mathbb{R}^3)$ and $\eta(\Omega)$, depend on T and therefore so does $\eta = \eta(T)$. To show the inequality $T \ll \eta(\Omega)(T)\ln^{-1}(1/\delta)$ has a solution, it suffices to show that $\eta(\Omega) = \eta(\Omega)(T)$ has a non-zero limit as $T \to 0$. One way to arrange this is to select $\eta(\Omega)(0)$ to be nonzero at $T = 0$ by choosing an appropriate Hamiltonian h_{per}. Then, by using Proposition 7, we can obtain κ_{per} which yields such a solution.

Remarks on Assumptions [A4] and [A6]

In comparison to Assumption [A4], suppose that β satisfies

$$\frac{C\ln(\delta^{-1})}{\eta(\Omega)} < \beta. \tag{3.26}$$

Then, by Lemma 59, [A6] has the upper bound

$$\|\text{xc}\|_{W^{1,\infty}} < \delta^{-2}\delta^{C/2} = \delta^{\frac{C}{2}-2}. \tag{3.27}$$

In particular, C can be at most 4 for xc to be on the order of $O(1)$. Note that $C = 3$ in [A4]. However, this bound is not necessarily optimum. Similarly, the bound for Assumption [A4] is also not necessarily optimum.

[1] For $h_{\text{per}} = -\Delta + V_{\text{per}}$, the BF fiber acting on $L^2_{\text{per}}(\mathbb{R}^3)$ is $h_{\text{per},k} = (-i\nabla - k)^2 + V_{\text{per}}$.

Dielectric constant in the limit $T \to 0$

In the limit $T \to 0$ and if $\text{xc} = 0$, our expression for the dielectric constant ϵ agrees with [10] (see Appendix A below)

Physical dimensions

Now, we give an estimate on the upper bound of T in Assumption [A4]. The physical cell size of common crystals is on the order of 10^{-10} m [47]. The gap size is on the order of $1eV$ [47]. Since the Boltzmann constant is of the order $10^{-4}eV/K$. Assumption [A4] requires

$$\beta \asymp C(10^{-4}eV/K)(1eV)^{-1}|\ln(10^{-10})| = C10^{-3}\ln(10)K^{-1}. \tag{3.28}$$

for some large constant $3 < C < 4$. This gives an approximate upper bound for T:

$$T < \frac{10^3}{3\ln(10)}K < 145K \tag{3.29}$$

3.4 Literature

We begin with $T = 0$. In the closely related Thomas-Fermi-Dirac-von Weiszäcker model on $\mathbb{R}^3$ with local density exchange-correlation term xc, the existence and uniqueness of solutions were obtained in [31] . For the full KS equation and for κ being a finite sum of delta functions on $\mathbb{R}^3$, the existence result for exchange-correlation terms depending on ρ and its derivatives was proved in [1]. In the periodic case $\kappa = \kappa_{\text{per}}$, the existence of periodic solutions from certain trace classes was obtained in [14] and [13] for the Hartree-Fock equation (1.41).

For the case where $T > 0$, F. Nier [43] proved the existence and uniqueness of the the KS equation (2.1) without the exchange-correlation term via variational techniques.

Later, Prodan and Nordlander [46] provided another existence and uniqueness result with the exchange-correlation term in the case where $\kappa = \kappa_{\text{per}}$ is small. In this case, the associated potential term $\phi_{\text{per}} + \text{xc}(\rho_{\text{per}})$ is small as well. (As was pointed by A. Levitt, a result for small $\kappa = \kappa_{\text{per}}$ would not work in Theorem 5 above as Assumption [A3] fails for it.)

The results given in Theorem 6 was proven in [16]. Papers [1, 13, 14, 16] use variational techniques and did not provide uniqueness results.

A. Levitt [32] proved the screening of small defects for the reduced HF equation at $T > 0$.

For $T = 0$, similar and related results to Theorem 5 were proven in [12, 8, 9, 10, 11, 18, 19, 22].

Chapter 4

Densities and the Bloch-Floquet decomposition

4.1 Densities

Let $C_c(\mathbb{R}^3)$ denote the space of compactly supported continuous functions on $\mathbb{R}^3$. An operator A on $L^2(\mathbb{R}^3)$ is said to be locally trace class if and only if fA is trace class for all $f \in C_c(\mathbb{R}^3)$

For a locally trace class operator A, we define its density den$[A]$ to be a regular countably additive complex Borel measure satisfying

$$\int \mathrm{den}(A) f = \mathrm{Tr}(fA), \tag{4.1}$$

$$\forall f \in C_c(\mathbb{R}^3). \tag{4.1a}$$

If $\mathrm{Tr}(fA)$ is continuous in f in the $C_c(\mathbb{R}^3)$-topology, the Riesz representation theorem shows that (4.1) and (4.1a) define den$[A]$ uniquely. In our case, we will frequently stipulate stronger regularity assumptions on A, implying that den$[A]$ is actually in a reasonable function space. (e.g. Lemma 9 below).

Let $\mathcal{L}$ be a Bravais lattice on $\mathbb{R}^3$ and Ω a fundamental domain of $\mathcal{L}$ as in Chapter 3. Denote $|S|$ to be the volume of a measurable set $S \subset \mathbb{R}^3$ and note that $|\Omega|$ is independent of the choice of the fundamental cell Ω. Let T_s be the translation operator

$$T_s : f(x) \mapsto f(x - s). \tag{4.2}$$

We say that a function $f : \mathbb{R}^3 \to \mathbb{C}$ is $\mathcal{L}$-periodic iff it is invariant under the translations action of T_s for all lattice elements $s \in \mathcal{L}$. We define the space

$$L^p_{\text{per}}(\mathbb{R}^3) = \{f \in L^p_{\text{loc}}(\mathbb{R}^3) : f \text{ is } \mathcal{L}\text{-periodic}\} \tag{4.3}$$

with the norm of $L^p(\Omega)$ for some Ω. The norms for $L^p_{\text{per}}(\mathbb{R}^3)$ and $L^p(\mathbb{R}^3)$ are distinguished by the subindices L^p_{per} and L^p.

We say that a bounded operator A on $L^2(\mathbb{R}^3)$ is $\mathcal{L}$-periodic if and only if $[A, T_s] = 0$ for all $s \in \mathcal{L}$ where T_s is the translation operator defined in (4.2).

Let I^p be the standard p-Schatten space of bounded operators on $L^2(\mathbb{R}^3)$ with the p-Schatten norm

$$\|A\|^p_{I^p} := \text{Tr}_{L^2}((A^*A)^{p/2}). \tag{4.4}$$

Next, let χ_S denote the characteristic function of a set $S \subset \mathbb{R}^3$ and let I^p_{per} be the space of bounded, $\mathcal{L}$-periodic operators A on $L^2(\mathbb{R}^3)$ with $\|A\|_{I^p_{\text{per}}} < \infty$ where

$$\|A\|^p_{I^p_{\text{per}}} := \text{Tr}_{\Omega}((A^*A)^{p/2}) := \frac{1}{|\Omega|}\text{Tr}_{L^2}(\chi_\Omega (A^*A)^{p/2} \chi_\Omega) \tag{4.5}$$

We remark that the I^2_{per} norm does not depend on the choice of Ω since A is $\mathcal{L}$-periodic. We have the following estimates for the densities in terms of Schatten norms.

Lemma 9. *Let A be a locally trace class operator on $L^2(\mathbb{R}^3)$ and $\epsilon > 0$. We have the following statements.*

1. *If $(1 - \Delta)^{3/4+\epsilon} A \in I^2$ or I^2_{per}, then $\text{den}[A] \in L^2(\mathbb{R}^3)$ or $L^2_{\text{per}}(\mathbb{R}^3)$ respectively.*

Moreover,

$$\|\operatorname{den}[A]\|_{L^2} \lesssim \|(1-\Delta)^{3/4+\epsilon}A\|_{I^2} \tag{4.6}$$

$$\|\operatorname{den}[A]\|_{L^2_{\text{per}}} \lesssim |\Omega|^{1/2}\|(1-\Delta)^{3/4+\epsilon}A\|_{I^2_{\text{per}}} \tag{4.7}$$

2. *If* $(1-\Delta)^{1/4+\epsilon}A \in I^{6/5}$*, then* $\operatorname{den}[A] \in \dot{H}^{-1}(\mathbb{R}^3)$ *(where* $\dot{H}^s(\mathbb{R}^3)$ *is defined in* (3.10)*). Moreover,*

$$\|\operatorname{den}[A]\|_{\dot{H}^{-1}} \lesssim \|(1-\Delta)^{1/4+\epsilon}A\|_{I^{6/5}} \tag{4.8}$$

Proof. We prove (4.7) and (4.8) only; (4.6) is similar and easier. We begin with (4.7). Since the operator $(1-\Delta)^{1/4+\epsilon}A$ is $\mathcal{L}$-periodic, its density, if it exists, is also $\mathcal{L}$-periodic. By the L^2_{per}-L^2_{per} duality, relation (4.1), $\operatorname{den}[A] \in L^2_{\text{per}}$ and (4.7) holds if and only if

$$\operatorname{Tr}(Af) \lesssim |\Omega|^{1/2}\|f\|_{L^2_{\text{per}}}\|(1-\Delta)^{3/4+\epsilon}A\|_{I^2_{\text{per}}} \tag{4.9}$$

for all $f \in L^2(\mathbb{R}^3)$ with support in Ω, where we recall $\|f\|_{L^2_{\text{per}}} = \|f\chi_\Omega\|_{L^2}$. Since the support of f is in Ω, by the Hölder's inequality for the trace-per-volume norm,

$$\frac{1}{|\Omega|}|\operatorname{Tr}(Af)| = \frac{1}{|\Omega|}|\operatorname{Tr}(Af\chi_\Omega)| \tag{4.10}$$

$$\lesssim \|A(1-\Delta)^{4/3+\epsilon}\|_{I^2_{\text{per}}}\|(1-\Delta)^{-3/4-\epsilon}f\|_{I^2_{\text{per}}}. \tag{4.11}$$

By the Kato-Seiler-Simon inequality

$$\|f(x)g(-i\nabla)\|_{I^p} \lesssim \|f\|_{L^p}\|g\|_{L^p} \tag{4.12}$$

for $2 \leq p < \infty$ (see [49]; one can also replace I^p and L^p by their periodic versions I^p_{per} and L^p_{per}, respectively.), we obtain (4.9). Thus, (4.7) is proved.

Now we prove (4.8) as above. By the H^1-H^{-1} duality, it suffices to show that

$$\operatorname{Tr}(Af) \lesssim \|f\|_{\dot{H}^1}\|(1-\Delta)^{1/4+\epsilon}A\|_{I^{6/5}} \tag{4.13}$$

for all $f \in \dot{H}^1 \cap C_c(\mathbb{R}^3)$ and for $\epsilon > 0$. By the non-abelian Hölder inequality with

$1 = \frac{1}{6} + \frac{1}{6/5}$ ([49]),

$$\mathrm{Tr}(fA) \lesssim \|f(1-\Delta)^{-1/4-\epsilon}\|_{I^6} \|(1-\Delta)^{1/4+\epsilon} A\|_{I^{6/5}}. \tag{4.14}$$

The Kato-Seiler-Simon inequality (4.12) shows

$$\mathrm{Tr}(fA) \lesssim \|f\|_{L^6} \|(1-\Delta)^{1/4+\epsilon} A\|_{I^{6/5}}. \tag{4.15}$$

Now, applying the Hardy-Littlewood inequality (for $d = 3$; see [38])

$$\|f\|_{L^6} \lesssim \|\nabla f\|_{L^2} \tag{4.16}$$

to $\|f\|_{L^6}$ in (4.15), we obtain (4.13). The proof of Lemma 9 is completed by the H^1-H^{-1} duality and the fact that $\dot{H}^1 \cap C_c(\mathbb{R}^3)$ is dense in H^1. □

4.2 Bloch-Floquet Decomposition

Define the (fiber integral) space

$$\mathcal{H}^{\oplus}_{\mathcal{L}} = \{f \in L^2_{\mathrm{loc}}(\mathbb{R}^3_k \times \mathbb{R}^3_x) : T^x_s f = f \tag{4.17}$$

$$\text{and } T^k_r f = e^{-2\pi i r \cdot x} f,\ \forall s \in \mathcal{L}, \forall r \in \mathcal{L}^*\} \tag{4.18}$$

where T^k_s is the translation in the k-variable by s and T^x_r is the translation in the x-variable by r (see (4.2)). We write $f = f_k(x) \in \mathcal{H}^{\oplus}_{\mathcal{L}}$ as

$$\int^{\oplus}_{\mathbb{R}^3/\mathcal{L}^*} f_k \, d\hat{k} = \int^{\oplus}_{\Omega^*} f_k \, d\hat{k}, \tag{4.19}$$

for some choice of a fundamental cell Ω^* of the reciprocal lattice $\mathcal{L}^*$ and $d\hat{k} := |\Omega^*|^{-1} dk$.

We use the Bloch-Floquet decomposition U_{BF} mapping from $L^2(\mathbb{R}^3)$ into $\mathcal{H}_{\mathcal{L}}^{\oplus}$ as

$$U_{\mathrm{BF}} f := \int_{\Omega^*}^{\oplus} d\hat{k} f_k \,, \tag{4.20}$$

$$f_k(x) := \sum_{t\in\mathcal{L}} e^{-2\pi i k(x+t)} f(x+t) \tag{4.21}$$

and the inverse Bloch-Floquet transform

$$U_{\mathrm{BF}}^{-1}\big(\int_{\Omega^*}^{\oplus} d\hat{k} f_k\big)(x) := \int_{\Omega^*} d\hat{k}\, e^{2\pi i k x} f_k(x),\ \forall x \in \mathbb{R}^3. \tag{4.22}$$

Lemma 10. *We have, for any $f \in L^2(\mathbb{R}^3)$,*

$$\int_{\Omega} f_k(x) dx = \hat{f}(k) \tag{4.23}$$

Proof. By (4.21) and a change of variable, we see that

$$\int f_k(x) dx := \int_{\Omega_\delta} \sum_{t\in\mathcal{L}} e^{-2\pi i k(x+t)} f(x+t) dx \tag{4.24}$$

$$= \sum_{t\in\mathcal{L}} \int_{t+\Omega} e^{-2\pi i k x} f(x) dx \tag{4.25}$$

$$= \int e^{-2\pi i k x} f(x) dx. \tag{4.26}$$

Equation (4.23) follows from the definition of the Fourier transform. □

Let $\langle f\rangle_S = |S|^{-1} \int_S f(x)dx$, the average of f on a set S, and χ_S be the indicator (characteristic) function of S.

Lemma 11. *Let $f \in L^2(\mathbb{R}^3)$ and f_k be its k-th fiber $\mathcal{L}$-Bloch-Floquet decomposition. Then for any $S \subset \Omega^*$,*

$$\chi_S(-i\nabla) f = U_{\mathrm{BF}}^{-1} \int_S^{\oplus} d\hat{k}\, \langle f_k\rangle_\Omega. \tag{4.27}$$

Proof. Let $f \in L^2(\mathbb{R}^3)$ with the k-th fiber f_k. Then Lemma 10 shows that

$$\langle f_k \rangle_\Omega = |\Omega|^{-1} \hat{f}(k). \tag{4.28}$$

Using the definition of the inverse Bloch transform in (4.22) and (4.28), we see that

$$\begin{aligned} U_{\mathrm{BF}}^{-1} \left(\int_S^\oplus d\hat{k}\, \langle f_k \rangle_\Omega \right) &= \int_{\Omega^*} d\hat{k}\, e^{2\pi i k x} \langle f_k \rangle_\Omega \\ &= \int_S d\hat{k}\, |\Omega|^{-1} e^{2\pi i k x} \hat{f}(k) \end{aligned} \tag{4.29}$$

Since $d\hat{k} = |\Omega^*|^{-1} dk = |\Omega| dk$, the last equation yields

$$U_{\mathrm{BF}}^{-1} \int_S^\oplus d\hat{k}\, \langle f_k \rangle_\Omega = \int_S dk\, e^{2\pi i k x} \hat{f}(k) = \chi_S(-i\nabla) f, \tag{4.30}$$

which gives (4.27). □

Let $P_r = \chi_{B(r)}(-i\nabla)$ where $B(r)$ is the ball of radius r centered at the origin (see (5.39)). Lemma 10 and 11 imply

Corollary 12. *Let $f \in L^2(\mathbb{R}^3)$ and $B(r) \subset \Omega^*$, then*

$$(P_r f)_k = |\Omega|^{-1} \hat{f}(k) \chi_{B(r)}(k). \tag{4.31}$$

Any $\mathcal{L}$-periodic operator A has a Bloch-Floquet decomposition [48] in the sense that

$$A = U_{\mathrm{BF}}^{-1} \int_{\Omega^*}^\oplus d\hat{k} A_k U_{\mathrm{BF}}, \tag{4.32}$$

where A_k are operators (called k-fibers of A) on L^2_{per} and the operator $\int_{\Omega^*}^\oplus d\hat{k}\, A_k$ acts on $\int_{\Omega^*}^\oplus d\hat{k} f_k \in \mathcal{H}_{\mathcal{L}}^\oplus$ as

$$\int_{\Omega^*}^\oplus d\hat{k} A_k \cdot \int_{\Omega^*}^\oplus d\hat{k} f_k = \int_{\Omega^*}^\oplus d\hat{k} A_k f_k. \tag{4.33}$$

Definition (4.33) implies the following relations for any $\mathcal{L}$-periodic operators A and

B

$$(Af)_k = A_k f_k, \tag{4.34}$$

$$(AB)_k = A_k B_k. \tag{4.35}$$

Furthermore, we have

Lemma 13. *Let A be an $\mathcal{L}$-periodic operator and A_k, its k-fibers in its Bloch-Floquet decomposition. Then $A_k = e^{-2\pi ixk} A_0 e^{2\pi ixk}$.*

Proof. We compute $(Af)_k$. Let T_s denote the translation operator (4.2). Let A_0 denote the 0-th fiber of A in its Bloch-Floquet decomposition. By (4.21) and the periodicity of A,

$$(Af)_k = \sum_{t\in\mathcal{L}} e^{-2\pi ik(x+t)} T_{-t} Af \tag{4.36}$$

$$= \sum_{t\in\mathcal{L}} e^{-2\pi ikx} A e^{-2\pi ikt} T_{-t} f \tag{4.37}$$

$$= e^{-2\pi ikx} A_0 e^{2\pi ikx} \sum_{t\in\mathcal{L}} e^{-2\pi ik(x+t)} T_{-t} f \tag{4.38}$$

$$= e^{-2\pi ikx} A_0 e^{2\pi ikx} f_k. \tag{4.39}$$

□

Now, we have the following result.

Lemma 14. *Let A be an $\mathcal{L}$-periodic operator and A_k, its k-fibers in its Bloch-Floquet decomposition. Then*

$$P_r A P_r = b(-i\nabla) P_r \tag{4.40}$$

where $b(k) = \langle A_k \mathbf{1} \rangle_\Omega$, $1 \in L^2_{\text{per}}(\mathbb{R}^3)$ is the constant function 1.

Proof. Let f_k be the k-th fiber of the Bloch-Floquet function f. We apply Lemma 11 with $S = B(r)$ and $f = AP_r\varphi$ (so that $\chi_S(-i\nabla) = P_r$) to obtain

$$P_r A P_r \varphi = U_{\mathrm{BF}}^{-1} \int_{\Omega^*}^{\oplus} d\hat{k}\, \langle (AP_r\varphi)_k \rangle_\Omega. \tag{4.41}$$

By Corollary 12 and equation (4.41), we find

$$P_r A P_r \varphi = |\Omega|^{-1} U_{\mathrm{BF}}^{-1} \int_{B(r)}^{\oplus} d\hat{k}\, \langle A_k 1 \rangle_\Omega \hat{\varphi}(k) \tag{4.42}$$

where $1 \in L^2_{\mathrm{per}}(\mathbb{R}^3)$ is the constant function equal to 1. Using the definition (4.22) of the inverse Bloch-Floquet transform and that $d\hat{k} = |\Omega|^{-1} dk$, we deduce (4.40). □

4.3 Passing to the Macroscopic Variable

Define the microscopic lattice $\mathcal{L}_\delta := \delta\mathcal{L}$ and let $\mathcal{L}_\delta^*$ be its reciprocal lattice. Define the rescaling operator

$$U_\delta : f(x) \mapsto \delta^{-3/2} f(\delta^{-1} x) \tag{4.43}$$

mapping from the microscopic to the macroscopic scale. A change of variable in (4.1) gives the following

Lemma 15. *For any operator A on $L^2(\mathbb{R}^3)$, we have*

$$\delta^{-3/2} U_\delta \,\mathrm{den}[A] = \mathrm{den}[U_\delta A U_\delta^*]. \tag{4.44}$$

Finally, note that A is an $\mathcal{L}$-periodic operator iff $U_\delta A U_\delta^*$ be an $\mathcal{L}_\delta$-periodic operator. Lemma 14 implies

Lemma 16. *Let A be an $\mathcal{L}$-periodic operator and A_k, its k-fibers in its Bloch-Floquet decomposition. Then*

$$P_r U_\delta A U_\delta^* P_r = b(-i\delta\nabla) P_r \tag{4.45}$$

where $b(k) = \langle A_k \mathbf{1} \rangle_\Omega$, $1 \in L^2_{\mathrm{per}}(\mathbb{R}^3)$ is the constant function 1.

Proof. Let $A_\delta = U_\delta A U_\delta^*$. By $U_\delta^* P_r U_\delta = P_{\delta r}$ and Lemma 14, we have

$$P_r U_\delta A U_\delta^* P_r = U_\delta P_{\delta r} A P_{\delta r} U_\delta^* = U_\delta b(-i\nabla) P_{\delta r} U_\delta^*.$$

Using $U_\delta P_{\delta r} U_\delta^* = P_r$ and $U_\delta b(-i\nabla) U_\delta^* = b(-i\delta\nabla)$ gives (4.40). □

Chapter 5

Dielectric Response: Proof of Theorem 5

In this section, we prove Theorem 5 modulo several auxiliary technical statements proved in Section 5.2. To simplify the exposition, we omit the exchange term xc. We explain in Section 5.3 how to deal with this term.

5.1 Core proof

In this section, we prove Theorem 5 modulo several auxiliary technical statements proved in Section 5.2. To simplify the exposition, we omit the exchange-correlation term xc. We explain in Section 5.3 how to deal with this term.

5.1.1 Linearized Map

Our starting point is equation (2.10), which we reproduce here

$$-\Delta\phi = 4\pi(\kappa - \mathrm{den}[f_{\mathrm{FD}}(\beta(h^\phi - \mu))]), \tag{5.1}$$

where (recall, for xc = 0)

$$h^\phi := -\Delta - \phi. \tag{5.2}$$

For simplicity, we do not display the factor 4π *and only restore it in exact formulae in Proposition 23 below.* In the xc $=0$ case, we consider (5.1) on the function space $\phi \in H^2_{\mathrm{per}}(\mathbb{R}^3) + \dot{H}^1(\mathbb{R}^3)$. For such ϕ's, the operator h^ϕ is self-adjoint and bounded below so that functions of h^ϕ above are well-defined by the spectral theory.

Our first step is to investigate the linearized map

$$M := d_\phi \, \mathrm{den}[f_{\mathrm{FD}}(\beta(h^\phi - \mu))]\big|_{\phi=\phi_{\mathrm{per}}}. \tag{5.3}$$

To derive basic properties of M, we find an explicit formula for it. We write $f_{\mathrm{FD}}(\beta(h^\phi - \mu))$ using the Cauchy-integral formula

$$f_{\mathrm{FD}}(\beta(h^\phi - \mu)) = \frac{1}{2\pi i}\int_\Gamma dz f_{\mathrm{FD}}(\beta(z-\mu))(z-h^\phi)^{-1} \tag{5.4}$$

where Γ is a contour around the spectrum of h^ϕ not containing the poles of f_{FD} which are located at $\mu + i\pi(2k+1)\beta^{-1}$, $k \in \mathbb{Z}$, see Figure 5.1 below. Here we use that h^ϕ is bounded from below, has a gap, and μ is in the gap. And since $1 \ll \beta$, we have

$$|f_{\mathrm{FD}}(\beta(z-\mu))| \lesssim \min(1, e^{-\beta \mathrm{Re} z}) \tag{5.5}$$

assuring the convergence of the integral. Moreover, under Assumption [A2],

$$\sup_{z\in\Gamma} \|(z-h)^{-1}\|_\infty = O(\max(1/\eta(\mathbb{R}^3), 1)). \tag{5.6}$$

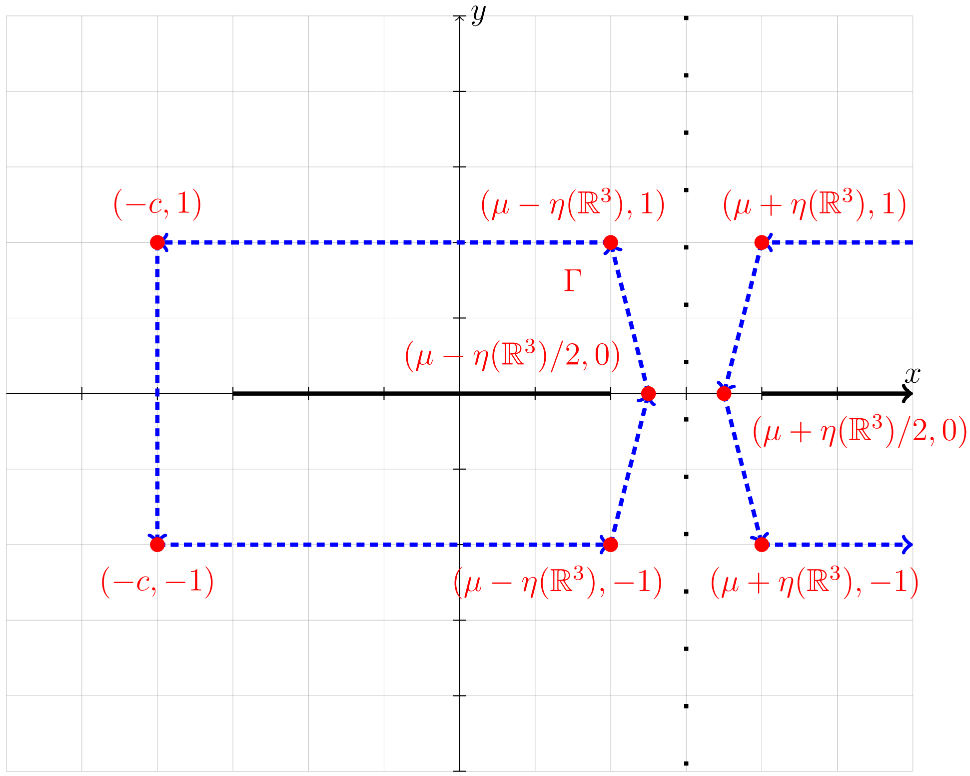

Figure 5.1: We identify the complex plane $\mathbb{C}$ with $\mathbb{R}^2$ via $z = x + iy$ for $(x, y) \in \mathbb{R}^2$ in the diagram above. The contour Γ is denoted by the blue dashed line. The spectrum of h^ϕ is denoted by solid black line. The poles of $f_{\text{FD}}(\beta(z-\mu))$ are denoted by the black dots. The number c denotes the lower bound $h^\phi > -c+1$.

To simplify the expressions below, we will introduce the following notation.

$$\oint := \frac{1}{2\pi i} \int_\Gamma dz f_{\text{FD}}(\beta(z-\mu)) \tag{5.7}$$

where Γ is the contour given in Figure 5.1.

Furthermore, for any operator h, we denote $h^L : \alpha \to h\alpha$ and $h^R : \alpha \to \alpha h$. Let us also denote the $\mathcal{L}$-periodic resolvent and Hamiltonian

$$r_{\text{per}}(z) = (z - h_{\text{per}})^{-1}, \quad h_{\text{per}} := h_{\phi_{\text{per}}} = -\Delta + \phi_{\text{per}}. \tag{5.8}$$

By Theorem 6, the electrostatic potential, $\phi_{\text{per}}(y)$ associated with the solution $\rho_{\text{per}}(y)$

(c.f. (2.12)) satisfies

$$\phi_{\text{per}} \in H^2_{\text{per}}(\mathbb{R}^3) \tag{5.9}$$

Hence the operator h^{δ}_{per} is self-adjoint and the operator functions above are well-defined.

The next proposition gives an explicit form for M and states its properties (also see [10]).

Proposition 17. *Let Assumption [A1] hold. Then*

1. *The operator M has the following explicit representation*

$$Mf := \text{den}\left[\oint r_{\text{per}}(z) f r_{\text{per}}(z)\right] \tag{5.10}$$

$$= \text{den}\left[\frac{\tanh(\beta(h^L_{\text{per}} - \mu)) - \tanh(\beta(h^R_{\text{per}} - \mu))}{h^L_{\text{per}} - h^R_{\text{per}}} f\right], \tag{5.11}$$

   where $f \in L^2(\mathbb{R}^3)$ on the right hand side is considered as a multiplication operator.

2. *The operator M is bounded, self-adjoint, and positive on $L^2(\mathbb{R}^3)$. Moreover, M is $\mathcal{L}$-periodic (c.f. Section 4.1).*

Proof of Proposition 17. In this proof, we *omit the subscript* "per" in h_{per} and $r_{\text{per}}(z)$. We begin with item (1). Equation (5.10) follows from definition (5.3), the Cauchy formula in (5.4)

$$f_{\text{FD}}(\beta(h - \mu)) = \oint (z - h)^{-1} = \oint r(z), \tag{5.12}$$

and a simple differentiation of the resolvent.

Using the Cauchy integral formula, we observe that for any operator α,

$$\oint (z - h)^{-1} \alpha (z - h)^{-1} = \oint (z - h^L)^{-1} (z - h^R)^{-1} \alpha$$

$$= \frac{\tanh(\beta(h^L - \mu)) - \tanh(\beta(h^R - \mu))}{h^L - h^R} \alpha \tag{5.13}$$

This gives (5.11). Item (1) is now proved.

Now we prove item (2). Since $h = h_{\text{per}}$ is self-adjoint and bounded below, $c - 1 + h$ is invertible for sufficiently large c. For each function $f \in L^2(\mathbb{R}^3)$, we define

$$\alpha_f := (c+h)^{-1/2} f (c+h)^{-1/2}. \tag{5.14}$$

The Kato-Seiler-Simon inequality (4.12) shows that α_f is Hilbert-Schmidt and

$$\|\alpha_f\|_{I^2} \lesssim \|f\|_{L^2} \tag{5.15}$$

(the I^2 norm is given in (4.4)). Together with (4.1), we write

$$\langle f, Mg\rangle = -\oint \operatorname{Tr}(\alpha_f^*(c+h)r(z)\alpha_g r(z)(c+h))\,. \tag{5.16}$$

Moreover, by (5.13), we have that

$$\langle f, Mg\rangle = \operatorname{Tr}\left(\alpha_f^* \tilde{M} \alpha_g\right), \tag{5.17}$$

$$\tilde{M} := -\frac{\tanh(\beta(h^L-\mu)) - \tanh(\beta(h^R-\mu))}{(c+h^L)^{-1} - (c+h^R)^{-1}}. \tag{5.18}$$

Since the function $G : \mathbb{R}^2 \to \mathbb{R}$,

$$G(x,y) := -\frac{\tanh(\beta(x-\mu)) - \tanh(\beta(y-\mu))}{(x+c)^{-1} - (y+c)^{-1}} \tag{5.19}$$

is bounded on the set $x, y \geq -c+1$, we see that M is bounded due to (5.15) and (5.17). Moreover, we can also see from expressions (5.17) - (5.19) that M is symmetric since G is real and h is self-adjoint. Since M is bounded, it is self-adjoint. Since the function G in (5.19) is positive for $x, y \geq -c+1$, equation (5.17) and spectral theorem on I^2 show that $\langle f, Mf\rangle = \operatorname{Tr}\left(\alpha_f^* \tilde{M} \alpha_f\right) > 0$ for any nonzero $f \in L^2(\mathbb{R}^3)$. This shows that M is positive.

Finally, formula (5.10) and the fact $h = h_{\text{per}}$ and $r = r_{\text{per}}(z)$ are $\mathcal{L}$-periodic show that M is $\mathcal{L}$-periodic. The proof of Proposition 17 is complete. □

The next proposition gives the Bloch-Floquet decomposition of the operator M.

Proposition 18. *The operator M has a Bloch-Floquet decomposition* (4.32) *whose $k-$fiber, M_k, acting on $L^2_{\text{per}}(\mathbb{R}^3)$ is given by*

$$M_k f = -\,\text{den}\left[\oint r_{\text{per},0}(z) f r_{\text{per},k}(z)\right] \tag{5.20}$$

where $f \in L^2_{\text{per}}(\mathbb{R}^3)$ and, on $L^2_{\text{per}}(\mathbb{R}^3)$,

$$r_{\text{per,k}}(z) = (z - h_{\text{per,k}})^{-1}, \tag{5.21}$$

$$h_{\text{per,k}} = (-i\nabla - k)^2 + \phi_{\text{per}}\,. \tag{5.22}$$

Proof of Proposition 18. Let T_s be given in (4.2) and $\varphi \in L^2(\mathbb{R}^3)$. To compute k-fibers of M, we note $T_{-t}\,\text{den}[A] = \text{den}\,[T_t^* A T_t]$ and $[T_t, r_{\text{per}}(z)] = 0$ for all $t \in \mathcal{L}$. Using these relations, the definition of the Bloch-Floquet decomposition (4.21) and equation (5.10), we obtain

$$\begin{aligned}&(M\varphi)_k(x)\\ &= -\sum_{t\in\mathcal{L}} e^{-ik(x+t)} \oint T_{-t}\,\text{den}\,[r_{\text{per}}(z)\varphi r_{\text{per}}(z)]\\ &= -\sum_{t\in\mathcal{L}} e^{-ik(x+t)} \oint \text{den}\,[T_t^* r_{\text{per}}(z)\varphi r_{\text{per}}(z) T_t]\,.\end{aligned} \tag{5.23}$$

Since $r_{\text{per}}(z)$ is $\mathcal{L}$-periodic, (5.23) shows

$$\begin{aligned}&(M\varphi)_k(x)\\ &= -\sum_{t\in\mathcal{L}} e^{-ik(x+t)} \oint \text{den}\,[r_{\text{per}}(z)(T_{-t}\varphi) r_{\text{per}}(z)]\,.\end{aligned} \tag{5.24}$$

Using that $\text{den}[A]f = \text{den}[Af] = \text{den}[fA]$ for any operator A on $L^2(\mathbb{R}^3)$ and any sufficiently regular function f on $\mathbb{R}^3$, we insert the constant factor of e^{-ikt} into den in (5.24). We obtain

$$\begin{aligned}&(M\varphi)_k(x)\\ &= -\,e^{-ikx} \oint \text{den}\left[r_{\text{per}}(z) \sum_{t\in\mathcal{L}} e^{-ikt} (T_{-t}\varphi) r_{\text{per}}(z)\right]\end{aligned} \tag{5.25}$$

This and the definition of the Bloch-Floquet decomposition of φ, (4.21), imply

$$(M\varphi)_k(x) = -\oint \mathrm{den}\left[r_{\mathrm{per}}(z)\varphi_k e^{ikx} r_{\mathrm{per}}(z)e^{-ikx}\right] \tag{5.26}$$

Since $e^{ikx}(-i\nabla)e^{-ikx} = -i\nabla - k$, and therefore $e^{ikx}r_{\mathrm{per}}(z)e^{-ikx} = r_{\mathrm{per},k}(z)$, this gives (5.20). $\square$

5.1.2 Lyapunov-Schmidt Decomposition

This step is to pass from the microscopic coordinate y to the macroscopic one, $x = \delta y$. We rescale the $\mathcal{L}$-periodic microscopic charge distribution, κ_{per}, as

$$\kappa^{\delta}_{\mathrm{per}}(x) := \delta^{-3}\kappa_{\mathrm{per}}(\delta^{-1}x) = \delta^{-3/2}U_\delta\kappa_{\mathrm{per}} \tag{5.27}$$

where U_δ is the $L^2(\mathbb{R}^3)$-unitary scaling map defined in (4.43) (note that the L^1-norm, hence total charge, is preserved under this scaling). Let

$$\kappa^{\delta}(x) = \kappa^{\delta}_{\mathrm{per}}(x) + \kappa'(x) \tag{5.28}$$

be the macroscopic perturbed background potential. Accordingly, we rescale equation (5.1) by applying $\delta^{-3/2}U_\delta$ to their left and right hand sides. Using Lemma 15, we arrive at the rescaled electrostatic potential equation

$$-\Delta\phi^{\delta} = 4\pi\kappa^{\delta} - F_\delta(\phi^{\delta}), \tag{5.29}$$

$$F_\delta(\phi^{\delta}) = 4\pi\,\mathrm{den}[f_{FD}(\beta(-\delta^2\Delta - \delta\phi^{\delta} - \mu))]. \tag{5.30}$$

We will consider (5.29) on the space $(H^2_{\mathrm{per}} + H^2)(\mathbb{R}^3)$.

We remark that the macroscopic quantities (with superscripts δ) and the microscopic quantities (with subscripts δ) are related as follows

$$\kappa^{\delta} = \delta^{-3/2}U_\delta\kappa_\delta, \qquad \phi^{\delta} = \delta^{1/2}U_\delta\phi_\delta. \tag{5.31}$$

From now on, all quantities and equations are in the macroscopic variable x unless stated otherwise.

Let $\phi^{\delta}_{\text{per}} = \delta^{1/2} U_\delta \phi_{\text{per}}$, where ϕ_{per} is the periodic potential associated to the periodic solution $(\rho_{\text{per}}, \mu_{\text{per}})$ of (2.1) with periodic background charge κ_{per} given in Theorem 6. Let

$$\varphi \equiv \varphi^{\delta} := \phi^{\delta} - \phi^{\delta}_{\text{per}}. \tag{5.32}$$

We rewrite equation (5.29) by expanding the r.h.s. around $\phi^{\delta}_{\text{per}}$ to obtain

$$K_\delta \varphi = 4\pi\kappa' + N_\delta(\varphi) \tag{5.33}$$

where

$$K_\delta = -\,\Delta + M_\delta\,, \quad \text{with} \quad M_\delta = d_\varphi F_\delta(\phi^{\delta}_{\text{per}}). \tag{5.34}$$

and N_δ is defined by the expression.

As was mentioned in the introduction, we prove Theorem 5 by decomposing φ in (5.32) in small and large momentum parts (c.f. [11]). We use rough estimates for high momenta while we expand in δ and use a perturbation argument for low momenta.

We begin with a discussion of the linearized map, K_δ. Since we rescaled equation (2.1) by applying $\delta^{-3/2} U_\delta$ to it and rescaled the microscopic potentials via (5.31), it follows that

$$F_\delta = \delta^{-3/2} U_\delta \circ F_1 \circ (\delta^{-1/2} U^{*}_{\delta}) \tag{5.35}$$

where $F_1 = F_{\delta=1}$. Thus, by the definition of M_δ in (5.34) and the fact it is linear, it can be written as

$$M_\delta = \delta^{-2} U_\delta M U^{*}_{\delta}, \tag{5.36}$$

where $M := M_{\delta=1}$ and is given by (5.3).

Recall that an operator A on $L^2(\mathbb{R}^3)$ is said to be $\mathcal{L}$-periodic iff it commutes with the translations T_s (see (4.2)) by all lattice elements $s \in \mathcal{L}$. As an immediate consequence of Proposition 17, representation (5.10), and the rescaling (5.36), we have the following result

Proposition 19. *Let Assumption [A1] hold. Then M_δ is $\mathcal{L}_\delta$-periodic, positive (so that $K_\delta = -\Delta + M_\delta > -\Delta$), bounded on $L^2(\mathbb{R}^3)$ with an $O(\delta^{-2})$ bound, and has the following representation*

$$M_\delta \varphi = -\delta \, \mathrm{den} \left[\oint r^\delta_{\mathrm{per}}(z) \varphi r^\delta_{\mathrm{per}}(z) \right] , \tag{5.37}$$

where the resolvent operator $r^\delta_{\mathrm{per}}(z)$ acting on $L^2(\mathbb{R}^3)$ is given by

$$r^\delta_{\mathrm{per}}(z) = (z - h^\delta_{\mathrm{per}})^{-1}, \qquad h^\delta_{\mathrm{per}} = -\delta^2 \Delta - \delta \phi^\delta_{\mathrm{per}}. \tag{5.38}$$

To separate small and large momenta, we now perform a Lyapunov-Schmidt reduction. Let χ_Q be the characteristic function of a set $Q \subset \mathbb{R}^3$. Let Ω^*_δ denote the fundamental domain of $\mathcal{L}^*_\delta$ as in Subsection 4.2. We recall the definition of the orthogonal projection onto small momenta (as [11])

$$P_r = \chi_{B(r)}(-i\nabla) , \tag{5.39}$$

where $B(r)$ is the ball of radius r centered at the origin. We choose r such that $B(r) \subset \Omega^*_\delta$ and

$$a := \delta r = O(1) \text{ small} \tag{5.40}$$

is fixed. Below, we use the convention that $\lesssim$ is independent of a, r, δ, and β. Let

$$\bar{P}_r = 1 - P_r \tag{5.41}$$

be the orthogonal projection onto the large momenta. We decompose

$$\varphi = \varphi_s + \varphi_l \tag{5.42}$$

where $\varphi_s = P_r \varphi$ and $\varphi_l = \bar{P}_r \varphi$. Here s stands for small momentum and l stands for large momentum. We split (5.33) as

$$P_r K_\delta(\varphi_s + \varphi_l) = P_r \kappa' + P_r N_\delta(\varphi) \tag{5.43}$$
$$\bar{P}_r K_\delta(\varphi_s + \varphi_l) = \bar{P}_r \kappa' + \bar{P}_r N_\delta(\varphi)\,. \tag{5.44}$$

We solve (5.44) for φ_l on the ball

$$B_{l,\delta} :=\{\varphi \in \bar{P}_r H^1(\mathbb{R}^3) : \|\varphi\|_{\dot{H}^1} \le c_l\}, \tag{5.45}$$
$$\text{where } 1 \ll c_l \ll \delta^{-1/2} \tag{5.46}$$

while keeping φ_s fixed in the deformed ball

$$B_{s,\delta} :=\{\varphi \in P_r H^1(\mathbb{R}^3) : \|\varphi\|_{B_{s,\delta}} \le c_s\}, \tag{5.47}$$
$$\text{where } 1 \ll c_s \lesssim a^2 c_l \ll a^2 \delta^{-1/2} \tag{5.48}$$

with the norm

$$\|\varphi\|^2_{B_{s,\delta}} := \delta^{-2}\|V\|_{L^1_{\text{per}}}\|\varphi\|^2_{L^2} + \|\nabla\varphi\|^2_{L^2}\,. \tag{5.49}$$

where

$$V(x) = -\operatorname{den}\left[\beta f'_{FD}(\beta(h_{\text{per,xc},0} - \mu))\right] \ge 0. \tag{5.50}$$

Note that the H^1 and $\dot{H}^1$ norms are equivalent on $B_{l,\delta}$. Moreover, $\bar{P}_r \dot{H}^1(\mathbb{R}^3) = \bar{P}_r H^1(\mathbb{R}^3)$.

Proposition 20. *Let Assumptions [A1] - [A5] hold. Assume $\varphi_s \in B_{s,\delta}$. If* (5.40) *holds, then equation* (5.44) *on $B_{l,\delta}$ has a unique solution $\varphi_l = \varphi_l(\varphi_s)$ and this solution satisfies*

$$\|\varphi_l\|_{\dot{H}^1} \lesssim a^{-1}(\delta + \|\varphi_s\|_{B_{s,\delta}} + \delta^{1/2}\|\varphi_s\|^2_{B_{s,\delta}}) \tag{5.51}$$
$$\lesssim a^{-1}(\delta + o(\delta^{-1/2})) \tag{5.52}$$

This proposition is proven is Subsection 5.2.1. A key to this proof is the following simple lemma.

Lemma 21. *Let Assumptions [A1] hold and let r be chosen according to* (5.40)*. Then,*

$\bar{K}_\delta := \bar{P}_r K_\delta \bar{P}_r$ is invertible on the range of $\bar{P}_r$ and for $f \in$ ran $\bar{P}_r$,

$$\|\bar{K}_\delta^{-1} f\|_{\dot{H}^1} \lesssim a^{-1}\delta \|f\|_{L^2}\,. \tag{5.53}$$

Proof of Lemma 21. By Proposition 19, we see that $-\Delta + M_\delta > -\Delta$. Consequently,

$$\|\nabla \bar{K}_\delta^{-1} f\|_{L^2}^2 = \langle \bar{K}_\delta^{-1} f, (-\Delta)\bar{K}_\delta^{-1} f\rangle_{L^2} \tag{5.54}$$

$$\leq \langle \bar{K}_\delta^{-1} f, \bar{K}_\delta \bar{K}_\delta^{-1} f\rangle_{L^2} = \langle f, \bar{K}_\delta^{-1} f\rangle_{L^2}. \tag{5.55}$$

Using, on the other hand, that $\langle u, \bar{K}_\delta u\rangle_{L^2} \geq r^2 \|\bar{P} u\|_{L^2}^2$ and letting $\bar{P} u := \bar{K}_\delta^{-1/2} f$, we conclude that (5.53) holds by (5.40). □

Let $\varphi_l = \varphi_l(\varphi_s)$ be the solution to equation (5.44) given in Proposition 20 with $\varphi_s \in B_{s,\delta}$. Equation (5.44) can be written as

$$\varphi_l = \bar{K}_\delta^{-1}(-M_\delta \varphi_s + \bar{P}_r \kappa + \bar{P}_r N_\delta(\varphi_s + \varphi_l)) \tag{5.56}$$

where $\bar{P}_r$ is defined in (5.41) and, for an operator A on $L^2(\mathbb{R}^3)$,

$$\bar{A} := \bar{P}_r A \bar{P}_r \tag{5.57}$$

We substitute this expression into equation (5.43). After some algebraic manipulation, we arrive at the following equation

$$\ell \varphi_s = -Q\kappa + QN(\varphi(\varphi_s)), \tag{5.58}$$

where $\varphi(\varphi_s) = \varphi_s + \varphi_l(\varphi_s)$ with $\varphi_l(\varphi_s)$ being the solution of (5.44), and

$$\ell := P_r K_\delta P_r - P_r M_\delta \bar{K}_\delta^{-1} M_\delta P_r, \tag{5.59}$$

$$Q := P_r - P_r M_\delta \bar{K}_\delta^{-1}\,. \tag{5.60}$$

In Subsection 5.2.3 we prove the following

Proposition 22. *Let Assumptions [A1] - [A5] and equation* (5.40) *hold. Equation* (5.58) *has a unique solution $\varphi_s \in B_{s,\delta}$.*

As a result of Propositions 20 and 22 and equation (5.42), equation (5.33) has the unique solution $\varphi \in (L^2 + \dot{H}^1 + \dot{H}^2)(\mathbb{R}^3)$. This proves the existence and uniqueness of the solution $\phi_\delta \in (H^2_{\text{per}} + L^2 + \dot{H}^1 + \dot{H}^2)(\mathbb{R}^3)$ of (2.10) with κ given in (3.5). This and equation (2.8) implies the existence and uniqueness of the solution $\rho_\delta \in (L^2_{\text{per}} + L^2 + \dot{H}^{-1} + \dot{H}^{-2})(\mathbb{R}^3)$ of equation (2.1) with κ given in (3.5). This completes the proof of item (1) of Theorem 5.

Now, we address item (2) of Theorem 5. First, we extract leading order behavior by expanding the operator ℓ in δ.

Let $K_{1,k}$ denote the k-fiber of $K \equiv K_{\delta=1}$. In particular, $K_{1,0} = K_{1,k=0}$ is the 0-fiber of K, acting on L^2_{per}. We also let Π_0 denote the projection onto constant functions on $L^2_{\text{per}}(\mathbb{R}^3)$ and $\bar{\Pi}_0 := 1 - \Pi_0$. Finally, we define

$$\bar{K}_{1,0} := \bar{\Pi}_0 K_{1,0} \bar{\Pi}_0. \tag{5.61}$$

With these notations, we have

Proposition 23. *Let Assumptions [A1] - [A4] hold. Then on ran P_r, the operator ℓ in* (5.59) *is purely a function of $-i\nabla$ and has the expansion*

$$\ell = c_0 - \nabla(\epsilon + \epsilon_1)\nabla + O(\delta^2(-i\nabla)^4) \tag{5.62}$$

where $c_0 = \delta^{-2}|\Omega|^{-1}\|V\|_{L^1_{\text{per}}} + O(\delta^{-2}C_\beta e^{-2\eta(\Omega)\beta})$ are real numbers, with V given in (5.50) *and the constant C_β being at most polynomial in β, and ϵ and $\epsilon_1 = O(C_\beta e^{-\eta(\Omega)\beta})$ are real matrices, with ϵ satisfying*

$$\epsilon := 1 + \epsilon' - \epsilon'' \geq 1, \tag{5.63}$$

$$\epsilon' = -\frac{4\pi}{|\Omega|}\mathrm{Tr}_{L^2_{\text{per}}} \oint r^2_{\text{per},0}(z)(-i\nabla)r_{\text{per},0}(z)(-i\nabla)r_{\text{per},0}(z), \tag{5.64}$$

$$\epsilon'' = \frac{16\pi^2}{|\Omega|}\langle \rho_1, \bar{K}^{-1}_{1,0}\rho_1\rangle_{L^2_{\text{per}}}. \tag{5.65}$$

where $r_{\text{per},0}$ and $h_{\text{per},0}$ denote the restrictions of r_{per} and h_{per} (see (5.8)*) to $L^2_{\text{per}}(\mathbb{R}^3)$*

respectively, $\bar{K}_{1,0}$ *is given in* (5.61)*, the inverse of* $\bar{K}_{1,0}^{-1}$ *is taken on the range of* $\bar{\Pi}_0$*, and*

$$\rho_1 = 2\,\mathrm{den} \oint r_{\mathrm{per},0}^2(z)(-i\nabla) r_{\mathrm{per},0}(z)\,. \tag{5.66}$$

Proof of Proposition 23. For simplicity, we do not display the factor 4π in M_δ and only restore it in the statements of Proposition 23. Let 1 denote the constant function $1 \in L^2_{\mathrm{per}}(\mathbb{R}^3)$. Since M_δ is $\mathcal{L}_\delta$-periodic by Proposition 19, Lemma 16 shows that

$$\ell = \delta^{-2} b(-i\delta\nabla) P_r, \tag{5.67}$$

where $b(k) = \langle (\ell\mid_{\delta=1})1\rangle_\Omega$. This shows that ℓ is purely a function of $-i\nabla$, proving the first claim of the Proposition. Using equations (4.35) and (5.59) we find that the explicit form of $b(k)$:

$$b(k) = |\Omega|^{-1}(\langle 1, M_{1,k}1\rangle_{L^2_{\mathrm{per}}} - \langle 1, M_{1,k}((\bar{K}_1)_k)^{-1} M_{1,k}1\rangle_{L^2_{\mathrm{per}}}) \tag{5.68}$$

$$= : b_1(k) - b_2(k). \tag{5.69}$$

Here $M_{1,k}$ and $(\bar{K}_1)_k$ are the k-th Bloch-Floquet fiber of $M_{\delta=1}$ and $\bar{K}_{\delta=1}$ (c.f. the Bloch-Floquet decomposition in Section 4.2). Equation (5.62) is obtained by expanding $b(k)$ to the 4-th order in k.

Lemma 13 implies that

$$M_{1,k} = e^{-ixk} M_{1,0} e^{ixk} \quad \text{and} \quad K_{1,k} = e^{-ixk} K_{1,0} e^{ixk}, \tag{5.70}$$

where $M_{1,0} = M_{1,k=0}$ and $K_{1,0} = K_{1,k=0}$.

Next, we claim that $(\bar{K}_1)_k = e^{-ixk}\bar{K}_{1,0}e^{ixk}$, where, recall, $(\bar{K}_1)_k = (\bar{K}_1)_k$ and $\bar{K}_{1,0} = \bar{\Pi}_0 K_{1,0} \bar{\Pi}_0$ (see (5.61)). Let $\Pi_a := (P_a)_{k=0}$. Then $\Pi_a = \chi_{B(a)}(-i\nabla)$ on $L^2_{\mathrm{per}}(\mathbb{R}^3)$ where $\chi_{B(a)}$ is the characteristic function on the ball of radius a centred at the origin, $B(a) \subset \mathbb{R}^3$. Since the spectrum of $-i\nabla$ on $L^2_{\mathrm{per}}(\mathbb{R}^3)$ is discrete, for a small, $\Pi_a = \Pi_0$, independent of a, and is the projection onto constant functions in $L^2_{\mathrm{per}}(\mathbb{R}^3)$. It follows from (4.35) that

$$(\bar{K}_1)_{k=0} = (\bar{P}_a)_{k=0}(K_1)_{k=0}(\bar{P}_a)_{k=0}$$

$$= \bar{\Pi}_0 (K_1)_{k=0} \bar{\Pi}_0 = \bar{K}_{1,0} \tag{5.71}$$

which proves our claim.

It follows from (5.68) - (5.71) that

$$b(k) = b_1(k) - b_2(k), \tag{5.72}$$

$$b_1(k) := |\Omega|^{-1}(\langle 1, M_{1,k}1\rangle_{L^2_{\text{per}}}$$
$$= |\Omega|^{-1}\langle 1, e^{-ixk}M_{1,0}e^{ixk}1\rangle_{L^2_{\text{per}}}, \tag{5.73}$$

$$b_2(k) := \langle 1, M_{1,k}((\bar{K}_1)_k)^{-1}M_{1,k}1\rangle_{L^2_{\text{per}}})$$
$$= |\Omega|^{-1}\langle 1, e^{-ixk}M_{1,0}(\bar{K}_{1,0})^{-1}M_{1,0}e^{ixk}1\rangle_{L^2_{\text{per}}}, \tag{5.74}$$

where $\bar{K}_{1,0}$ is given in (5.61).

To expand $b(k)$ in k around $k = 0$, we show first that

$$b(-k) \text{ is real and even, } \; b(-k) = b(k). \tag{5.75}$$

We prove claim (5.75) for b_2 only as the case for b_1 is easier. By Proposition 17, $M_{1,0}$ and $K_{1,0}$ are self-adjoint, therefore $b_2(k) \in \mathbb{R}$. Consequently, (5.74) shows

$$b_2(-k) = \overline{b_2(-k)} \tag{5.76}$$

$$= |\Omega|^{-1}\langle 1, \mathcal{C}e^{ixk}M_{1,0}(\bar{K}_{1,0})^{-1}M_{1,0}e^{-ixk}1\rangle_{L^2_{\text{per}}} \tag{5.77}$$

where $\mathcal{C}$ is the complex conjugation operator. Since $M_{1,0}$ and $K_{1,0}$ are functions of $-\Delta$ and $-\Delta - \phi_{\text{per}}$, which commute with $\mathcal{C}$, the operators $M_{1,0}$ and $K_{1,0}$ also commute with $\mathcal{C}$. Thus, (5.77) shows

$$b_2(-k) = |\Omega|^{-1}\langle 1, e^{-ixk}M_{1,0}(\bar{K}_{1,0})^{-1}M_{1,0}e^{ixk} \cdot 1\rangle_{L^2_{\text{per}}}$$
$$= b_2(k). \tag{5.78}$$

By a similar proof, $b_1(k)$ is even in k. This proves (5.75). Consequently, the expansions of $b_1(k)$ and $b_2(k)$ in k have only even powers of k.

By Proposition 19, M_δ is $\mathcal{L}_\delta$-periodic. Hence, M_δ has a Bloch-Floquet decomposition

(4.32) with $\mathcal{L} = \mathcal{L}_\delta$. In an analogy to $L^2_{\text{per}}(\mathbb{R}^3)$ given in (3.1), we let

$$L^2_{\text{per},\delta}(\mathbb{R}^3) := \{ f \in L^2_{\text{loc}}(\mathbb{R}^3) : f \text{ is } \mathcal{L}_\delta\text{-periodic } \}. \tag{5.79}$$

Recall that $\phi^\delta_{\text{per}}(x) = \delta^{-1}\phi_{\text{per}}(\delta^{-1}x)$. The next lemma gives an explicit form for the k-fiber of M_δ.

Lemma 24. *Let Assumption [A1] hold. Then M_δ has a Bloch-Floquet decomposition* (4.32) *with $\mathcal{L} = \mathcal{L}_\delta$, whose $k-$fiber $M_{\delta,k}$ acting on $L^2_{\text{per},\delta}$ (see* (5.79)*) is given by*

$$M_{\delta,k} f = -\,\delta \,\text{den}\left[\oint r^\delta_{\text{per},0}(z) f r^\delta_{\text{per},k}(z) \right] \tag{5.80}$$

where $f \in L^2_{\text{per},\delta}$ and, on $L^2_{\text{per},\delta}$,

$$r^\delta_{\text{per},k} = (z - h^\delta_{\text{per},k})^{-1}, \tag{5.81}$$

$$h^\delta_{\text{per},k} = \delta^2(-i\nabla - k)^2 + \delta\phi^\delta_{\text{per}}\,. \tag{5.82}$$

Proof. This follows from Proposition 18 and the rescaling relation (5.36). □

Now, we expand $b(k) = b_1(k) - b_2(k)$ in k. First, we claim that

$$b_1(0) = |\Omega|^{-1}\|V\|_{L^1_{\text{per}}} \tag{5.83}$$

$$b_1(k) - b_1(0) = \tilde{\epsilon}|k|^2 + k\cdot\epsilon' k + O(|k|^4) \tag{5.84}$$

where V and ϵ' are given in (5.50) and (5.64), respectively, and

$$\tilde{\epsilon} = O(C_\beta e^{-\eta(\Omega)\beta}) \tag{5.85}$$

is a real matrix, where C_β is at most polynomial in β. We absorb $\tilde{\epsilon}$ into ϵ_1 in (5.62).

Using definition of b_1 in (5.69) and Lemma 24, we see that

$$b_1(k) = -|\Omega|^{-1}\langle 1, \oint r_{\text{per},0}(z) 1 r_{\text{per},k}(z)\rangle_{L^2(\Omega)} \tag{5.86}$$

$$= -|\Omega|^{-1}\text{Tr}_\Omega \oint r_{\text{per},0}(z) 1 r_{\text{per},k}(z) \tag{5.87}$$

where 1 is the constant function $1 \in L^2_{\text{per}}(\mathbb{R}^3)$. Setting $k = 0$ and using the Cauchy-formula for derivatives, we obtain

$$b_1(0) = -\langle \oint r^2_{\text{per},0}(z)\rangle_\Omega = \langle V\rangle_\Omega \tag{5.88}$$

where V is given in (5.50). Since $f' < 0$, we see that $V \geq 0$. Thus $b_1(0)$ has the form (5.83).

Next, recall that $h_{\text{per},k} = (-i\nabla - k)^2 - \phi_{\text{per}}$ (see (5.82)). We have

$$h_{\text{per},k} - h_{\text{per},k=0} = -2(-i\nabla)\cdot k + |k|^2. \tag{5.89}$$

It follows by the resolvent identity that

$$\begin{aligned} b_1(k) - b_1(0) = &- |\Omega|^{-1}\text{Tr}_{L^2_{\text{per}}} \oint r_{\text{per},0}(z) r_{\text{per},k}(z) \\ &\times [-2(-i\nabla)\cdot k + |k|^2] r_{\text{per},0}(z). \end{aligned} \tag{5.90}$$

Since $b(k)$ is even, the expansion of $b_1(k)$ around $k = 0$ has no odd terms in k. It follows from (5.90) that

$$b_1(k) - b_1(0) = -\text{Tr}_{L^2_{\text{per}}} \oint r^3_{\text{per},0}(z)|k|^2 \tag{5.91}$$

$$- k\cdot \text{Tr}_{L^2_{\text{per}}} \oint r^2_{\text{per},0}(z)(-i\nabla) r_{\text{per},0}(z)(-i\nabla) r_{\text{per},0}(z) k \tag{5.92}$$

$$+ O(|k|^4), \tag{5.93}$$

which gives (5.84). This concludes the expansion of $b_1(k)$ and proves (5.64). The estimate of $\tilde{\epsilon}$ follows by first rewriting it using the Cauchy-integral formula as

$$\tilde{\epsilon} = -\frac{1}{2}\text{Tr}_{L^2_{\text{per}}} \beta^2 f''_{\text{FD}}(\beta(h_{\text{per}} - \mu)). \tag{5.94}$$

and then following the proof of Lemma 59 with f'_{FD} replaced by f''_{FD}, we see that $\tilde{\epsilon} = O(C_\beta e^{-\eta(\Omega)\beta})$. Thus, we absorb $\tilde{\epsilon}$ into ϵ_1 in (5.62).

Next we prove the expansion

$$b_2(k) = k\cdot(\epsilon'' + \epsilon'_1)k + O(|k|^4) + O(C_\beta e^{-2\eta(\Omega)\beta}) \tag{5.95}$$

where ϵ'' is given in (5.65), $\epsilon_1' = O(C_\beta e^{-\eta(\Omega)\beta})$ is a real matrix which we absorb into ϵ_1 in (5.62), and C_β is at most polynomial in β.

To expand $b_2(k)$ in k, we recall from (5.74) that

$$b_2(k) = |\Omega|^{-1}\langle 1, (M\bar{K}^{-1}M)_k 1\rangle_{L^2_{\text{per}}} \tag{5.96}$$

$$= |\Omega|^{-1}\langle M_{1,k}1, (\bar{K}^{-1})_k M_{1,k}1\rangle_{L^2_{\text{per}}}, \tag{5.97}$$

where, recall, $M_{1,k}$ and $K_{1,k}$ are the k-th Bloch-Floquet fiber of $M \equiv M_{\delta=1}$ and $K \equiv K_{\delta=1}$. Letting

$$\rho_k = (\bar{P}_a)_k M_{1,k}1 \in L^2_{\text{per},\delta}\,, \tag{5.98}$$

where $L^2_{\text{per},\delta}$ is given in (5.79), a is given in (5.40), and P_a is defined in (5.39), we find

$$b_2(k) = |\Omega|^{-1}\langle \rho_k, (\bar{K}^{-1})_k \rho_k\rangle_{L^2_{\text{per}}}\,. \tag{5.99}$$

To extract leading order terms, we expand in k. Let $V(x)$ be given in (5.50). By definitions (5.98) and (5.80) and Lemma 24, we have

$$\rho_k = (\bar{P}_a)_k V + \rho_k', \tag{5.100}$$

$$\rho_k' := (\bar{P}_a)_k \,\text{den} \oint r^2_{\text{per},0}(z)(2(-i\nabla)k + k^2) r_{\text{per},k}(z). \tag{5.101}$$

Finally, using the decomposition (5.100), we see that b_2 given in (5.97) becomes

$$|\Omega| b_2(k) = \langle \rho_k', (\bar{K}^{-1})_k \rho_k'\rangle + \langle V, (\bar{K}^{-1})_k V\rangle + 2\text{Re}\langle V, (\bar{K}^{-1})_k \rho_k'\rangle. \tag{5.102}$$

We expand the first term in (5.102). Using (5.100), the fact b_2 is even, and $(\bar{P}_a)_{k=0} = (\bar{P}_{a=0})_{k=0}$ if a is sufficiently small (since on L^2_{per} the spectrum of $-i\nabla$ is discrete), we see that

$$\langle \rho_k', (\bar{K}^{-1})_k \rho_k'\rangle = -k\epsilon'' k + O(k^4) \tag{5.103}$$

where ϵ'' is given in (5.65).

By (5.102), this shows that

$$|\Omega|b_2(k) = -\, k\epsilon'' k + O(k^4) + \mathrm{Rem}, \tag{5.104}$$

$$\mathrm{Rem} := \langle V, (\bar{K}^{-1})_k V\rangle + 2\mathrm{Re}\langle V, (\bar{K}^{-1})_k \rho_k' \rangle. \tag{5.105}$$

Now we estimate the terms in (5.105). By Lemma 59 and since $b_2(k)$ is even in k, (5.105) is bounded as

$$\begin{aligned} |\mathrm{Rem}| \lesssim & \|V\|^2_{L^2_{\mathrm{per}}} + \|V\|_{L^2_{\mathrm{per}}} |k|^2 + O(k^4) \\ = & O(C_\beta e^{-2\eta(\Omega)\beta}) + O(C_\beta e^{-\eta(\Omega)\beta}|k|^2) + O(k^4) \end{aligned} \tag{5.106}$$

where C_β is at most polynomial in β. We identify the first term in (5.106) with the last term in (5.95), while absorbing the second and third terms in (5.106) into ϵ_1' and the second terms on the r.h.s. of (5.106).

Equations (5.104) - (5.106) prove (5.95). This completes the expansion of (5.74) and proves the formulae for and estimates of the terms ϵ' and ϵ_1 in the statement of Proposition 23. Equation (5.68), (5.69), (5.83), (5.84), and (5.95) yield equation (5.62).

Let ϵ be given in (5.63)-(5.65). The next lemma shows that $\epsilon \geq 1$ which completes the proof of Proposition 23. □

Lemma 25. *The 3×3 matrix ϵ is positive definite and $\epsilon \geq 1$.*

We prove this lemma in Subsection 5.2.5 using the Feshbach-Schur map. Here we present the main idea. For any projection P and operator H on $L^2(\mathbb{R}^3)$, the Feshbach-Schur map $F_P(H)$ is defined as

$$F_P(H) := PHP - PH\bar{P}\bar{H}^{-1}\bar{P}HP. \tag{5.107}$$

where $\bar{P} = 1 - P$, $\bar{H} = \bar{P}H\bar{P}$, and $\bar{H}^{-1}$ is defined on the range of $\bar{P}$. The Feshbach-Schur map has the property [25]

$$-\lambda \notin \sigma(H) \iff -\lambda \notin \sigma(F_P(H+\lambda) - \lambda P). \tag{5.108}$$

for any $\lambda \geq 0$. That is,

$$H \geq 0 \iff F_P(H+\lambda) - \lambda P \geq 0 \tag{5.109}$$

for all $\lambda > 0$.

With the Laplacian Δ, we define

$$K_{\epsilon,\delta} = K_\delta + c\Delta. \tag{5.110}$$

Since $M_\delta > 0$ by Proposition 17, we have that $K_{c,\delta} > 0$ for all $c \in [0,1)$. Consequently, (5.109) shows that, for any $\lambda > 0$,

$$F_P(K_{c,\delta}+\lambda) - \lambda P \geq 0. \tag{5.111}$$

By using Lemma 16 to expand $F_P(K_{c,\delta}+\lambda) - \lambda P$ on the left hand side of (5.111) in δ, one can show that

$$\begin{aligned} &F_P(K_{c,\delta}+\lambda) - \lambda P \\ &\qquad = -\nabla(\epsilon - c)\nabla P + o(1) \text{ small in } \delta, \end{aligned} \tag{5.112}$$

which together with (5.111) implies that $\epsilon - c \geq 0, \forall c \in [0,1)$ and therefore $\epsilon \geq 1$ giving Lemma 25.

Next, we use Proposition 23 to extract the leading order terms in ℓ. We define

$$\ell = \ell_0 + \ell', \tag{5.113}$$

$$\ell_0 := c_0 - \nabla(\epsilon + \epsilon_1)\nabla \tag{5.114}$$

where the c_0 and ϵ_1 are given in Proposition 23 and ℓ' is defined by this expression. We remark that $\epsilon_1 = O(C_\beta e^{-\eta(\Omega)\beta})$ and $c_0 = \delta^{-2}|\Omega|\|V\|_{L^1_{\text{per}}} + O(\delta^{-2}C_\beta e^{-2\eta(\Omega)\beta})$ with $\|V\|_{L^1_{\text{per}}} = O(C_\beta e^{-\eta(\Omega)\beta})$ (see Lemma 59) and C_β at most polynomial in β. Moreover, ℓ is the Feshbach-Schur map of $-\Delta + M_\delta$ with projection P_r. We remark that ℓ' is the $O(\delta^2(-i\nabla)^4)$ portion of ℓ on the range of P_r.

To construct an expansion of φ_s, we let φ_0 be the solution to the equation

$$\ell_0 \varphi_0 = \kappa' \tag{5.115}$$

(this solution exists since $c_0 > 0$ and $\epsilon + \epsilon_1 > 0$ and by applying Lemma 33 proved in Section 5.2.3 below) and write

$$\varphi_s = P_r \varphi_0 + \varphi_1 \tag{5.116}$$

where φ_1 is defined by this expression. In Subsection 5.2.3 below we prove the following

Lemma 26. *The function* φ_1 *in* (5.116) *obeys the estimate*

$$\|\varphi_1\|_{B_{s,\delta}} \lesssim a^{-2} \delta^{1/2} \tag{5.117}$$

As a result, due to (5.42) and (5.116), the solution φ of equation (5.33) can be written as

$$\varphi = P_r \varphi_0 + \varphi_1 + \varphi_l \tag{5.118}$$

and $\varphi_1 \in B_{s,\delta}$ and $\varphi_l \in B_{l,\delta}$ satisfying estimates (5.117) and (5.52), respectively.

Finally, we prove item (2) of Theorem 5, with φ_0, φ_1, and φ_l satisfying (5.115), (5.199), and (5.44), respectively, we peel off all δ (hence β) dependence of ℓ_0 and φ_0. Set ϕ_0 to be the solution of the equation

$$-\operatorname{div} \epsilon \nabla \phi_0 = \kappa' \tag{5.119}$$

where ϵ is given in (5.63). We write $\varphi_0 = \phi_0 + \varphi_0'$. Then φ_0' is given by the equation

$$\varphi_0' = \ell_0^{-1} (\ell_0 + \operatorname{div} \epsilon \nabla) \phi_0 \, . \tag{5.120}$$

We would like to estimate the $\dot{H}^1$ norm of φ_0' using (5.120). To achieve this, we note that

$$\nabla \ell_0^{-1} \lesssim \nabla (\delta^{-2} |\Omega|^{-1} \|V\|_{L^1_{\text{per}}} - \nabla \epsilon \nabla)^{-1} \lesssim (\delta^{-2} |\Omega|^{-1} \|V\|_{L^1_{\text{per}}})^{-1/2} \tag{5.121}$$

by Proposition 23. Applying (5.121) to (5.120) and using Lemma 56, we see that

$$\|\varphi_0'\|_{\dot H^1} \lesssim \delta C_\beta e^{\frac{1}{2}\eta(\Omega)\beta} \|(\ell_0 + \operatorname{div}\epsilon\nabla)\phi_0\|_{L^2}\,. \tag{5.122}$$

where C_β is at most polynomial in β. Together with Definition (5.114), this shows

$$\|\varphi_0'\|_{\dot H^1} \lesssim \delta C_\beta e^{\frac{1}{2}\eta(\Omega)\beta} \|(\delta^{-2}|\Omega|^{-1}\|V\|_{L^1_{\text{per}}} + \lambda_0 - \nabla\epsilon_1\nabla)\phi_0\|_{L^2}. \tag{5.123}$$

By Proposition 23 and Lemma 59, $\|V\|_{L^1_{\text{per}}}, \epsilon_1 = O(C_\beta e^{-\eta(\Omega)\beta})$ and $\lambda_0 = O(C_\beta e^{-2\eta(\Omega)\beta})$. Equation (5.123) and (5.119) imply

$$\|\varphi_0'\|_{\dot H^1} \lesssim O(\delta^{-1} C_\beta e^{-\frac{1}{2}\eta(\Omega)\beta}) \lesssim \delta^{1/2} \tag{5.124}$$

by Assumption [A4].

Consequently, we write

$$\varphi = \varphi_0 - \bar P_r \varphi_0 + P_r \varphi_0' + \varphi_1 + \varphi_l \tag{5.125}$$

and set

$$\varphi_{\text{rem},1} = -\bar P_r \varphi_0 + P_r \varphi_0' + \varphi_1, \tag{5.126}$$

$$\varphi_{\text{rem},2} = \varphi_l\,. \tag{5.127}$$

To control the term $-\bar P_r \varphi_0$, let

$$\nabla^{-1} := \nabla(-\Delta)^{-1} \tag{5.128}$$

and we note that

$$\|\nabla \bar P_r \varphi_0\|_{L^2} = \|\bar\nabla P_r \ell_0^{-1}\kappa\|_{L^2} \tag{5.129}$$

$$\lesssim \|\bar P_r \nabla^{-1}\kappa\|_{L^2} \lesssim \delta\|\kappa\|_{L^2}\,. \tag{5.130}$$

Moreover, Lemma 26 shows that $\|\varphi_1\|_{\dot H^1} \lesssim \delta^{1/2}$. Combining with (5.124), we see that $\|\varphi_{\text{rem},1}\|_{\dot H^1} \lesssim \delta^{1/2}$. Since φ_l is in the range of $\bar P_r$, Proposition 20 gives the estimate

$$\|\varphi_{\text{rem},2}\|_{L^2} = \|\nabla^{-1}\nabla\varphi_{\text{rem},2}\|_{L^2} \lesssim \delta\|\varphi_{\text{rem},2}\|_{\dot H^1} \lesssim \delta. \tag{5.131}$$

This completes the proof of part (2) of Theorem 5. □

5.2 Technicalities for Theorem 5

5.2.1 Proof of Proposition 20

Proof of Proposition 20. In order to convert (5.44) into a fixed point problem, we use that, by Proposition 19, $\bar{K}_\delta := \bar{P}_r K_\delta \bar{P}_r$ is invertible on the range of $\bar{P}_r$ (see (5.41)). Thus, we write

$$\varphi_l = \Phi_l(\varphi_l) \tag{5.132}$$

where

$$\begin{aligned}\Phi_l(\varphi_l) :=& \bar{K}_\delta^{-1}(-M_\delta\varphi_s + \bar{P}_r\kappa') + \bar{K}_\delta^{-1}\bar{P}_r N_\delta(\varphi)\\ =&: \Phi_s + \Phi'(\varphi_l)\end{aligned} \tag{5.133}$$

and $\varphi = \varphi(\varphi_l) := \varphi_s + \varphi_l$. This is a fixed point problem for φ_l. We will solve this problem on the ball $B_{l,\delta}$ defined in (5.45)). We start with linear estimates.

Lemma 27. *Let Assumptions [A1] - [A4] hold and let r be chosen according to* (5.40). *Then*

$$\|\bar{K}_\delta^{-1} M_\delta P_r f\|_{B_{l,\delta}} \lesssim a^{-1}\|f\|_{B_{s,\delta}} \tag{5.134}$$

where a is given in (5.40), *$B_{s,\delta}$ and $B_{l,\delta}$ are given in* (5.45) *and* (5.49), *respectively.*

For the sake of continuity, this lemma is proved immediately after the current proof. Lemmas 21 and 27 show that

$$\|\bar{K}_\delta^{-1}\kappa\|_{\dot{H}^1} \lesssim a^{-1}\delta\|\kappa\|_{L^2} \lesssim a^{-1}\delta \tag{5.135}$$

$$\|\bar{K}_\delta^{-1} M_\delta P_r \varphi_s\|_{\dot{H}^1} \lesssim a^{-1}\|\varphi_s\|_{B_{s,\delta}}\,. \tag{5.136}$$

Consequently, the constant term Φ_s in (5.133) is bounded as follows.

$$\|\Phi_s\|_{\dot{H}^1} \lesssim a^{-1}(\delta + \|\varphi_s\|_{B_{s,\delta}}) \tag{5.137}$$

Now we consider the nonlinear terms. Let $\psi \in B_{l,\delta}$. Applying Lemmas 21 to equation (5.133), and using the relation $\delta r =: a \asymp 1$ (see (5.40)), we see that

$$\|\Phi'(\psi)\|_{\dot{H}^1} \lesssim a^{-1}\delta \|N_\delta(\varphi_s + \psi_1)\|_{L^2}. \tag{5.138}$$

Since $\|\varphi_s\|_{B_{s,\delta}}$ and $\|\psi\|_{\dot{H}^1}$ are $o(\delta^{-1/2})$ by definition (see (5.47) and (5.45)), we can apply equation (B.21) to (5.138). Consequently,

$$\|\Phi'(\psi)\|_{\dot{H}^1} \lesssim a^{-1}\delta^{1/2}(\|\varphi_s\|^2_{B_{s,\delta}} + \|\psi\|^2_{B_{l,\delta}}). \tag{5.139}$$

Similarly, let $\psi_1, \psi_2 \in B_{l,\delta}$. By Lemma 21 and the relation (5.40), we have

$$\begin{aligned} &\|\Phi'(\psi_1) - \Phi'(\psi_2)\|_{B_{l,\delta}} \\ =&\|\bar{K}_\delta^{-1}(\bar{P}_r N_\delta(\varphi_s + \psi_1) - \bar{P}_r N_\delta(\varphi_s + \psi_2))\|_{B_{l,\delta}} &(5.140) \\ \lesssim& a^{-1}\delta\|N_\delta(\varphi_s + \psi_1) - N_\delta(\varphi_s + \psi_2)\|_{L^2} &(5.141) \end{aligned}$$

By equation (B.21),

$$\|\Phi'(\psi_1) - \Phi'(\psi_2)\|_{B_{l,\delta}} \lesssim a^{-1}\delta^{1/2}(\|\varphi_s\|_{B_{s,\delta}} + \|\psi_1\|_{B_{s,\delta}} + \|\psi_2\|_{B_{s,\delta}})\|\psi_1 - \psi_2\|_{\dot{H}^1}. \tag{5.142}$$

In conjunction, equations (5.133), (5.137), (5.139), and (5.142) show that for $\psi_1, \psi_2 \in B_{s,\delta}$,

$$\|\Phi_l(\psi_1)\|_{B_{l,\delta}} \lesssim a^{-1}(\delta + \|\varphi_s\|_{B_{s,\delta}} + \delta^{1/2}\|\varphi_s\|^2_{B_{s,\delta}} + \delta^{1/2}\|\psi_1\|^2_{\dot{H}^1}) \tag{5.143}$$

$$\|\Phi_l(\psi_1) - \Phi_l(\psi_2)\|_{B_{l,\delta}} \lesssim a^{-1}\delta^{1/2}(\|\varphi_s\|_{B_{s,\delta}} + \|\varphi_1\|_{B_{s,\delta}} + \|\varphi_2\|_{B_{s,\delta}})\|\varphi_1 - \varphi_2\|_{\dot{H}^1}. \tag{5.144}$$

By (5.46) and (5.48), equation (5.143) shows that if $\psi \in B_{l,\delta}$, then

$$\|\Phi_l(\psi)\|_{B_{l,\delta}} \lesssim a^{-1}(\delta + c_s + \delta^{1/2}c_s^2 + \delta^{1/2}c_l^2) \tag{5.145}$$
$$\lesssim a^{-1}\delta + ac_l + a^3\delta^{1/2}c_l^2 + a^{-1}\delta^{1/2}c_l^2 \tag{5.146}$$
$$\lesssim a^{-1}\delta + (a + o(1))c_l \tag{5.147}$$

Thus, Φ_l maps $B_{l,\delta}$ into itself if $a = O(1)$ is small. Similarly, if $\psi_1, \psi_2 \in B_{l,\delta}$, their $B_{s,\delta}$ norms is $o(\delta^{-1/2})$. It follows by (5.144) that Φ_l is a contraction on $B_{l,\delta}$. By the fixed point theorem, (5.133) has a solution $\varphi_l = \varphi_l(\varphi_s)$ on $B_{l,\delta}$ provided $\varphi_s \in B_{s,\delta}$. Thus, (5.44) is solved.

The estimate in Proposition 20 is proved by Lemma 28 below. The proof of Lemma is defered to Subsection 5.2.2.

Lemma 28. *Let $\psi_1, \psi_2 \in B_{s,\delta}$ and $\varphi_l(\psi_1), \varphi_l(\psi_2) \in B_{l,\delta}$ denote the solution to* (5.44) *as given in Proposition 20. Then*

$$\|\varphi_l(\psi_1)\|_{\dot{H}^1} \lesssim a^{-1}(\delta + \|\psi_1\|_{B_{s,\delta}} + \delta^{1/2}\|\psi_1\|^2_{B_{s,\delta}}) \tag{5.148}$$
$$\|\varphi_l(\psi_1) - \varphi_l(\psi_2)\|_{\dot{H}^1} \lesssim a^{-1}\|\psi_1 - \psi_2\|_{B_{s,\delta}} \tag{5.149}$$

□

Our goal now is to prove Lemma 27, which was stated in the proof of Proposition 20 and whose proof is defered until now. Recall the definitions of $L^2_{\mathrm{per},\delta}$ in (5.79) and of the k-fiber $M_{\delta,k}$ of M_δ in (5.80). We decompose the operator $M_{\delta,k}$ acting on $L^2_{\mathrm{per},\delta}$ as

$$M_{\delta,k} =: M_{\delta,0} + M'_{\delta,k}\,, \tag{5.150}$$

where $M_{\delta,0} = M_{\delta,k=0}$ and $M'_{\delta,k}$ is defined by the expression (5.150). We define operators M_0 and M'_δ on $L^2(\mathbb{R}^2)$ via

$$M_0 := \int_{\Omega^*_\delta}^{\oplus} d\hat{k}\, M_{\delta,0}\varphi, \tag{5.151}$$

$$M'_\delta := \int_{\Omega^*_\delta}^{\oplus} d\hat{k}\, M'_{\delta,k}\varphi\,. \tag{5.152}$$

By Lemma 24 and definition (5.150), the latter operators satisfy

$$M_\delta = M_0 + M'_\delta \,. \tag{5.153}$$

Lemma 29. *M_0 (see (5.151)) restricted to the range of P_r is a multiplication operator given by*

$$(M_0 P_r \varphi)(x) = V_\delta(x)(P_r\varphi)(x), \tag{5.154}$$

where

$$V_\delta(x) = -\delta^{-2}\,\mathrm{den}\left[\beta f'_{FD}(\beta(h_{\mathrm{per},0} - \mu))\right](\delta^{-1}x)\,. \tag{5.155}$$

and $h_{\mathrm{per},0}$ is given in (5.22) (with $k = 0$).

Proof. By (5.80) and definition of M_0 in (5.151), we see that

$$M_0 P_r \varphi = -\int_{\Omega_\delta^*}^{\oplus} d\hat{k}\,\delta\,\mathrm{den}\left[\oint r^\delta_{\mathrm{per},0}(z)(P_r\varphi)_k r^\delta_{\mathrm{per},0}(z)\right]. \tag{5.156}$$

By Corollary 12 and the Cauchy integral formula,

$$\begin{aligned} M_0 P_r \varphi &= -\int_{\Omega_\delta^*}^{\oplus} d\hat{k}\,\delta\,\mathrm{den}\left[\oint (r^\delta_{\mathrm{per},0}(z))^2\right]|\Omega_\delta|^{-1}\hat{\varphi}(k) & (5.157)\\ &= -\int_{\Omega_\delta^*}^{\oplus} d\hat{k}\,\beta f_{\mathrm{FD}}(\beta(h^\delta_{\mathrm{per},0} - \mu))|\Omega_\delta|^{-1}\hat{\varphi}(k). & (5.158)\end{aligned}$$

where $r^\delta_{\mathrm{per},0}(z)$ and $h^\delta_{\mathrm{per},0}$ are given by (5.81) and (5.82) respectively. Applying the inverse Bloch-Floquet transform (4.22), (5.158) implies

$$\begin{aligned} M_0 P_r \varphi = -\delta\,\mathrm{den}[\beta f'_{FD}(\beta(h^\delta_{\mathrm{per},0} - \mu))]&\\ \times \int_{\Omega_\delta^*} d\hat{k}\, e^{-ikx}|\Omega_\delta|^{-1}\hat{\varphi}(k).& \qquad (5.159)\end{aligned}$$

Since $d\hat{k}$ is normalized by the volume of Ω_δ, (5.159) shows

$$M_0 P_r \varphi = -\,\delta\,\mathrm{den}\left[\beta f'_{FD}(\beta(h^\delta_{\mathrm{per},0} - \mu))\right] P_r\varphi. \tag{5.160}$$

By Lemma 15 and recalling the definition of U_δ from (4.43), we see that

$$\delta\,\mathrm{den}\left[\beta f'_{FD}(\beta(h^{\delta}_{\mathrm{per},0}-\mu))\right] \tag{5.161}$$
$$=\delta\,\mathrm{den}\left[U_\delta\beta f'_{FD}(\beta(h_{\mathrm{per},0}-\mu))U^*_\delta\right] \tag{5.162}$$
$$=\delta^{-2}\,\mathrm{den}\left[\beta f'_{FD}(\beta(h_{\mathrm{per},0}-\mu))\right](\delta^{-1}x)\,, \tag{5.163}$$

where $h_{\mathrm{per},0}=h^{\delta=1}_{\mathrm{per},0}$, which together with (5.160) gives (5.154)-(5.155). □

Lemma 30. *For M_0 given in* (5.151) *and with $V(x)$ given in* (5.50)*, we have that*

$$\|\bar{P}_r\nabla^{-1}M_0P_r\varphi\|_{L^2}\lesssim a^{-1}\delta^{-1}\|V\|_{L^2_{\mathrm{per}}}\|P_r\varphi\|_{L^2}. \tag{5.164}$$

where ∇^{-1} is given in (5.128) *and a is given in* (5.40).

Proof. Let V_δ be given in (5.155). Since the Bloch-Floquet decomposition is unitary, we see, by Lemma 29 and Corollary 12, that

$$\|M_0P_r\varphi\|^2_{L^2}=\|V_\delta P_r\varphi\|^2_{L^2} \tag{5.165}$$
$$=\int_{\Omega^*_\delta}d\hat{k}\|V_\delta|\hat{\varphi}(k)||\Omega_\delta|^{-1}\|^2_{L^2_{\mathrm{per},\delta}}, \tag{5.166}$$

where $L^2_{\mathrm{per},\delta}$ is given in (5.79). Using the fact that $d\hat{k}=|\Omega^*_\delta|^{-1}dk$ and $|\Omega_\delta|=\delta^3|\Omega|$, (5.166) implies

$$\|M_0P_r\|^2_{L^2}=\delta^{-3}|\Omega|\|V_\delta\|^2_{L^2_{\mathrm{per},\delta}}\|P_r\varphi\|^2_{L^2}. \tag{5.167}$$

By a change of variable, we see that

$$\|V_\delta\|_{L^2_{\mathrm{per},\delta}}=\delta^{-1/2}\|V\|_{L^2_{\mathrm{per}}} \tag{5.168}$$

where V is given by (5.50). Combing with (5.167), the fact $\bar{P}_r(-i\nabla)^{-1}\lesssim r^{-1}$ (where ∇^{-1} is given in (5.128) and see (5.40)), and $a=\delta r$, Lemma 30 is proved. □

Lemma 31. *Let $M'_{\delta,k}$ be given in* (5.150)*, we have that*

$$M'_{\delta,k}\varphi=-\,\delta\,\mathrm{den}\oint\left[r^{\delta}_{\mathrm{per}}(z)\varphi r^{\delta}_{\mathrm{per}}(z)\right.$$
$$\left.\times(2(-i\delta\nabla)\delta k-\delta^2k^2)r^{\delta}_{\mathrm{per},k}(z)\right] \tag{5.169}$$

Proof. By (5.80) and (5.150), we have that

$$M'_{\delta,k}\varphi = -\,\delta\,\mathrm{den}\left[\oint r_{\mathrm{per},0}(z)\varphi(r^{\delta}_{\mathrm{per},k}(z) - r^{\delta}_{\mathrm{per},0}(z))\right]. \tag{5.170}$$

Since $r^{\delta}_{\mathrm{per},k}(z) - r_{\mathrm{per},0}(z) = r^{\delta}_{\mathrm{per},0}(z)(2(-i\delta\nabla)\delta k - \delta^2 k^2)r^{\delta}_{\mathrm{per},k}(z)$, this gives (5.169). □

Lemma 32. *Let M'_δ be given by* (5.152). *Then*

$$\|\bar{P}_r\nabla^{-1}M'_\delta P_r\nabla^{-1}\varphi\|_{L^2} \lesssim a^{-1}\|P_r\varphi\|_{L^2} \tag{5.171}$$

where ∇^{-1} is defined in (5.128) *and a is given in* (5.40).

Proof. Let ∇^{-1} be given in (5.128), and $k^{-1} := k/|k|^2$. Let $\varphi \in L^2(\mathbb{R}^3)$. By Corollary 12, we have

$$(P_r\nabla^{-1}\varphi)_k = k^{-1}\hat{\varphi}(k)|\Omega_\delta|^{-1}\chi_{B(r)}(k). \tag{5.172}$$

This gives $M'_\delta P_r\nabla^{-1}\varphi = |\Omega_\delta|^{-1}\int^{\oplus}_{B(r)} d\hat{k} M'_{\delta,k}k^{-1}\hat{\varphi}(k)$. Since the Bloch-Floquet decomposition is unitary, we see, using (5.172), that

$$\|M'_\delta P_r\nabla^{-1}\varphi\|^2_{L^2} \tag{5.173}$$

$$= |\Omega_\delta|^{-2}\int_{B_r} d\hat{k}\,\|M'_{\delta,k}1\|^2_{L^2_{\mathrm{per},\delta}}|k|^{-2}|\hat{\varphi}(k)|^2 \tag{5.174}$$

Since $d\hat{k} = |\Omega^*_\delta|^{-1}dk = |\Omega_\delta|dk$ and $|\Omega_\delta| = \delta^3|\Omega|$, (5.174) is bounded as

$$\|M'_\delta P_r\nabla^{-1}\varphi\|^2_{L^2} \lesssim \delta^{-3}\sup_{k\in B_r}\left(\|M'_{\delta,k}1\|^2_{L^2_{\mathrm{per},\delta}}|k|^{-2}\right)\|P_r\varphi\|^2_{L^2} \tag{5.175}$$

where $1 \in L^2_{\mathrm{per},\delta}$ is the constant function 1 and $L^2_{\mathrm{per},\delta}$ is given in (5.79). By the rescaling relation (5.36) and (5.169), we see that

$$\|M'_{\delta,k}1\|_{L^2_{\mathrm{per},\delta}} = \|U^*_\delta M'_{\delta,k}U_\delta\cdot U^*_\delta 1\|_{L^2_{\mathrm{per}}} \tag{5.176}$$

$$= \delta^{3/2-2}\|M'_{1,k}1\|_{L^2_{\mathrm{per}}} \tag{5.177}$$

$$= \delta^{-1/2}\Big\|\,\mathrm{den}\Big[\oint r^2_{\mathrm{per}}(z)(-2(-i\nabla)\delta k + \delta^2|k|^2)r_{\mathrm{per},\delta k}(z)\Big]\Big\|_{L^2_{\mathrm{per}}}. \tag{5.178}$$

By (5.178), for $|k| \leq r$,

$$\|M'_{\delta,k}1\|_{L^2_{\text{per}}}|k|^{-1} \lesssim \delta^{-1/2+1} + \delta^{-1/2+2}r \tag{5.179}$$

$$= \delta^{1/2} + \delta^{3/2}r\,. \tag{5.180}$$

By (5.40) and (5.175), equation (5.180) shows that

$$\|M'_\delta P_r \nabla^{-1}\varphi\|_{L^2} \lesssim \delta^{-1}. \tag{5.181}$$

The proof of Lemma 32 is complete after noting that $\|\bar{P}_r\nabla^{-1}\|_\infty \lesssim r^{-1}$ (see (5.39)) and $a = \delta r$. □

Finally, we are ready for the Proof of Lemma 27.

Proof of Lemma 27. Using ∇^{-1} from (5.128), we write $\nabla\bar{K}_\delta^{-1}M_\delta f = \nabla\bar{K}_\delta^{-1}\nabla\cdot(\nabla^{-1}M_\delta)f$. Proposition 19 shows that $\nabla\bar{K}_\delta^{-1}\nabla \leq 1$. It follows

$$\|\nabla\bar{K}_\delta^{-1}M_\delta f\|_{L^2} \lesssim \|\bar{P}_r\nabla^{-1}M_\delta f\|_{L^2}. \tag{5.182}$$

Decomposing M_δ according to (5.153), we see that

$$\begin{aligned}\|\nabla^{-1}\bar{P}_r M_\delta P_r\varphi\|_{L^2} \leq &\|\nabla^{-1}\bar{P}_r M_0 P_r\varphi\|_{L^2} \\ &+ \|\nabla^{-1}\bar{P}_r M'_\delta P_r\varphi\|_{L^2}.\end{aligned} \tag{5.183}$$

By Lemma 30 and 32, we see that (5.183) can be bounded by

$$\|\bar{K}_\delta^{-1}M_\delta f\|_{\dot{H}^1} \lesssim \delta^{-1}a^{-1}\|V\|_{L^2_{\text{per}}}\|f\|_{L^2} + a^{-1}\|\nabla f\|_{L^2} \tag{5.184}$$

where V is given in (5.50). Using $\|V\|_{L^2_{\text{per}}} \leq \|V\|_{L^\infty}^{1/2}\|V\|_{L^1_{\text{per}}}^{1/2}$ and (5.184), we see that

$$\begin{aligned}&\|\bar{K}_\delta^{-1}M_\delta f\|_{\dot{H}^1} \\ &\lesssim a^{-1}(\|V\|_{L^\infty}^{1/2}(\delta^{-1}\|V\|_{L^1_{\text{per}}}^{1/2}\|f\|_{L^2}) + \|\nabla f\|_{L^2})\,.\end{aligned} \tag{5.185}$$

By the gap Assumption [A3], Lemma 59 implies (5.134) and so Lemma 27 is proved. □

5.2.2 Proof of Lemma 28

Proof. Since $\varphi_l(\psi_1), \varphi_l(\psi_2)$ satisfy (5.44) (hence (5.133)). Thus, by equations (5.143) and (5.144),

$$\|\varphi_l(\psi_1)\|_{\dot{H}^1} \lesssim a^{-1}(\delta + \|\psi_1\|_{B_{s,\delta}} + \delta^{1/2}\|\psi_1\|^2_{B_{s,\delta}} + \delta^{1/2}\|\varphi_l(\psi_1)\|^2_{\dot{H}^1}) \tag{5.186}$$

Since $\varphi_l(\psi_1) \in B_{l,\delta}$, its $B_{l,\delta}$ norm is at most $c_l = o(\delta^{-1/2})$ (see (5.47)). It follows that

$$\|\varphi_l(\psi_1)\|_{\dot{H}^1} \lesssim a^{-1}(\delta + \|\psi_1\|_{B_{s,\delta}} + \delta^{1/2}\|\psi_1\|^2_{B_{s,\delta}}) + o(1)\|\varphi_l(\psi_1)\|_{\dot{H}^1} \tag{5.187}$$

Moving the term $o(1)\|\varphi_l(\psi_1)\|_{\dot{H}^1}$ to the left hand side of (5.187) proves (5.148).

Similarly, if $\psi_1, \psi_2 \in B_{s,\delta}$, then

$$\begin{aligned}\|\varphi_l(\psi_1) - \varphi_l(\psi_2)\|_{\dot{H}^1} \lesssim & \|\bar{K}_\delta^{-1} M_\delta(\psi_1 - \psi_2)\|_{\dot{H}^1} \\ & + \|\bar{K}_\delta^{-1}\bar{P}[N_\delta(\psi_1 + \varphi_l(\psi_1)) - N_\delta(\psi_2 + \varphi_l(\psi_2))]\|_{\dot{H}^1}\end{aligned} \tag{5.188}$$

By Proposition 19, Lemmas 27, and equation (B.21),

$$\begin{aligned}&\|\varphi_l(\psi_1) - \varphi_l(\psi_2)\|_{\dot{H}^1} \\ \lesssim & a^{-1}\|\psi_1 - \psi_2\|_{B_{s,\delta}} \\ & + a^{-1}\delta^{1/2}(\|\psi_1 + \varphi_l(\psi_1)\|_{B_{s,\delta}} + \|\psi_1 + \varphi_l(\psi_1)\|_{B_{s,\delta}}) && (5.189) \\ & \times \|\psi_1 - \psi_2 + \varphi_l(\psi_1) - \varphi_l(\psi_2)\|_{B_{s,\delta}} && (5.190)\end{aligned}$$

Since $\psi_1, \psi_2, \varphi_l(\psi_1), \varphi_l(\psi_2)$ has $B_{s,\delta}$ norm at most $o(\delta^{-1/2})$, we see that

$$\begin{aligned}&\|\varphi_l(\psi_1) - \varphi_l(\psi_2)\|_{\dot{H}^1} \\ \lesssim & a^{-1}\|\psi_1 - \psi_2\|_{B_{s,\delta}} \\ & + a^{-1}o(1)(\|\psi_1 - \psi_2\|_{B_{s,\delta}} + \|\varphi_l(\psi_1) - \varphi_l(\psi_2)\|_{B_{s,\delta}}).\end{aligned} \tag{5.191}$$

Moving the $a^{-1}o(1)\|\varphi_l(\psi_1) - \varphi_l(\psi_2)\|_{B_{s,\delta}}$ term to the left hand side of (5.191) proves (5.149). Lemma 28 is now proved.

□

5.2.3 Proof of Proposition 22

We begin with the following

Lemma 33. *Let Assumptions [A1] - [A4] and equation* (5.40) *hold. Let* ℓ, ℓ_0, ℓ' *be given in* (5.59), (5.114), *and* (5.113) *respectively. Then*

$$|\ell'| \lesssim \delta^2(-i\nabla)^4, \tag{5.192}$$

$$\ell_0 \gtrsim -\Delta + \delta^{-2}\|V\|_{L^1_{\text{per}}}, \tag{5.193}$$

$$\ell \gtrsim -\Delta + \delta^{-2}\|V\|_{L^1_{\text{per}}}. \tag{5.194}$$

Proof. The first inequality (5.192) is a direct consequence of Proposition 23 and definition (5.113). By Proposition 23, and Lemma 25, we see that

$$\ell_0 \geq -C_1\Delta + C_2\delta^{-2}\|V\|_{L^1} \tag{5.195}$$

for some δ, r-independent $O(1)$ constant $C_1 > 0$ (see (5.40) for the definition of r). This proves 5.193.

Finally, we prove the last inequality (5.194). By (5.113) and (5.192),

$$\ell = \ell_0 + \ell' \tag{5.196}$$

$$\geq -C_1\Delta + C_2\delta^{-2}\|V\|_{L^1} - O(\delta^2(-i\nabla)^4)P_r \tag{5.197}$$

for some constants $C_1, C_2 > 0$ independent of δ and r. Since $-i\nabla P_r \leq r$ and $a := \delta r = O(1)$ is small (see (5.39) and (5.40)), (5.197) implies

$$\ell \geq -C_1\Delta + C_2\delta^{-2}\|V\|_{L^1_{\text{per}}} - O(a^2(-i\nabla)^2)P_r. \tag{5.198}$$

This implies (5.194). □

Now, we prove Proposition 22. Inserting (5.116) into equation (5.58) and decompose $\ell = \ell_0 + \ell'$ (see (5.59)) as in (5.113) and decompose $\varphi = P_r\varphi_0 + \varphi_1$ as in (5.115), we obtain the equivalent equation for φ_1:

$$\ell\varphi_1 = -\ell'\varphi_0 - P_r M_\delta \bar{K}_\delta^{-1}\kappa' + QN_\delta(\tilde{\varphi})\,, \tag{5.199}$$

where

$$\tilde{\varphi} = \tilde{\varphi}(\varphi_1) := P_r\varphi_0 + \varphi_1 + \varphi_l(P_r\varphi_0 + \varphi_1), \tag{5.200}$$

and $\varphi_l = \varphi_l(f)$ is the solution to equation (5.44) given by Proposition 20 with $f \in B_{s,\delta}$. Now we are ready for the proof.

Proof of Proposition 22. We use Lemma 33 to invert ℓ_0 (see (5.114)) in (5.115) to obtain

$$\varphi_0 := \ell_0^{-1}\kappa'\,. \tag{5.201}$$

Furthermore, we invert ℓ (see (5.59)) using Lemma 33 in equation (5.199) to find

$$\varphi_1 = \Phi_1(\varphi_1)\,, \tag{5.202}$$

where

$$\begin{aligned} \Phi_1(\varphi_1) :=& -\ell^{-1}[\ell'\ell_0^{-1}\kappa' + P_r M_\delta \bar{K}_\delta^{-1}\kappa'] + \ell^{-1}QN(\tilde{\varphi}) & (5.203)\\ =:& \Phi_{\kappa'} + \Phi(\varphi_1) & (5.204) \end{aligned}$$

with $\tilde{\varphi}$, ℓ', and Q given in (5.200), (5.192), and (5.60) respectively. Now, (5.202) is our desired fixed point problem for φ_1.

We show that Φ_1 is a contraction on $B_{s,\delta}$ (see (5.47)) and therefore (5.202) has a fixed point on $B_{s,\delta}$. We estimate (5.204) term by term. By Lemma 47 of Appendix B, we see that

$$\|\Phi_{\kappa'}\|_{L^2} \lesssim \delta^2\|\kappa\|_{L^2} + r^{-2}\|V\|_1^{-1/2}\|\kappa\|_{L^2}, \tag{5.205}$$

$$\|\nabla\Phi_{\kappa'}\|_{L^2} \lesssim \delta^2\|\nabla\kappa\|_{L^2} + a^{-2}\delta\|\kappa\|_{L^2}\,. \tag{5.206}$$

By choice of the weighted $B_{s,\delta}$ norm (see (5.49)), we see that

$$\|\Phi_{\kappa'}\|_{B_{s,\delta}} \lesssim a^{-2}\delta\|\kappa\|_{H^1\cap H^{-1}}. \tag{5.207}$$

This finishes the estimate for $\Phi_{\kappa'}$ in (5.204).

Now we turn our attention to the nonlinear estimates. First we estimate the pre-factor $\ell^{-1}Q$ in Φ (see (5.203)).

Lemma 34. *Let Assumptions [A1] - [A4] hold, then*

$$\|\ell^{-1}Qf\|_{B_{s,\delta}} \lesssim \|f\|_{\dot{H}^{-1}} + a^{-2}\delta\|f\|_{L^2} \tag{5.208}$$

Proof. Let ∇^{-1} be given in (5.128). Since ℓ is purely a function of $-i\nabla$, Lemma 33 shows that

$$\|\ell^{-1}P_rf\|_{L^2} \lesssim \|(-\Delta+\delta^{-2}\|V\|_{L^1_{\text{per}}})^{-1}f\|_{L^2} \tag{5.209}$$
$$= \|(-\Delta+\delta^{-2}\|V\|_{L^1_{\text{per}}})^{-1}\nabla\cdot\nabla^{-1}f\|_{L^2} \tag{5.210}$$
$$\lesssim \delta\|V\|^{-1/2}_{L^1_{\text{per}}}\|f\|_{\dot{H}^{-1}}. \tag{5.211}$$

Similarly, Lemma 33 shows

$$\|\nabla\ell^{-1}P_rf\|_{L^2} = \|\nabla\ell^{-1}\nabla\cdot\nabla^{-1}P_rf\|_{L^2} \lesssim \|f\|_{\dot{H}^{-1}}. \tag{5.212}$$

Combining with (B.2) and (B.3), we see that

$$\|\ell^{-1}(P_r - P_rM_\delta\bar{K}_\delta^{-1})f\|_{L^2} \tag{5.213}$$
$$\lesssim \delta\|V\|^{-1/2}_{L^1_{\text{per}}}\|f\|_{\dot{H}^{-1}} + r^{-2}\|V\|^{-1/2}_{L^1_{\text{per}}}\|f\|_{L^2} \tag{5.214}$$

and

$$\|\ell^{-1}(P_r - P_rM_\delta\bar{K}_\delta^{-1})f\|_{\dot{H}^1} \tag{5.215}$$
$$\lesssim \|f\|_{\dot{H}^{-1}} + a^{-2}\delta\|f\|_{L^2}. \tag{5.216}$$

Recalling the definition of the norm $B_{s,\delta}$ in (5.49), Lemma 34 is proved by (5.214) and (5.216). □

As a corollary, we have an estimate for the nonlinearity in Φ.

Lemma 35. *Let Assumptions [A1] - [A4] hold and* $\psi_1, \psi_2 \in B_{s,\delta}$*, then*

$$\|\ell^{-1} Q N(\psi_1)\|_{B_{s,\delta}} \lesssim a^{-2}\delta^{1/2}\|\psi_1\|^2_{B_{s,\delta}} \tag{5.217}$$

$$\|\ell^{-1} Q[N(\psi_1) - N(\psi_2)]\|_{B_{s,\delta}} \lesssim a^{-2}\delta^{1/2}(\|\psi_1\|_{B_{s,\delta}} + \|\psi_2\|_{B_{s,\delta}})\|\psi_1 - \psi_2\|_{B_{s,\delta}}. \tag{5.218}$$

where ℓ*,* Q*, and* N_δ *are given in* (5.59), (5.60)*, and* (5.33) *respectively. In particular,*

$$\|\ell^{-1} Q N(\psi_1)\|_{B_{s,\delta}} \ll \|\psi_1\|_{B_{s,\delta}} \tag{5.219}$$

$$\|\ell^{-1} Q N(\psi_1) - \ell^{-1} Q N(\psi_2)\|_{B_{s,\delta}} \ll \|\psi_1 - \psi_2\|_{B_{s,\delta}} \tag{5.220}$$

Proof. Equations (5.217) and (5.218) are direct consequences of Lemma 34 equations (B.21) and (B.22). Equations (5.219) and (5.220) follow from (5.217) and (5.218) since $\|\psi_1\|_{B_{s,\delta}}, \|\psi_2\|_{B_{s,\delta}} \ll \delta^{-1/2}$. □

Let $\varphi_1, \varphi_2 \in B_{s,\delta}$, Lemma 35 and definition (5.204) show that

$$\|\Phi(\varphi_1)\|_{B_{s,\delta}} \lesssim a^{-2}\delta^{1/2}\|\tilde{\varphi}(\varphi_1)\|^2_{B_{s,\delta}} \tag{5.221}$$

$$\begin{aligned}&\|\Phi(\varphi_1) - \Phi(\varphi_2)]\|_{B_{s,\delta}} \\ &\quad\lesssim a^{-2}\delta^{1/2}(\|\tilde{\varphi}(\varphi_1)\|_{B_{s,\delta}} + \|\tilde{\varphi}(\varphi_2)\|_{B_{s,\delta}})\|\tilde{\varphi}(\varphi_1) - \tilde{\varphi}(\varphi_2)\|_{B_{s,\delta}}\end{aligned} \tag{5.222}$$

Next, we estimate $\tilde{\varphi}(\varphi_1)$ (see (5.200)) in terms of φ_1 in (5.200).

Lemma 36. *Let Assumptions [A1] - [A4] hold. If* $\varphi_1, \varphi_2 \in B_{s,\delta}$*, then*

$$\|\tilde{\varphi}(\varphi_1)\|_{B_{s,\delta}} \lesssim 1 + a^{-1}\|\varphi_1\|_{B_{s,\delta}} \tag{5.223}$$

$$\|\tilde{\varphi}(\varphi_1) - \tilde{\varphi}(\varphi_2)\|_{B_{s,\delta}} \lesssim a^{-1}\|\varphi_1 - \varphi_2\|_{B_{s,\delta}} \tag{5.224}$$

Proof. We prove (5.223) first. By definition (5.200) of $\tilde{\varphi}$,

$$\begin{aligned}&\|\tilde{\varphi}(\varphi_1)\|_{B_{s,\delta}} \\ &\lesssim \|P_r\varphi_0\|_{B_{s,\delta}} + \|\varphi_1\|_{B_{s,\delta}} + \|\varphi_l(P_r\varphi_0 + \varphi_1)\|_{B_{s,\delta}}.\end{aligned} \tag{5.225}$$

By definition (5.115) of φ_0 and Lemma 33, we see

$$\|\tilde{\varphi}(\varphi_1)\|_{B_{s,\delta}} \lesssim 1 + \|\varphi_1\|_{B_{s,\delta}} + \|\varphi_l(P_r\varphi_0 + \varphi_1)\|_{B_{s,\delta}}. \tag{5.226}$$

Applying (5.148) to (5.226), equation (5.223) is proved.

Now, we prove (5.224). By definition (5.200),

$$\begin{aligned} &\|\tilde{\varphi}(\varphi_1) - \tilde{\varphi}(\varphi_2)\|_{B_{s,\delta}} \\ =&\|\varphi_1 - \varphi_2\|_{B_{s,\delta}} && (5.227) \\ &+ \|[\varphi_l(P_r\varphi_0 + \varphi_1) - \varphi_l(P_r\varphi_0 + \varphi_2)]\|_{B_{s,\delta}}. && (5.228) \end{aligned}$$

It suffices that we bound (5.228). By (5.201), $\|\varphi_0\|_{H^1} \lesssim \|\kappa\|_{H^{-2}} = O(1)$. Since $\varphi_i \in B_{s,\delta}$, we see that $\|P_r\varphi_0 + \varphi_i\|_{B_{s,\delta}} \lesssim 1 + \|\varphi_i\|_{B_{s,\delta}} \ll \delta^{-1/2}$. Thus, (5.224) is proved by invoking Lemma 28.

□

For any $\varphi_1, \varphi_2 \in B_{s,\delta}$, Lemmas 35 and 36 prove that

$$\|\Phi_1(\varphi_1)\|_{B_{s,\delta}} \lesssim a^{-2}\delta^{1/2} + a^{-3}\delta^{1/2}\|\varphi_1\|^2_{B_{s,\delta}}, \tag{5.229}$$

$$\|\Phi_1(\varphi_1) - \Phi_1(\varphi_1)\|_{B_{s,\delta}} \lesssim a^{-3}\delta^{1/2}(1 + \|\varphi_1\|_{B_{s,\delta}} + \|\varphi_2\|_{B_{s,\delta}})\|\varphi_1 - \varphi_2\|_{B_{s,\delta}} \tag{5.230}$$

This shows that $\Phi_1(\varphi_1)$ (see (5.202)) is a contraction and has a fixed point on $B_{s,\delta}$. □

5.2.4 Proof of Lemma 26

Proof of Lemma 26. Let φ_1 be a solution to (5.57) (equivalently, to (5.202)) as given in Proposition 22. In particular, $\|\varphi_1\|_{B_{s,\delta}} = o(\delta^{-1/2})$. By (5.229), we see that

$$\begin{aligned} \|\varphi_1\|_{B_{s,\delta}} \lesssim& a^{-2}\delta^{1/2} + a^{-3}\delta^{1/2}\|\varphi_1\|^2_{B_{s,\delta}} \\ \lesssim& a^{-2}\delta^{1/2} + o(1)\|\varphi_1\|_{B_{s,\delta}} && (5.231) \end{aligned}$$

Moving the term $o(1)\|\varphi_1\|_{B_{s,\delta}}$ to the right of (5.231) proves the estimate (5.117) and Lemma 26 is proved. □

5.2.5 Proof of Lemma 25

We expand the left hand side of (5.111) in $\lambda > 0$. Let $P = P_s$ (see (5.39)) for some real number $s > 0$, unrelated to r. Using definition (5.107) and the resolvent identity, we obtain

$$
\begin{aligned}
&F_P(K_{c,\delta}+\lambda) - \lambda P && (5.232)\\
=&PK_{c,\delta}P - PM_\delta(\bar{K}_{c,\delta}+\lambda\bar{P})^{-1}M_\delta P && (5.233)\\
=&F_P(K_{c,\delta}) + \lambda PM_\delta\bar{K}_{c,\delta}^{-1}(\bar{K}_{c,\delta}+\lambda\bar{P})^{-1}M_\delta P && (5.234)\\
=&F_P(K_{c,\delta}) + \lambda PM_\delta\bar{K}_{c,\delta}^{-2}M_\delta P\\
&-\lambda^2 PM_\delta(\bar{K}_{c,\delta})^{-2}(\bar{K}_{c,\delta}+\lambda\bar{P})^{-1}M_\delta P. && (5.235)
\end{aligned}
$$

By the choice of $P = P_s$ (see (5.39)), we see that $\bar{K}_{c,\delta} \gtrsim s^2$. Since $M_\delta \lesssim \delta^{-2}$, we see that the last term in (5.235) is bounded by $O(\lambda^2\delta^{-4}s^{-6})$. Thus, (5.232) - (5.235) implies

$$
\begin{aligned}
F_P(K_{c,\delta}+\lambda) - \lambda P = F_P(K_{c,\delta}) &+ \lambda PM_\delta(\bar{K}_{c,\delta})^{-2}M_\delta P && (5.236)\\
&+ O(\lambda^2\delta^{-4}s^{-6})P. && (5.237)
\end{aligned}
$$

Next, we expand $PM_\delta(\bar{K}_{c,\delta})^{-2}M_\delta P$ in δ. This computation is identical to the computation of ϵ'' in Proposition 23. Using ρ_1 in (5.66), we see that

$$
\begin{aligned}
&PM_\delta(\bar{K}_{c,\delta})^{-2}M_\delta P && (5.238)\\
&\quad = -\delta^2\nabla\epsilon_3\nabla P + O(\delta^4(-i\nabla)^4 P + C_\beta e^{-\eta(\Omega)\beta}) && (5.239)
\end{aligned}
$$

where we note that there is no odd power $\delta(-i\nabla)$ as the proof of Proposition 23,

$$
\epsilon_3 := |\Omega|^{-1}\langle\rho_1, (\bar{K}_{c,\delta=1,0})^{-2}\rho_1\rangle_{L^2_{\text{per}}} > 0, \qquad (5.240)
$$

where $K_{c,\delta=1,0}$ is the 0-th fiber of $K_{c,\delta=1}$, $\bar{K}_{c,\delta=1,0} = \bar{\Pi}_0 K_{c,\delta=1,0}\bar{\Pi}_0$. Here $\bar{\Pi}_0 = 1 - \Pi_0$ and Π_0 is the projection in L^2_{per} onto constants. The inverse $(\bar{K}_{c,\delta=1,0})^{-2}$ is taken on the range of $\bar{\Pi}_0$. Here C_β is at most polynomial in β, and $\eta(\Omega)$ is given in the paragraph right before Assumption [A3]. Lemma 59 implies that the error term $C_\beta e^{-\eta(\Omega)\beta}$ in (5.239) is much smaller than any power of δ. So we absorbed this term into the error $O(\lambda^2\delta^{-4}s^{-6})$. Equations (5.236) - (5.240) imply that

$$F_P(K_{c,\delta}+\lambda)-\lambda P = F_P(K_{c,\delta}) - \lambda\delta^2\nabla\epsilon_3\nabla P + O(\delta^4(-i\nabla)^4 P) + O(\lambda\delta^{-4}s^{-6}P). \tag{5.241}$$

Now, we expand the term $F_P(K_{c,\delta})$ (defined in (5.110)) from (5.241) in c. A simple computation shows that

$$F_P(K_{c,\delta}) = F_P(K_\delta) + c\Delta P \tag{5.242}$$
$$- \sum_{n\geq 1} c^n P M_\delta (\bar{K}_\delta^{-1}(-\Delta))^n \bar{K}_\delta^{-1} M_\delta P. \tag{5.243}$$

Since $\bar{K}_\delta \geq 0$, (5.243) is negative and we conclude

$$F_P(K_{c,\delta}) \leq F_P(K_\delta) + c\Delta P. \tag{5.244}$$

Finally, we expand $F_P(K_\delta)$ in δ. Since $F_P(K_\delta) = \ell$ when we set $r = s$ (see (5.59)), by Propositions 23, we see that

$$F_P(K_\delta) = -\nabla\epsilon\nabla P + O(\delta^2(-i\nabla)^4 P + C_\beta e^{-\eta(\Omega)\beta}(1-\Delta)P), \tag{5.245}$$

with the symbols defined in Propositions 23.

By Assumption [A4], $C_\beta e^{-\eta(\Omega)\beta} \ll 1$. We combine the error terms $O(C_\beta e^{-\eta(\Omega)\beta}\Delta P)$ and $O(\delta^4(-i\nabla)^4 P) = O(\tilde{a}^2\delta^2(-i\nabla)^2 P)$, where $\tilde{a} := \delta s$ (which is unrelated to the a in (5.40)), into one term $O(\tilde{a}^2(-i\nabla)^2 P)$. By (5.245) and (5.244),

$$-\nabla(\epsilon - c - O(\tilde{a}^2))\nabla P \tag{5.246}$$
$$= F_P(K_\delta) + c\Delta P + O(C_\beta e^{-\eta(\Omega)\beta})P \tag{5.247}$$
$$\geq F_P(K_{c,\delta}) + O(C_\beta e^{-\eta(\Omega)\beta})P. \tag{5.248}$$

By (5.241), (5.248) implies

$$-\nabla(\epsilon - c - O(\tilde{a}^2))\nabla P \tag{5.249}$$
$$\geq F_P(K_{c,\delta} + \lambda) - \lambda P + \lambda\delta^2\nabla\epsilon_3\nabla P$$
$$+ O(\lambda^2\delta^{-4}s^{-6})P + O(C_\beta e^{-\eta(\Omega)\beta})P. \tag{5.250}$$

Finally using (5.111), (5.250) shows

$$-\nabla(\epsilon - c - O(\tilde{a}^2))\nabla P \tag{5.251}$$
$$\geq \lambda\delta^2\nabla\epsilon_3\nabla P + O(\lambda^2\delta^{-4}s^{-6})P + O(e^{-\eta(\Omega)\beta})P. \tag{5.252}$$

Since ϵ_3 is $O(1)$, we absorb the term $\lambda\delta^2\nabla\epsilon_3\nabla P$ in (5.252) into the error $\nabla O(\tilde{a}^2)\nabla$ in (5.253). It follows that

$$-\nabla(\epsilon - c - O(\tilde{a}^2))\nabla P$$
$$\geq O(\lambda^2\delta^{-4}s^{-6}) + O(e^{-\eta(\Omega)\beta})P. \tag{5.253}$$

We note that the expressions for ϵ_0 in Propositions 23 are independent of δ and s. The s-dependence occurs only in the projection $P \equiv P_s$. In particular, the expression (5.253) holds for all $s \in (0, \delta^{-1})$. Taking $s \to \infty$, $\delta \to 0$ while $\tilde{a} := \delta s \to 0$, $\delta^{-4}s^{-6} \to 0$, $e^{-\eta(\Omega)\beta} \to 0$ and taking into account that P_s converges strongly to $\mathbf{1}$, we see that $\epsilon - c \geq 0$ for all $c \in [0, 1)$, and therefore $\epsilon \geq 1$, as claimed.

5.3 Inclusion of the exchange term

We sketch the main ideas of the proof of Theorem 5 with xc $\neq 0$ under the additional Assumption [A6]. For notation simplicity, we drop 4π in (2.8).

We begin with equation (2.10), which we rewrite as

$$-\Delta\phi = \kappa - \text{den}[f_{\text{FD}}(\beta(h^\phi - \mu)], \tag{5.254}$$

where

$$h^{\phi} = -\Delta - \phi + \mathrm{xc}(-\Delta\phi + \kappa). \tag{5.255}$$

We define the relevant macroscopic quantities κ^{δ} and ϕ^{δ} according to (5.31) (see also the paragraph immediately before (5.31)). By (3.5), we have $\kappa^{\delta} = \kappa^{\delta}_{\mathrm{per}} + \kappa'$. To study perturbations from the periodic case, we define

$$\varphi := \phi^{\delta} - \phi^{\delta}_{\mathrm{per}}. \tag{5.256}$$

After applying $\delta^{-3/2}U_{\delta}$ (see (4.43)) to equation (5.254), which brings us to equation (3.15), and subtracting $\rho^{\delta}_{\mathrm{per}}$ from both the right and left sides of the resulting equation, we obtain

$$-\Delta\varphi = \kappa' + F_{\delta}(\varphi, \kappa') \tag{5.257}$$

where, since $\rho^{\delta}_{\mathrm{per}} = f_{\mathrm{FD}}(\beta(h^{\delta}_{\mathrm{per,xc}} - \mu))$ by definition,

$$F_{\delta}(\varphi, \kappa') = \mathrm{den}[f_{\mathrm{FD}}(\beta(h^{\delta}_{\mathrm{tot}} - \mu)) - f_{\mathrm{FD}}(\beta(h^{\delta}_{\mathrm{per,xc}} - \mu))], \tag{5.258}$$

$$h^{\delta}_{\mathrm{per,xc}} = -\delta^2\Delta - \delta\phi^{\delta}_{\mathrm{per}} + \mathrm{xc}(\delta^3\rho^{\delta}_{\mathrm{per}}), \tag{5.259}$$

$$h^{\delta}_{\mathrm{tot}} = -\delta^2\Delta - \delta\phi^{\delta} + \mathrm{xc}(\delta^3(-\Delta\phi^{\delta} + \kappa^{\delta})). \tag{5.260}$$

Following (5.33), we rewrite (5.257) as

$$\tilde{K}_{\delta}\varphi = \kappa'' + N_{\kappa',\delta}(\varphi) \tag{5.261}$$

where

$$\kappa'' = \kappa' + F_{\delta}(0, \kappa'), \tag{5.262}$$

$$\tilde{K}_{\delta} = -\Delta + \tilde{M}_{\delta}, \tag{5.263}$$

$$\tilde{M}_{\delta} = -d_{\varphi}F_{\delta}(0, \kappa') \tag{5.264}$$

and $N_{\kappa',\delta}$ is defined by the expression. Equation (5.261) is in the same form as equation (5.33) in the proof for xc = 0. We remark that since κ' always occurs in $F_{\delta}(0, \kappa')$ as $\delta^3\kappa'$ (see (5.258) - (5.260)). Since $F_{\delta}(0, 0) = 0$, we have

$$\|F_{\delta}(0, \kappa')\|_{H^2} = \|F_{\delta}(0, \kappa') - F_{\delta}(0, 0)\|_{H^2} = O(\delta), \tag{5.265}$$

proved in a similar way as the estimates $\|M_\delta\|_\infty \lesssim \delta^{-2}$ in Proposition 19.

The idea of the proof is the same as Section 5.1. To recapitulate, recall that $P_r = \chi_{B(r)}(-i\nabla)$ (see (5.39) and r is chosen as in (5.40)). We solve equation (5.261) on the range of P_r and $\bar{P}_r$ by expanding in δ around $\delta = 0$ on the range of P_r while controlling the subleading part on $\bar{P}_r$. To begin, we prove Proposition 37 below, which is an analogue of Proposition 23.

Let

$$M_{\delta,\kappa'} f := -\,\delta\,\mathrm{den}\left[\oint r^\delta_{\kappa'}(z) f r^\delta_{\kappa'}(z)\right] \tag{5.266}$$

$$K_{\delta,\kappa'} := -\,\Delta + M_{\delta,\kappa'} \tag{5.267}$$

where

$$r^\delta_{\kappa'}(z) = (z - h^\delta_{\kappa'})^{-1}, \tag{5.268}$$

$$h^\delta_{\kappa'} = -\delta^2\Delta - \delta\phi^\delta_{\mathrm{per}} + \mathrm{xc}(\delta^3(\rho^\delta_{\mathrm{per}} + \kappa')). \tag{5.269}$$

By a computation similar to Proposition 17, we see from (5.264) that

$$\tilde{M}_\delta = M_{\delta,\kappa'} + M_\delta S_{\delta,\rho^\delta_{\mathrm{per}},\kappa'} =: M_{\delta,\kappa'} + \tilde{M}'_\delta \tag{5.270}$$

where

$$S_{\delta,\rho,\kappa} f := \mathrm{xc}'(\delta^3(\rho+\kappa))(\delta^2\Delta f). \tag{5.271}$$

Proposition 37. *Let Assumptions [A1], [A2], and [A4] - [A6] hold. Then the linear operator $K_{\delta,\kappa'}$ (see (5.267)) is self-adjoint on $L^2(\mathbb{R}^3)$ and $K_{\delta,\kappa'} \geq -\Delta$. Moreover, for $\tilde{K}_\delta$ defined in (5.263),*

$$\|\tilde{K}_\delta f\|_{L^2} \geq C(c - \|ex'\|_{L^\infty})\|\Delta f\|_{L^2} \tag{5.272}$$

for some constants $c, C > 0$.

A sketch of the proof of Proposition 37 is given in Section 5.3.1. We remark that $\tilde{M}_\delta$ is no longer self-adjoint due to the presence of the xc term (see (5.270)). Nevertheless, Proposition 37 assures us that we can use the same proof strategy as in the proof of Theorem 5. Our next goal is to prove a version of Proposition 20. We decompose (5.261) by the projection P_r of (5.39) as

$$P_r K_\delta \varphi_s + P_r K_\delta \varphi_l = P_r \kappa'' + P_r N_{\kappa',\delta}(\varphi) \tag{5.273}$$

$$\bar{P}_r K_\delta \varphi_s + \bar{P}_r K_\delta \varphi_l = \bar{P}_r \kappa'' + \bar{P}_r N_{\kappa',\delta}(\varphi)\,, \tag{5.274}$$

where $\bar{P}_r$ is defined in (5.41). Recall the homogeneous spaces $\dot{H}^s(\mathbb{R}^3)$, $s \geq 0$, defined in (3.10). This time, we solve for φ_l on the ball

$$B^2_{l,\delta} := \{\varphi \in \bar{P}_r(\dot{H}^2(\mathbb{R}^3) \cap \dot{H}^2(\mathbb{R}^3)) : a^{-1}\delta\|\varphi\|_{\dot{H}^2} \ll c_l\} \tag{5.275}$$

where c_l is given in (5.46), with the norm

$$\|\varphi\|^2_{B_{l,\delta}} = a^{-2}\delta^2\|\varphi\|^2_{\dot{H}^2}\,, \tag{5.276}$$

where a is given in (5.40), for a given φ_s in the deformed ball

$$B^2_{s,\delta} := \{\varphi \in H^1(\mathbb{R}^3) : \|\varphi\|_{B_{s,\delta}} \ll c_s\}, \tag{5.277}$$

where c_s and V are given by (5.48) and (3.9) respectively, with the norm

$$\|\varphi\|^2_{B_{s,\delta}} = \delta^{-2}\|V\|_{L^1_{\text{per}}}\|\varphi\|^2_{L^2} + \|\nabla\varphi\|^2_{L^2} + a^{-2}\delta^2\|\Delta\varphi\|^2_{L^2}\,, \tag{5.278}$$

where a is given in (5.40).

Proposition 38. *Let Assumptions [A1] - [A6] hold and $\varphi_s \in B^2_{s,\delta}$. Then there exists a unique solution $\varphi_l = \varphi_l(\varphi_s)$ solving equation (5.274) on $B^2_{l,\delta}$. Moreover,*

$$\|\varphi_l\|_{B^2_{l,\delta}} \lesssim a^{-1}(\delta + \|\varphi_s\|_{B^2_{s,\delta}} + \delta^{1/2}\|\varphi_s\|^2_{B^2_{s,\delta}}) \tag{5.279}$$

$$\lesssim a^{-1}(\delta + o(\delta^{-1/2})) \tag{5.280}$$

The proof of this proposition is sketched in Section 5.3.1. Next, we insert the solution $\varphi_l = \varphi_l(\varphi_s)$ from Proposition 38 into equation (5.273). For an operator A on $L^2(\mathbb{R}^3)$, let $\bar{A} := \bar{P}_r A \bar{P}_r$ where $\bar{P}_r$ is defined in (5.41). By Proposition 37, $\tilde{K}$ is invertible on the range of $\bar{P}_r$. We may define in the same way as (5.59) and (5.60) the following quantities.

$$\ell := P_r(-\Delta + \tilde{M}_\delta)P_r - P_r\tilde{M}_\delta\overline{\tilde{K}_\delta}^{-1}\tilde{M}_\delta P_r \tag{5.281}$$

$$Q := P_r - P_r\tilde{M}_\delta\overline{\tilde{K}_\delta}^{-1}. \tag{5.282}$$

We remark that ℓ is the Feshbach-Schur map of $-\Delta + \tilde{M}_\delta$ with projection P_r. After some algebraic manipulations, the insertion of $\varphi_l = \varphi_l(\varphi_s)$ into equation (5.273) yields

$$\ell\varphi_s = Q\kappa'' + QN_{\kappa',\delta}(\varphi(\varphi_s)) \tag{5.283}$$

where

$$\varphi(\varphi_s) = \varphi_s + \varphi_l(\varphi_s). \tag{5.284}$$

To extract leading order terms, we use the following proposition, where a sketch of the proof is given in Section 5.3.1. Let

$$h_{\text{per,xc}} = -\Delta - \phi_{\text{per}} + \text{xc}(\rho_{\text{per}}) \text{ and}$$
$$r_{\text{per,xc}}(z) := (z - h_{\text{per,xc}})^{-1}. \tag{5.285}$$

Recall that $r_{\text{per,xc,0}}$ and $h_{\text{per,xc,0}}$ denote the restrictions of $r_{\text{per,xc}}$ and $h_{\text{per,xc}}$ to $L^2_{\text{per}}(\mathbb{R}^3)$, respectively. We define similarly $\mathcal{K}_1 = K_{\delta=1,\kappa'=0}$ where $K_{\delta,\kappa'} := -\Delta + M_{\delta,\kappa'}$ (see (5.266)). Let $(\mathcal{K}_1)_k$ denote the k-fiber of $\mathcal{K}_1$. In particular $(\mathcal{K}_1)_0 = (\mathcal{K}_1)_{k=0}$ is the 0-fiber of $\mathcal{K}_1$ acting on L^2_{per}. Finally, we define

$$\overline{\mathcal{K}}_{1,0} := \bar{\Pi}_0(\mathcal{K}_1)_0\bar{\Pi}_0 \tag{5.286}$$

where Π_0 is defined in the paragraph immediately before (5.61).

Proposition 39. *Let Assumptions [A1] - [A6] hold. On the range of P_r, the operator ℓ in* (5.59) *has the expansion*

$$\ell = \delta^{-2}|\Omega|^{-1}\|V\|_{L^1_{\text{per}}} - \nabla\epsilon\nabla + R + O(\delta^2(-i\nabla)^4) \tag{5.287}$$

where $O(\delta^2(-i\nabla)^4)$ is measured in the operator norm, V is given in (3.9),

$$\epsilon := 1 + \epsilon' - \epsilon'' \geq 1 \tag{5.288}$$

$$\epsilon' = -\frac{4\pi}{|\Omega|}\mathrm{Tr}_{L^2_{\mathrm{per}}(\mathbb{R}^3)} \oint r^2_{\mathrm{per},xc,0}(z)(-i\nabla) \times r_{\mathrm{per},xc,0}(z)(-i\nabla) r_{\mathrm{per},xc,0}(z) \tag{5.289}$$

$$\epsilon'' = \frac{(4\pi)^2}{|\Omega|}\langle \rho_1, (\overline{\mathcal{K}}_{1,0})^{-1}\rho_1\rangle_{L^2_{\mathrm{per}}} \tag{5.290}$$

with $\overline{\mathcal{K}}_{1,0}$ given in (5.286)*, the inverse of $(\overline{\mathcal{K}}_{1,0})^{-1}$ is taken on the range of $\bar{\Pi}_0$,*

$$\rho_1 = 2\,\mathrm{den} \oint r^2_{\mathrm{per},xc,0}(z)(-i\nabla) r_{\mathrm{per},xc,0}(z)\,, \tag{5.291}$$

and

$$\|Rf\|_{L^2} \ll \|(\delta^{-2}\|V\|_{L^1_{\mathrm{per}}} - \Delta) f\|_{L^2} \tag{5.292}$$

where the real number C_β is at most polynomial in β.

Using Proposition 39, we decompose

$$\ell = \ell_0 + \ell', \tag{5.293}$$
$$\ell_0 := \delta^{-2}|\Omega|^{-1}\|V\|_{L^1_{\mathrm{per}}} - \nabla\epsilon\nabla + R$$

where ϵ and R are defined in Propositions 38 and ℓ' is defined by the expression (5.293). The following Lemma summarizes the properties of the above terms.

Lemma 40. *Let Assumptions [A1] - [A6] hold, then*

1. *ℓ_0 is invertible and $\|\ell_0^{-1} f\|_{\dot{H}^s} \lesssim \|(\delta^{-2}\|V\|_{L^1} - \Delta)^{-1} f\|_{\dot{H}^s}$ for $s \in \mathbb{Z}$.*
2. *ℓ is invertible and $\|\ell^{-1} f\|_{\dot{H}^s} \lesssim \|\ell_0^{-1} f\|_{\dot{H}^s}$ for $s = 0, 1, 2$.*
3. *$\|\ell' f\|_{L^2} \lesssim \delta^2\|\nabla^4 f\|_{L^2}$.*

Lemma is a direct consequence of Proposition 39. The proof is similar to Lemma 33. It is omitted here.

To construct an expansion of φ_s, we let φ_0 be the solution to the equation

$$\ell_0\varphi_0 = \kappa''. \tag{5.294}$$

and write

$$\varphi_s = P_r\varphi_0 + \varphi_1 \tag{5.295}$$

where φ_1 is defined by this expression. In Subsection 5.3.1 below, we prove the following Proposition.

Proposition 41. *Let Assumptions [A1] - [A6] hold. Equation* (5.283) *has a unique solution* $\varphi_s \in B^2_{s,\delta}$ *of the form* (5.295) *with* φ_1 *obeying the estimate*

$$\|\varphi_1\|_{B_{s,\delta}} \lesssim \delta^{1/2} \tag{5.296}$$

The proof of Proposition 41 follows the proofs in Section 5.2.3. From here, by following the same argument verbatim as was used in the paragraphs after Proposition 22 and (5.265), Theorem 5 with exchange term xc $\neq 0$ is proved. □

5.3.1 Appendix: supplementary proofs for Section 5.3

Proof of Proposition 37. The first claim in Proposition (37) is just the result of Proposition (17) and (19) with ρ^δ_{per} replaced by $\rho^\delta_{\text{per}} + \text{xc}(\delta^3(\rho^\delta_{\text{per}} + \kappa'))$. To see the inequality (5.272), we only have to note that in the decomposition (5.270),

$$\tilde{M}'_\delta = M_{\delta,\kappa'}(\text{xc}'(\delta\rho^\delta_{\text{per}} + \delta^3\kappa')(\delta^2\Delta)). \tag{5.297}$$

A slight modification of Proposition (17) shows that $\|M_{\delta,\kappa'}\|_\infty \lesssim \delta^{-2}$, which cancels with the δ^2 in $\delta^2\Delta$ in (5.297). It follows that

$$\|\tilde{M}'_\delta f\|_\infty \lesssim \|\text{xc}'\|_{L^\infty}\|\Delta f\| \tag{5.298}$$

for all $f \in H^2$. Together with the first claim in Proposition (37) that $K_\delta \geq -\Delta$ and decomposition (5.270), inequality 5.272 is proved. □

Proof of Proposition 38. It suffices to prove analogous versions of the linear estimates (Lemma 21, Lemma 27) and nonlinear estimates (Proposition 48) and Proposition 38 will follow by the same fixed point argument as in Proposition 20. So we will only prove these auxiliary results here in this proof and refer the reader to the proof of Proposition 20 for the related details. Recall that $\bar{A}$ of an operator A on $L^2(\mathbb{R}^3)$ is given in (5.57). We have the following result.

Lemma 42 (Analogue of Lemma 21)**.** *Let Assumptions [A1] - [A6] hold, then*

$$\|\nabla^s \overline{\tilde{K}_\delta}^{-1} f\|_{L^2} \lesssim \|\bar{P}_r \nabla^{s-2} f\|_{L^2} \tag{5.299}$$

for $s = 0, 1, 2$ *and* $f \in \dot{H}^{s-2}(\mathbb{R}^3)$.

Proof. The case for $s = 2$ is just a restatement of Proposition 37. We consider the case where $s = 0$. We decompose $\tilde{K} = -\Delta + M_{\delta,\kappa'} + \tilde{M}'_\delta$ (see (5.270)). By Proposition 37, the operator $-\Delta + M_{\delta,\kappa'}$ is self-adjoint. Recall that for any two self-adjoint operators A and B,

$$\|AB\|_\infty = \|BA\|_\infty. \tag{5.300}$$

Thus, by the result for $s = 2$ (with minor modifications), we see that

$$\|\overline{(-\Delta + M_{\delta,\kappa'})}^{-1} f\|_{L^2} \lesssim \|\nabla^{-2} f\|_{L^2}. \tag{5.301}$$

It follows by (5.298) and (5.301) that

$$\|\nabla^{-2}\overline{\tilde{K}_\delta} f\|_{L^2} \tag{5.302}$$
$$= \|\nabla^{-2}\overline{(-\Delta + M_{\delta,\kappa'})}(1 + \overline{(-\Delta + M_{\delta,\kappa'})}^{-1} M'_\delta) f\|_{L^2} \tag{5.303}$$
$$\gtrsim \|(1 + \overline{(-\Delta + M_{\delta,\kappa'})}^{-1} M'_\delta) f\|_{L^2} \tag{5.304}$$
$$\gtrsim \|f\|_{L^2} \tag{5.305}$$

by Assumption [A6]. (5.305) is equivalent to the case $s = 0$. The case for $s = 1$ is done by interpolation. □

Lemma 43 (Analogue of Lemma 27)**.** *Let Assumptions [A1] - [A6] hold and let r be the* *cut-off parameter for P_r. Then*

$$\|\overline{\tilde{K}_\delta}^{-1}\tilde{M}_\delta P_r f\|_{B^2_{l,\delta}} \lesssim a^{-1}\|f\|_{B^2_{s,\delta}} \tag{5.306}$$

where a is given in (5.40).

Proof. By definition (5.276) of the $B_{l,\delta}$ norm and Lemma 42,

$$\begin{aligned}\|\overline{\tilde{K}_\delta}^{-1}\tilde{M}_\delta P_r f\|_{B_{l,\delta}} :=& a^{-1}\delta\|\overline{\tilde{K}_\delta}^{-1}\tilde{M}_\delta P_r f\|_{\dot{H}^2} &(5.307)\\ \lesssim& a^{-1}\delta\|\bar{P}_r\tilde{M}_\delta P_r f\|_{L^2}. &(5.308)\end{aligned}$$

To estimate the last line, we further decompose $\tilde{M}_\delta$ into it periodic and perturbative (perturbation in κ' from $\kappa'=0$) parts in the decomposition (5.270). Since Using $M_{\delta,\kappa'=0}$ is periodic, we label

$$M_{\text{per},\delta} := M_{\delta,\kappa'=0} \tag{5.309}$$

to emphasis its periodicity. We remark that the operator M_δ defined in (5.34) is equal to $M_{\text{per},\delta}$ here if $\text{xc}=0$. We write

$$\begin{aligned}\tilde{M}_{\delta,\kappa'} =& M_{\text{per},\delta}(1+S_{\delta,\rho_{\text{per}},\kappa'=0}) + \text{perturbation} &(5.310)\\ =& M_{\text{per},\delta}[1+\text{xc}'(\delta^3(\rho_{\text{per}}))(-\delta^2\Delta)] + \text{perturbation} &(5.311)\\ =& M_{\text{per},\delta} + M_{\text{per},\delta}\text{xc}'(\delta^3\rho^\delta_{\text{per}})(-\delta^2\Delta) + \text{perturbation}. &(5.312)\end{aligned}$$

In this notation, the estimate associated to the first term $M_{\text{per},\delta}$ in (5.312) is just Lemma 27, which gives an upper bound as in the claimed estimate (5.306). To consider the rest of the terms, we make the following observation. Proposition (17) shows that $\|M_{\text{per},\delta}\|_\infty \lesssim \delta^{-2}$. Under the rescaling (4.43), each derivative on φ worths δ. Using this observation, we see that

$$\begin{aligned}&\|M_{\text{per},\delta}\text{xc}'(\delta^3\rho^\delta_{\text{per}})(-\delta^2\Delta)f\|_{L^2}\\ &\qquad\lesssim \|M_{\text{per},\delta}\|_\infty\|\delta^2\Delta f\|_{L^2} \lesssim \|f\|_{\dot{H}^2}. &(5.313)\end{aligned}$$

Now, we consider the perturbation term in (5.312). By definition, the perturbation is in κ' around $\kappa'=0$. Moreover, κ' always appear in $\tilde{M}_{\text{per},\delta}$ as $\delta^3\kappa'$ through the exchange term $\mathrm{xc}'(\delta^3\rho_{\mathrm{per}}^\delta + \delta^3\kappa')$ (see (5.266) - (5.271)). Thus

$$\begin{aligned} & \|\text{perturbation} \cdot f\|_{L^2} \\ \lesssim & \underbrace{\delta^{-2}}_{\text{by (5.35)}} (\|\delta^3\kappa'(\delta y)f\|_{L^2} + \|\delta^3\kappa'(\delta y)(\delta^2\Delta)f\|_{L^2}). \end{aligned} \tag{5.314}$$

We bound this using the $B_{s,\delta}$ norm. By the Hölder inequality with $\frac{1}{2} = \frac{1}{6} + \frac{1}{3}$, we see that

$$\|\delta^3\kappa'(\delta y)f\|_{L^2} + \|\delta^3\kappa'(\delta y)\Delta f\|_{L^2} \tag{5.315}$$
$$\lesssim \|\delta^3\kappa'(\delta y)\|_{L^3}\|f\|_{L^6} + \delta^3\|\kappa'\|_{L^\infty}\|f\|_{\dot{H}^2} \tag{5.316}$$
$$\lesssim \delta^2\|f\|_{L^6} + \delta^3\|f\|_{\dot{H}^2} \tag{5.317}$$

By Hardy-Littlewood's inequality (4.16), $\|f\|_{L^6} \lesssim \|f\|_{\dot{H}^1}$. Together with (5.314), equation (5.317) shows that

$$\|\text{perturbation} \cdot f\|_{L^2} \lesssim \|f\|_{B_{s,\delta}} \tag{5.318}$$

Combing Lemma 27, equations (5.308), (5.312), (5.313), and (5.318), Lemma 43 is now proved. □

Finally, we prove a nonlinear estimate. Following Proposition 48 and using (B.86), it suffices to prove a version of Lemma 51. Let

$$r_{\kappa'}(z) = (z - h_{\kappa'})^{-1}, \tag{5.319}$$
$$h_{\kappa'} = -\Delta - \phi_{\mathrm{per}} + \mathrm{xc}(\rho_{\mathrm{per}} + \delta^3\kappa'(\delta y)). \tag{5.320}$$

Expanding the nonlinearity in a similar way as (B.27), in the $\mathrm{xc} \neq 0$ case, we estimate the lowest order term

$$\begin{aligned} & N_{\kappa',2}(\phi) \\ := & \oint \mathrm{den}[r_{\kappa'}(z)[(\phi + \mathrm{xc}'(\rho_{\mathrm{per}} + \delta^3\kappa'(\delta y))\Delta\phi)r_{\kappa'}(z)]^2] \end{aligned} \tag{5.321}$$
$$+ \mathrm{den}[\oint r_{\kappa'}(z) \cdot \mathrm{xc}''(\rho_{\mathrm{per}} + \delta^3\kappa'(\delta y))(\Delta\phi)^2 \cdot r_{\kappa'}(z)]. \tag{5.322}$$

The term (5.321) is just (B.28) with ϕ replaced by $\phi + \mathrm{xc}'(\rho_{\mathrm{per}} + \delta^3\kappa'(\delta y))\Delta\phi$. The term

(5.322) is a new term and depends on the second order derivative of xc.

Lemma 44 (Analogue of Lemma 51). *Let Assumptions [A1] - [A6] hold. Assume that* $\|\nabla\phi\|_{L^2}$ *is small, then we have the estimate*

$$\|N_{\kappa',2}(\phi)\|_{L^2} \tag{5.323}$$

$$\lesssim \|\nabla\phi\|_{L^2}^2 + \|\Delta\phi\|_{L^2}^2 + C_{1,\beta}\|\nabla\phi\|_{L^2}^{4/3}\|\phi\|_{L^2}^{2/3} \tag{5.324}$$

where the constants associated with $\lesssim$ *are independent of* β*. Moreover, Lemma 54 applies to the constant* $C_{1,\beta}$*.*

Proof. The term associated to (5.321) is estimated in the exact same way as N_2 in Lemma 51 to produce an L^2-norm upper bound of

$$\|\nabla\phi\|_{L^2}^2 + \|\nabla^2\phi\|_{L^2}^2 + C_{1,\beta}\|\nabla\phi\|_{L^2}^{4/3}\|\phi\|_{L^2}^{2/3}. \tag{5.325}$$

So we focus on the second term in (5.322). We note that the second term is simply

$$M_{\kappa'}(\mathrm{xc}''(\rho_{\mathrm{per}} + \delta^3\kappa'(\delta y))(\Delta\phi)^2) \tag{5.326}$$

where $M_{\kappa'} = M_{\delta=1,\kappa'}$ is given in (5.266). By Proposition (17) (with $\delta = 1$), (5.326) is bounded by

$$\|M_{\kappa'}(\mathrm{xc}''(\rho_{\mathrm{per}}^{\delta} + \kappa')(\Delta\phi)^2)\|_{L^2} \lesssim \|\Delta\phi\|_{L^2}^2 \tag{5.327}$$

Together with equations (5.321), (5.322), and (5.325), Lemma 44 is now proved. □

By Lemmas 42, 43, and 44, Proposition 38 is now proved by the same fixed point argument as in Proposition 5.44. □

Proof of Proposition 39. We decompose ℓ (see (5.281)) as

$$\ell = \ell_{\mathrm{per}} + \ell'_{\kappa'} \tag{5.328}$$

where ℓ_{per} is ℓ with $\kappa' = 0$ and $\ell'_{\kappa'}$ is defined by this expression. The expansion (in δ) for ℓ_{per} is the same as in Proposition (23) but with ρ_{per} replaced by $\rho_{\mathrm{per}} + \mathrm{xc}(\rho_{\mathrm{per}})$. So we omit its computation here. We only remark that terms such as $\mathrm{xc}'(\rho_{\mathrm{per}})\Delta f$ do not appear in the leading terms coming from ℓ_{per} in the expansion since, under the rescaling (4.43), to every Δ is associated a factor of δ^2 (as in $\delta^2\Delta$), which is of higher order. The effect of this is an introduction of an error term that is proportional to δ^2 times the leading terms in (5.287), which we absorb into the remainder R (see (5.287)).

We show that $\ell'_{\kappa'}$ is small and does not contribute to the leading order expansion (in δ) of ℓ. For notation, let

$$G_{\kappa'} := \mathrm{xc}'(\delta^3(\rho^\delta_{\mathrm{per}} + \kappa'))(\delta^2\Delta\varphi) \text{ or } \varphi, \tag{5.329}$$

$$G_{\mathrm{per}} := \mathrm{xc}'(\delta^3\rho^\delta_{\mathrm{per}})(\delta^2\Delta\varphi) \text{ or } \varphi, \tag{5.330}$$

respectively. By (5.266) - (5.271), $\ell'_{\kappa'}$ consists of terms consisting factors of the form

$$\delta\,\mathrm{den}\left[\oint r^\delta_{\kappa'}(z)G_{\kappa'}r^\delta_{\kappa'}(z)\right] - \delta\,\mathrm{den}\left[\oint r^\delta_{\mathrm{per}}(z)G_{\mathrm{per}}r^\delta_{\mathrm{per}}(z)\right]. \tag{5.331}$$

By the resolvent identity, these terms can be written as

$$\begin{aligned} &= \oint \delta\,\mathrm{den}[r^\delta_{\kappa'}(z)(\mathrm{xc}(\delta^3(\rho^\delta_{\mathrm{per}} + \kappa')) - \mathrm{xc}(\delta^3\rho^\delta_{\mathrm{per}})) \\ &\qquad \times r^\delta_{\mathrm{per}}(z)G_{\kappa'}r^\delta_{\kappa'}(z) + \text{similar term}] && (5.332) \\ &\quad + \delta\,\mathrm{den}\left[\oint r^\delta_{\mathrm{per}}(z)(G_{\kappa'} - G_{\mathrm{per}})r^\delta_{\mathrm{per}}(z)\right] && (5.333) \\ &=: YG_{\kappa'} + M_{\mathrm{per},\delta}(G_{\kappa'} - G_{\mathrm{per}}) && (5.334) \end{aligned}$$

where $M_{\mathrm{per},\delta}$ is given in (5.312).

We first estimate $YG_{\kappa'}$ in the case where $G_{\kappa'}$ contains the exchange term. We note that

$$\|\mathrm{xc}(\delta^3(\rho^\delta_{\mathrm{per}} + \kappa')) - \mathrm{xc}(\delta^3\rho^\delta_{\mathrm{per}})\|_{L^\infty} \lesssim \delta^3\|\kappa'\|_{L^\infty}. \tag{5.335}$$

Thus, using Hölder inequality with $\frac{1}{2} = \frac{1}{2} + \frac{1}{\infty}$ (2-norm on the $G_{\kappa'}$ term and ∞-norm on κ' term), (5.329), (5.330), and (5.332), we see that

$$\|YG_{\kappa'}\|_{L^2} \lesssim \delta^3\|\Delta\varphi\|_{L^2}. \tag{5.336}$$

For the case $G_{\kappa'} = \varphi$, we expand $YG_{\kappa'}$ in orders of κ'. We will only estimate the leading order term as the higher order terms are done in a similar fashion. This term is

$$\oint \delta \operatorname{den}[r^{\delta}_{\mathrm{per,xc}}(z)(\mathrm{xc}'(\delta^3 \rho^{\delta}_{\mathrm{per}})\delta^3\kappa')r^{\delta}_{\mathrm{per,xc}}(z)\varphi r^{\delta}_{\mathrm{per,xc}}(z)] + \text{complex conjugate.} \tag{5.337}$$

We will not display the complex conjugate in the estimates below for simplicity. By the rescaling relations (5.35), (5.31), and Lemma (15), we see that

$$\|YG_{\kappa'}\|_{L^2} = \delta^{-3/2}\left\|\oint \operatorname{den}[r_{\mathrm{per,xc}}(z)(\mathrm{xc}'(\rho_{\mathrm{per}})\delta^3\kappa'(\delta x))r_{\mathrm{per,xc}}(z)\phi r_{\mathrm{per,xc}}(z)]\right\|_{L^2} \tag{5.338}$$

where $\phi = \delta^{-1/2}U^*_\delta\varphi$. So we estimate (5.338) by $\|\Delta\phi\|_{L^2}$. We first commute ϕ to the right end of the expression to obtain

$$\begin{aligned}
&\|YG_{\kappa'}\|_{L^2} \\
\leq &\delta^{-3/2}\left\|\oint \operatorname{den}[r_{\mathrm{per,xc}}(z)(\mathrm{xc}'(\rho_{\mathrm{per}})\delta^3\kappa'(\delta x))r^2_{\mathrm{per,xc}}(z)[-\Delta,\phi]r_{\mathrm{per,xc}}(z)]\right\|_{L^2} && (5.339)\\
&+\delta^{-3/2}\left\|\oint \operatorname{den}[r_{\mathrm{per,xc}}(z)(\mathrm{xc}'(\rho_{\mathrm{per}})\delta^3\kappa'(\delta x))r_{\mathrm{per,xc}}(z)^2]\phi\right\|_{L^2} && (5.340)
\end{aligned}$$

We apply Hölder with $\frac{1}{2} = \frac{1}{3} + \frac{1}{6}$ (3-norm on κ' and 6-norm on φ) to (5.339). By Lemma 9 and Hardy's inequality, we see that this term is bounded by

$$\begin{aligned}
\|(5.339)\|_{L^2} \lesssim &\delta^{-3/2}\|\delta^3\kappa'(\delta x)\|_{L^3}\|\nabla\phi\|_{L^6} && (5.341)\\
\lesssim &\delta^2\|\kappa'\|_{L^3}\|\Delta\varphi\|_{L^2}. && (5.342)
\end{aligned}$$

The term in (5.340) can be written as

$$\delta^{3/2}W_\delta(x)\phi(x) \tag{5.343}$$

where

$$W_\delta = \operatorname{den}[r_{\mathrm{per,xc}}(z)(\mathrm{xc}'(\rho_{\mathrm{per}})\kappa'(\delta x))r_{\mathrm{per,xc}}(z)^2]. \tag{5.344}$$

Thus, we see that (5.340) is bounded by

$$\delta^{3/2}\|W_\delta\|_{L^3}\|\phi\|_{L^6} \tag{5.345}$$

By Hardy's inequality, (5.340) is bounded by

$$\delta^{3/2}\|W_\delta\|_{L^3}\|\nabla\phi\|_{L^2}. \tag{5.346}$$

By Kato-Seiler-Simon's inequality ((4.12)), this translates to a bound of

$$\lesssim \delta^{3/2}\|\mathrm{xc}'\|_{L^\infty}\|\kappa'(\delta x)\|_{L^3}\|\nabla\varphi\|_{L^2} \tag{5.347}$$

$$\leq \delta\|\mathrm{xc}'\|_{L^\infty}\|\kappa'\|_{L^3}\|\nabla\varphi\|_{L^2} \tag{5.348}$$

for (5.340). By Young's inequality for products, we see that

$$|\nabla| \lesssim \delta^\alpha + \delta^{-\alpha}|\nabla|^2. \tag{5.349}$$

for any $\alpha > 0$. Combining with (5.348), we see that

$$\|(5.340)\|_{L^2} \lesssim \delta^{1+\alpha}\|\mathrm{xc}'\|_{L^\infty}\|\varphi\|_{L^2} + \|\mathrm{xc}'\|_{L^\infty}\delta^{1-\alpha}\|\Delta\varphi\|_{L^2} \tag{5.350}$$

Combining with (5.339) and (5.342), we see

$$\|YG_{\kappa'}\|_{L^2} \lesssim \delta^{1+\alpha}\|\mathrm{xc}'\|_{L^\infty}\|\varphi\|_{L^2} + \|\mathrm{xc}'\|_{L^\infty}\delta^{1-\alpha}\|\Delta\varphi\|_{L^2} \tag{5.351}$$

By choosing α such that $\delta^\alpha = \delta^{-1}\|V\|^{1/2}_{L^1_{\mathrm{per}}}$ and using [A6], we obtain

$$\|YG_{\kappa'}\|_{L^2} \ll \|(\delta^{-2}\|V\|_{L^1_{\mathrm{per}}} - \Delta)\varphi\|_{L^2}. \tag{5.352}$$

Next, we estimate the second term in (5.334). By (5.329) and (5.330), we see that the last term in (5.334) can be estimated as

$$\|M_{\mathrm{per},\delta}(G'_\kappa - G_{\mathrm{per}})\|_{L^2} \tag{5.353}$$

$$\lesssim \|M_{\mathrm{per},\delta}\|_\infty\|\mathrm{xc}(\delta^3(\rho^\delta_{\mathrm{per}} + \kappa')) - \mathrm{xc}(\delta^3\rho^\delta_{\mathrm{per}})\|_{L^\infty}\|\delta^2\Delta\varphi\|_{L^2} \tag{5.354}$$

$$\lesssim \delta^3\|\Delta\varphi\|_{L^2}. \tag{5.355}$$

since $\|M_{\mathrm{per},\delta}\|_\infty \lesssim \delta^{-2}$ by Proposition 17.

Collecting the terms (5.342), (5.352), and (5.355) proves (5.292). Proposition 39 is now proved. □

Proof of Proposition 41. We follow the proof of Proposition 22. The proof of this proposition is based on a linear (analogous to Lemma B.1 in the xc = 0 case) and a nonlinear estimate. We omit the proof for the nonlinear estimate and refer to Lemma 44 for the main ideas. The linear estimate is produced below in Lemma 45. To avoid the small, but cumbersome, $C_\beta e^{-\beta\eta(\mathbb{R}^3)}$ terms, they are not displayed below. □

Lemma 45 (Analogue of Lemma B.1)**.** *Let Assumptions [A1] - [A6] hold. Let $s = 0, 1$, or 2. Then*

$$\||\Delta|^{s/2}\ell^{-1}\ell'\ell_0^{-1}f\|_{L^2} \lesssim \delta^2\||\Delta|^{s/2}f\|_{L^2} \tag{5.356}$$

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

$$\|\ell^{-1}P_r\tilde{M}_\delta\overline{\tilde{K}_\delta}^{-1}f\|_{L^2} \lesssim \delta^2\|V\|_{L^1_{\mathrm{per}}}^{-1/2}\|f\|_{L^2} \tag{5.357}$$

$$\|\nabla\ell^{-1}P_r\tilde{M}_\delta\overline{\tilde{K}_\delta}^{-1}f\|_{L^2} \lesssim a^{-2}\delta\|f\|_{L^2} \tag{5.358}$$

$$\|\nabla^2\ell^{-1}P_r\tilde{M}_\delta\overline{\tilde{K}_\delta}^{-1}f\|_{L^2} \lesssim a^{-2}\|f\|_{L^2}\,. \tag{5.359}$$

where a is given in (5.40)*.*

Proof. We will only estimate the $\dot{H}^s$ case for $s = 2$. The cases for $s = 0, 1$ are similar to the ones in Lemma 47. By Lemma 40 and Proposition 39, we compute

$$\begin{aligned} \|\nabla^2\ell^{-1}\ell'\ell_0^{-1}f\|_{L^2} &\lesssim \|\ell'\ell_0^{-1}f\|_{L^2} && (5.360)\\ &\lesssim \delta^2\|\nabla^4\ell_0^{-1}f\|_{L^2} && (5.361)\\ &\lesssim \delta^2\|\nabla^2 f\|_{L^2} && (5.362) \end{aligned}$$

This proves (5.356). Now we prove (5.359), by Lemma 40 once more,

$$\|\nabla^2\ell^{-1}P_r\tilde{M}_\delta\overline{\tilde{K}_\delta}^{-1}f\|_{L^2} \lesssim \|P_r\tilde{M}_\delta\overline{\tilde{K}_\delta}^{-1}f\|_{L^2}. \tag{5.363}$$

Recall that (a slight modification of) Proposition (17) shows that $\|\tilde{M}_\delta\|_\infty \lesssim \delta^{-2}$. Thus, by definition of P_r in (5.40), Lemma 42, and (5.363), Lemma 45 is proved. □

Appendix A

$\epsilon(T) \to \epsilon(0)$ as $T \to 0$

Lemma 46. *Let $xc = 0$. Then $\epsilon(T) \to \epsilon(0)$ as $T \to 0$, where $\epsilon(0)$ is the dielectric constant for $T = 0$ obtained in [10].*

Proof. We see from (5.63) below that ϵ is of the form

$$\epsilon(T) = \epsilon(\beta) = \frac{1}{2\pi i} \int_{\Gamma} f_{\mathrm{FD}}(\beta(z-\mu))X(z) \tag{A.1}$$

where $X(z)$ is some holomorphic function on $\mathbb{C}\backslash\mathbb{R}$, independent of β, and remains holomorphic on the real axis where the gap of h_{per} occurs. On $\mathbb{R}$, we note that $f_{\mathrm{FD}}(\beta x)$ converges to the indicator function $\chi_{(-\infty,0)}$ as $\beta \to \infty$. If we take $\beta \to \infty$, the integral

$$\frac{1}{2\pi i} \int_{\Gamma} f_{\mathrm{FD}}(\beta(z-\mu))X(z) \tag{A.2}$$

converges to $\frac{1}{2\pi i}\int_{G_1} X(z)$ where G_1 is any contour around the part of the spectrum of h_{per} that is less than μ_{per}. This is the same expression as in [10] after inserting $1 = \sum_i |\varphi_i\rangle\langle\varphi_i|$ for each resolvent of h_{per} in $X(z)$ where the φ_i's are eigenvectors of h_{per}. $\square$

Appendix B

Estimates for Propositions 20 and 22

B.1 Linear estimates

Let the linear operators ℓ, ℓ_0, ℓ' be given in (5.59), (5.114), and (5.192) respectively. Moreover, recall the definitions of M_δ, K_δ, V, and P_r from (5.34), (5.34), (5.50), and (5.39) respectively. For any $s \in \mathbb{Z} \geq 0$, we denote ∇^s any product of partial derivatives of the total order s.

Lemma 47. *Let Assumptions [A1] - [A4] hold. Then*

$$|\Delta|^{s/2}\ell^{-1}\ell'\ell_0^{-1} \lesssim \delta^2|\Delta|^{s/2} \tag{B.1}$$

for any $s \in \mathbb{Z} \geq 0$. Moreover, for any $f \in L^2(\mathbb{R}^3)$,

$$\|\ell^{-1}P_r M_\delta \bar{K}_\delta^{-1} f\|_{L^2} \lesssim a^{-2}\delta^2\|V\|_1^{-1/2}\|f\|_{L^2}, \tag{B.2}$$

$$\|\nabla\ell^{-1}P_r M_\delta \bar{K}_\delta^{-1} f\|_{L^2} \lesssim a^{-2}\delta\|f\|_{L^2}\,. \tag{B.3}$$

Proof. Using Lemma 33, we see that, for $s \in \mathbb{Z} \geq 0$,

$$\begin{aligned} &|\Delta|^{s/2}\ell^{-1}\ell'\ell_0^{-1} \\ \lesssim &|\Delta|^{s/2}\frac{1}{-\Delta+\delta^{-2}\|V\|_{L^1}}\delta^2\Delta^2\frac{1}{-\Delta+\delta^{-2}\|V\|_{L^1}} && \text{(B.4)} \\ \lesssim &\delta^2|\Delta|^{s/2} && \text{(B.5)} \end{aligned}$$

Next, using $M_\delta = M_0 + M'_\delta$ (see (5.151) and (5.152)),

$$\begin{aligned} &|\Delta|^{s/2}\ell^{-1}P_r M_\delta \bar{K}_\delta^{-1} \\ &\quad = |\Delta|^{s/2}\ell^{-1}P_r M_0 \bar{K}_\delta^{-1} + |\Delta|^{s/2}\ell^{-1}P_r M'_\delta \bar{K}_\delta^{-1} && \text{(B.6)} \end{aligned}$$

for $s \geq 0$. By Lemma 33, we further note that

$$\begin{aligned} \ell^{-1} \lesssim &\frac{1}{\delta^{-2}\|V\|_{L^1_{\text{per}}} - \Delta} \\ \lesssim &\delta^2\|V\|_{L^1_{\text{per}}}^{-1} \text{ or } (\delta^2\|V\|_{L^1_{\text{per}}}^{-1})^{1/2}|\Delta|^{-1/2} && \text{(B.7)} \\ \nabla\ell^{-1} \lesssim &\frac{\nabla}{\delta^{-2}\|V\|_{L^1_{\text{per}}} - \Delta} \lesssim (\delta^2\|V\|_{L^1_{\text{per}}}^{-1})^{1/2} \text{ or } |\Delta|^{-1/2}\,. && \text{(B.8)} \end{aligned}$$

Let ∇^{-1} given in (5.128). Combining (B.7) and (B.8) with Lemma 30, by Proposition 19 and the choice of $\bar{P}_r$ in (5.41), we see that

$$\begin{aligned} &\||\Delta|^{s/2}\ell^{-1}P_r M_0 \bar{K}_\delta^{-1}\|_\infty \\ \leq &\||\Delta|^{s/2}\ell^{-1}\|_\infty \|P_r M_0 \nabla^{-1}\bar{P}_r\|_\infty \|\nabla \bar{K}_\delta^{-1}\nabla\|_\infty \|\bar{P}_r \nabla^{-1}\|_\infty && \text{(B.9)} \\ \lesssim &(\delta^2\|V\|_{L^1_{\text{per}}}^{-1})^{1-s/2} \cdot \delta^{-1}a^{-1}\|V\|_{L^2_{\text{per}}} \cdot 1 \cdot r^{-1} && \text{(B.10)} \\ = &\delta^{-s}r^{-2}\|V\|_{L^1_{\text{per}}}^{-1+s/2}\|V\|_{L^2_{\text{per}}}, && \text{(B.11)} \end{aligned}$$

where we used $a = \delta r$ (see (5.40)) to obtain (B.11). Similarly as the estimate for (B.11), but using Lemma 32 instead of Lemma 30, we see that

$$\begin{aligned} &\||\Delta|^{s/2}\ell^{-1}P_r M'_\delta \bar{K}_\delta^{-1}\|_\infty \\ \leq &\||\Delta|^{s/2}\ell^{-1}\nabla\|_\infty \|\nabla^{-1}P_r M'_\delta \nabla^{-1}\bar{P}_r\|_\infty \|\nabla \bar{K}_\delta^{-1}\nabla\|_\infty \|\bar{P}_r \nabla^{-1}\|_\infty && \text{(B.12)} \\ \lesssim &(\delta^2\|V\|_{L^1_{\text{per}}}^{-1})^{1/2-s/2} \cdot a^{-1} \cdot 1 \cdot r^{-1} && \text{(B.13)} \\ = &\delta^{-s}r^{-2}\|V\|_{L^1_{\text{per}}}^{-1/2+s/2}, && \text{(B.14)} \end{aligned}$$

where we used $a = \delta r$ in the last line. Applying (B.11) and (B.14) to (B.6), we see that

$$\begin{aligned}
&\|\ell^{-1} P_r M_\delta \bar{K}_\delta^{-1} f\|_{L^2} && \text{(B.15)}\\
\lesssim&(\|V\|_{L^1_{\text{per}}}^{-1/2}\|V\|_{L^2_{\text{per}}} r^{-2} + r^{-2})\|V\|_{L^1_{\text{per}}}^{-1/2}\|f\|_{L^2} && \text{(B.16)}\\
\lesssim&r^{-2}\|V\|_{L^1_{\text{per}}}^{-1/2}\|f\|_{L^2} && \text{(B.17)}
\end{aligned}$$

where the last line follows since $\|V\|_{L^1_{\text{per}}}^{-1/2}\|V\|_{L^2_{\text{per}}} \ll 1$ by Lemma 56 and 59. Similarly,

$$\begin{aligned}
&\|\nabla \ell^{-1} P_r M_\delta \bar{K}_\delta^{-1} f\|_{L^2} && \text{(B.18)}\\
\lesssim&(\|V\|_{L^1_{\text{per}}}^{-1/2}\|V\|_{L^2_{\text{per}}} \delta^{-1} r^{-2} + \delta^{-1} r^{-2})\|f\|_{L^2} && \text{(B.19)}\\
\lesssim&\delta^{-1} r^{-2}\|f\|_{L^2}\,. && \text{(B.20)}
\end{aligned}$$

This proves (B.2) and (B.3) and Lemma 47 is proved. □

B.2 Nonlinear Estimates

Let N_δ be given implicitly through (5.33) and recall the definition of the $B_{s,\delta}$ norm from (5.49). Let $\dot{H}^0 \equiv L^2$. We have the following estimates on N_δ.

Proposition 48. *Let Assumptions [A1] - [A4] hold. If* $\|\varphi_1\|_{B_{s,\delta}}, \|\varphi_2\|_{B_{s,\delta}} = o(\delta^{-1/2})$, *then we have the estimate*

$$\begin{aligned}
&\|N_\delta(\varphi_1) - N_\delta(\varphi_2)\|_{L^2}\\
&\qquad\lesssim \delta^{-1/2}(\|\varphi_1\|_{B_{s,\delta}} + \|\varphi_2\|_{B_{s,\delta}})\|\varphi_1 - \varphi_2\|_{\dot{H}^1}, && \text{(B.21)}\\
&\|N_\delta(\varphi_1) - N_\delta(\varphi_2)\|_{\dot{H}^{-1}}\\
&\qquad\lesssim \delta^{1/2}(\|\varphi_1\|_{B_{s,\delta}} + \|\varphi_2\|_{B_{s,\delta}})\|\varphi_1 - \varphi_2\|_{B_{s,\delta}}. && \text{(B.22)}
\end{aligned}$$

We prove a version of Proposition 48 with $\delta = 1$ first. Then we prove the full proposition at the end of the subsection by rescaling the obtained estimates. Let $N(\varphi) = N_{\delta=1}(\varphi)$. We have the following result.

Proposition 49. *Let Assumptions [A1] - [A4] hold. If* $\|\phi_1\|_{\dot{H}^1}, \|\phi_2\|_{\dot{H}^1} = o(1)$, *then we* *have the estimates, with* $k = 1, 2$,

$$\begin{aligned}
&\|N(\phi_1) - N(\phi_2)\|_{\dot{H}^{1-k}} \\
&\lesssim (\|\phi_1\|_{\dot{H}^1} + \|\phi_2\|_{\dot{H}^1})\|\phi_1 - \phi_2\|_{\dot{H}^1} \\
&+ C_{k,\beta}(\|\phi_1\|_{\dot{H}^1}^{1/3}\|\phi_1\|_{L^2}^{2/3} + \|\phi_2\|_{\dot{H}^1}^{1/3}\|\phi_2\|_{L^2}^{2/3})\|\phi_1 - \phi_2\|_{L^2} \\
&+ C_{k+1,\beta}(\|\phi_1\|_{\dot{H}^1}\|\phi_1\|_{L^2} + \|\phi_2\|_{\dot{H}^1}\|\phi_2\|_{L^2})\|\phi_1 - \phi_2\|_{\dot{H}^1}, \qquad \text{(B.23)}
\end{aligned}$$

where the constants $C_{j,\beta}$, $j = 1, 2, 3$, *depend only on* β *and are defined explicitly in* (B.34) - (B.36).

Proof of Proposition 49. Let h_{per} and $r_{\text{per}}(z)$ be given in (5.8). First we observe that the definition (5.33) implies

$$N(\phi) := \text{den}[\tilde{N}_2(\phi)] \qquad \text{(B.24)}$$

where

$$\tilde{N}_k(\phi) := \oint (z - h_{\text{per}} + \phi)^{-1}[(-\phi)r_{\text{per}}(z)]^k. \qquad \text{(B.25)}$$

By the resolvent expansion

$$\begin{aligned}
(z - h_{\text{per}} + \phi)^{-1} =& (z - h_{\text{per}})^{-1}[(-\phi)r_{\text{per}}(z)]^m \\
&+ \sum_{k=2}^{m-1} (z - h_{\text{per}} + \phi)^{-1}[(-\phi)r_{\text{per}}(z)]^k \qquad \text{(B.26)}
\end{aligned}$$

for any $m \geq 1$, we see that

$$N(\phi) = \text{den}[\tilde{N}_m(\phi)] + \sum_{k=2}^{m-1} \text{den}[N_k(\phi)], \qquad \text{(B.27)}$$

for any $m \geq 2$, where

$$N_k(\phi) := \oint r_{\text{per}}(z)[(-\phi)r_{\text{per}}(z)]^k. \qquad \text{(B.28)}$$

To estimate N_k, we will use the Schatten norm I^p (see (4.4)). In the special case

$p = \infty$, we denote $\|\cdot\|_{I^\infty}$ to be the operator norm $\|\cdot\|_\infty$. Let

$$P_- = \chi_{h_{\mathrm{per}}<\mu} \text{ and } P_+ = \chi_{h_{\mathrm{per}}\geq\mu} = 1 - P_-, \tag{B.29}$$

We start with the following lemma.

Lemma 50. *Let Assumptions [A1] - [A4] hold, we have the estimate*

$$\|[P_\pm, \phi]\|_{I^2} \lesssim \|\nabla\phi\|_{L^2}. \tag{B.30}$$

Proof of Lemma 50. Since the identity commutes with any operator and $P_+ = 1 - P_-$ (see (B.29)), we prove the lemma for P_- only. Since h_{per} (see (5.8)) has a gap at μ by [A3], the Cauchy integral formula implies

$$P_- = \frac{1}{2\pi i}\int_{\Gamma_1}(z - h_{\mathrm{per}})^{-1} = \frac{1}{2\pi i}\int_{\Gamma_1} r_{\mathrm{per}}(z) \tag{B.31}$$

where Γ_1 is the contour $\{t+i; -c \leq t < \mu\} \cup \{t-i; -c \leq t < \mu\} \cup \{-c - it + (1-t)i : t \in [0,1]\} \cup \{\mu - it + (1-t)i : t \in [0,1]\}$, where $c > 0$ is any constant such that $h_{\mathrm{per}} > -c+1$, and the contour is traversed counter-clock-wise. We see that

$$[P_-, \varphi] = \frac{1}{2\pi i}\int_{\Gamma_1}[r_{\mathrm{per}}(z), \varphi] \tag{B.32}$$

$$= \frac{1}{2\pi i}\int_{\Gamma_1} r_{\mathrm{per}}(z)[\nabla\cdot, \nabla\varphi]r_{\mathrm{per}}(z) + \frac{1}{2\pi i}\int_{\Gamma_1} r_{\mathrm{per}}(z)(2\nabla\varphi\cdot\nabla)r_{\mathrm{per}}(z). \tag{B.33}$$

Lemma 50 is now proved by an application of the Kato-Seiler-Simon inequality ((4.12)) to (B.33) and noting that Γ_1 is compact and has length $O(1)$. $\square$

We define explicit constants appearing in estimates below:

$$C_{1,\beta} = \sup_{f,g,h,*=\pm} \frac{\oint \mathrm{Tr}[fRP_*gRP_*hP_*R]}{\|f\|_{L^2}\|\nabla g\|_{L^2}^{4/3}\|h\|_{L^2}^{2/3}} \tag{B.34}$$

$$C_{2,\beta} = \sup_{f,g,h,*=\pm} \frac{\oint \mathrm{Tr}[fRP_*gRP_*hP_*R]}{\|\nabla f\|_{L^2}\|g\|_{L^2}^{5/3}\|\nabla h\|_{L^2}^{1/3}} \tag{B.35}$$

$$C_{3,\beta} = \sup_{f,g,h,u,*=\pm} \frac{\oint \mathrm{Tr}[fRP_*gRP_*hP_*RuRP_*]}{\|\nabla f\|_{L^2}\|\nabla g\|_{L^2}\|\nabla h\|_{L^2}\|u\|_{L^2}} \tag{B.36}$$

$$C_{4,\beta} = \sup_{f,g,h,u,v,*=\pm} \frac{\oint \mathrm{Tr}[fRP_*gRP_*hP_*RuRP_*RP_*v]}{\|\nabla f\|_{L^2}\|\nabla g\|_{L^2}\|\nabla h\|_{L^2}\|\nabla u\|_{L^2}\|v\|_{L^2}} \tag{B.37}$$

where the sup is taken over all possible f, g, h, u, v such that the denominators are finite, $R = r_{\mathrm{per}}(z)$ is given in (5.8), and the subscript $*$ in P_* is equal to $+$ or $-$ and the choice of $\pm$ remains constant through out each expression (the projections $P_\pm$ are given in (B.29)).

Motivated by Lemma 50, we estimate the leading term $\mathrm{den}[N_2(\phi)]$ from (B.27) below.

Lemma 51. *Let Assumptions [A1] - [A4] hold and let N_2 be given by* (B.28)*. Assume that $\|\nabla\phi\|_{L^2} = o(1)$, then we have the estimate*

$$\begin{aligned}&\|\,\mathrm{den}[N_2(\phi)]\|_{\dot{H}^{1-k}} \\ &\quad\lesssim \|\nabla\phi\|_{L^2}^2 + C_{k,\beta}\|\nabla\phi\|_{L^2}^{1/3}\|\phi\|_{L^2}^{5/3}, k = 1, 2,\end{aligned} \tag{B.38}$$

where the constants associated with $\lesssim$ are independent of β and the constants $C_{1,\beta}$ and $C_{2,\beta}$ are defined in (B.34) *and* (B.35).

Proof. We follow [11]. Let $R_\pm = r_{\mathrm{per}}(z)P_\pm$ where $P_\pm$ are given in (B.29) and $r_{\mathrm{per}}(z)$ be given by (5.8). For $a, b, c \in \{-, +\}$, we denote $N_2^{abc}(\phi)$ as

$$N_2^{abc}(\phi) = \oint R_a\phi R_b\phi R_c\,. \tag{B.39}$$

Since $P_- + P_+ = 1$ is the identity operator on $L^2(\mathbb{R}^3)$, we see that

$$N_2(\phi) = \sum_{a,b,c=+,-} N_2^{abc}(\phi)\,. \tag{B.40}$$

We estimate the terms individually.

Case 1: $-+-$ and $+-+$. We estimate the case for $-+-$, the other case is done similarly. Since $P_-P_+=0$, we write

$$N_2^{-+-}(\phi) = \oint R_-\phi R_+P_+\phi R_- \tag{B.41}$$
$$= \oint R_-[P_-,\phi]P_+R_+P_+[\phi,P_-]R_- \,. \tag{B.42}$$

By Lemmas 9 and equation (5.5), the explicit form of $N_2^{-+-}(\phi)$ in (B.42) shows

$$\|\operatorname{den}[N_2^{-+-}(\phi)]\|_{L^2} \lesssim \|(1-\Delta)^{3/4+\epsilon}N_2^{-+-}(\phi)\|_{I^2} \tag{B.43}$$
$$\lesssim \left|\oint\right| \|[P_-,\phi]P_+\|_{I^2}\|[P_-,\phi]P_+\|_{I^\infty}. \tag{B.44}$$

where recall

$$\left|\oint\right| := \frac{1}{2\pi}\int_\Gamma dz |f_{\mathrm{FD}}(\beta(z-\mu))|. \tag{B.45}$$

Since the operator norm is bounded by the I^2 norm, Lemma 50 and (B.44) show that

$$\|\operatorname{den}[N_2^{-+-}(\phi)]\|_{L^2} \lesssim \left|\oint\right| \|[P_-,\phi]P_+\|_{I^2}^2 \lesssim \|\nabla\phi\|_{L^2}^2 \,. \tag{B.46}$$

Similarly, using that $\|A\|_{I^{6/5}} \leq \|A\|_{I^1}$ for any operator A on $L^2(\mathbb{R}^3)$, Lemma 9 and equation (5.5), we see that

$$\|\operatorname{den}[N_2^{-+-}(\phi)]\|_{\dot{H}^{-1}} \lesssim \|(1-\Delta)^{1/2+\epsilon}N_2^{-+-}(\phi)\|_{I^{6/5}} \tag{B.47}$$
$$\lesssim \|(1-\Delta)^{1/2+\epsilon}N_2^{-+-}(\phi)\|_{I^1}. \tag{B.48}$$

Now, applying the non-abelian Hölder inequality with $1=\frac{1}{2}+\frac{1}{2}$ to (B.48), and using the explicit form (B.42) for N^{-+-}, we see that

$$\|\operatorname{den}[N_2^{-+-}(\phi)]\|_{\dot{H}^{-1}} \lesssim \left|\oint\right| \|[P_-,\phi]P_+\|_{I^2}^2 \lesssim \|\nabla\phi\|_{L^2}^2 \,. \tag{B.49}$$

By Lemmas 50, (5.6), (5.5), and (B.49) can be bounded as

$$\|\operatorname{den}[N_2^{-+-}(\phi)]\|_{\dot{H}^{-1}} \lesssim \|\nabla\phi\|_{L^2}^2 \,. \tag{B.50}$$

Case 2: $--+, +--, -++,$ **and** $++-$**.** We estimate the case for $--+$, the other cases are done similarly. Again, since $P_-P_+ = 0$, we write

$$N_2^{--+}(\phi) = \oint R_-\phi R_-\phi R_+ \tag{B.51}$$

$$= \oint R_-\phi R_-[\phi, P_-]R_+ \,. \tag{B.52}$$

We estimate the L^2 norm of $\mathrm{den}[N_2^{--+}(\phi)]$ first. By Lemma 9, (B.52) shows that

$$\| \mathrm{den}[N_2^{--+}(\phi)]\|_{L^2} \lesssim \left|\oint\right| \|\phi R_-\|_\infty \|[\phi, P_-]P_+\|_{I^2}. \tag{B.53}$$

where $\left|\oint\right|$ is defined in (B.45). By Lemma 50 and the fact $\|A\|_\infty \leq \|A\|_{I^p}$ for any $p \leq \infty$ for any operator A on $L^2(\mathbb{R}^3)$, equation (B.53) shows that

$$\| \mathrm{den}[N_2^{--+}(\phi)]\|_{L^2} \lesssim \left|\oint\right| \|R_-\phi\|_{I^6} \|\nabla\phi\|_{L^2}, \tag{B.54}$$

By the Kato-Seiler-Simon inequality (4.12) and (5.5), equation (B.54) becomes

$$\| \mathrm{den}[N_2^{--+}(\phi)]\|_{L^2} \lesssim \|\phi\|_{L^6} \|\nabla\phi\|_{L^2}. \tag{B.55}$$

Combining with Hardy-Littlewood's inequality (4.16), (B.55) gives

$$\| \mathrm{den}[N_2^{--+}(\phi)]\|_{L^2} \lesssim \|\nabla\phi\|^2_{L^2}. \tag{B.56}$$

To estimate the $\dot{H}^{-1}$ norm of $\mathrm{den}[N_2^{--+}(\phi)]$, we use H^1-H^{-1} duality. Using (4.1), we see that

$$\| \mathrm{den}[N_2^{--+}(\phi)]\|_{\dot{H}^{-1}} \tag{B.57}$$

$$= \sup_{f\in\dot{H}^1(\mathbb{R}^3), \|f\|_{\dot{H}^1}=1} \langle \mathrm{den}[N_2^{--+}(\phi)], f\rangle \tag{B.58}$$

$$= \sup_{f\in\dot{H}^1(\mathbb{R}^3), \|f\|_{\dot{H}^1}=1} \oint \mathrm{Tr}(R_-\phi R_-[\phi, P_-]R_+ f) \tag{B.59}$$

$$= \sup_{f\in\dot{H}^1(\mathbb{R}^3), \|f\|_{\dot{H}^1}=1} \oint \mathrm{Tr}(R_-\phi R_-[\phi, P_-]R_+[f, P_-]) \tag{B.60}$$

where the last line follows by the cyclicity of trace. Using the non-abelian Hölder's inequality with $1 = \frac{1}{\infty} + \frac{1}{2} + \frac{1}{2}$, we see that (B.60) gives

$$\begin{aligned} &\| \operatorname{den}[N_2^{--+}(\phi)]\|_{\dot{H}^{-1}} \\ &\leq \sup_{f\in \dot{H}^1, \|f\|_{\dot{H}^1}=1} \left|\oint\right| \|R_-\phi\|_\infty \|[\phi, P_-]\|_{I^2}\|[f, P_-]\|_{I^2}. \end{aligned} \tag{B.61}$$

where $\left|\oint\right|$ is defined in (B.45). Since $\|A\|_\infty \leq \|A\|_{I^p}$ for any $p \leq \infty$ and any operator A on $L^2(\mathbb{R}^3)$, we bound (B.61) as

$$\begin{aligned} &\| \operatorname{den}[N_2^{--+}(\phi)]\|_{\dot{H}^{-1}} \\ &\leq \sup_{f\in \dot{H}^1, \|f\|_{\dot{H}^1}=1} \left|\oint\right| \|R_-\phi\|_{I^6} \|[\phi, P_-]\|_{I^2}\|[f, P_-]\|_{I^2}. \end{aligned} \tag{B.62}$$

Applying Lemma 50, and (5.5), Kato-Seiler-Simon's inequality (4.12), and Hardy-Littlewood's inequality (4.16) to equation (B.62), we obtain

$$\| \operatorname{den}[N_2^{--+}(\phi)]\|_{\dot{H}^{-1}} \lesssim \|\nabla\phi\|_{L^2}^2. \tag{B.63}$$

Case 3: $---$ and $+++$. We prove the case for $---$ only and the other case is similar.

For the $\dot{H}^1$ norm estimate of $\operatorname{den}[N_2^{---}(\phi)]$, we use the $\dot{H}^1$-$\dot{H}^{-1}$ duality. Using the Hölder's inequality with $1 = \frac{1}{6} + \frac{1}{2} + \frac{1}{3}$, we see that, for any $f \in \dot{H}^1$,

$$\left|\oint \operatorname{Tr}(fR_-\phi R_-\phi R_-)\right| \lesssim \left|\oint\right| \|fR_-\|_{I^6}\|R_-\phi\|_{I^2}\|R_-\phi\|_{I^3} \tag{B.64}$$

where $\left|\oint\right|$ is given in (5.5). For any operator A on $L^2(\mathbb{R}^3)$, we note that

$$\|A\|_{I^3}^3 = \operatorname{Tr}(|A|^3) \leq \|A\|_\infty \operatorname{Tr}(|A|^2) = \|A\|_\infty\|A\|_{I^2}^2. \tag{B.65}$$

Applying (B.65) to $\|R_-\phi\|_{I^3}$ in (B.64), using Kato-Seiler-Simon's inequality (4.12), Lemma

50, and (5.5), equation (B.64) is bounded as

$$\left|\oint \mathrm{Tr}(fR_-\phi R_-\phi R_-)\right| \tag{B.66}$$

$$\lesssim \left|\oint\right| \|f\|_{L^6}\|\phi\|_{L^2}\|R_-\phi\|_{I^2}^{2/3}\|R_-\phi\|_{\infty}^{1/3} \tag{B.67}$$

$$\lesssim \|\nabla f\|_2\|\phi\|_{L^2}^{5/3}\|\nabla\phi\|_{L^2}^{1/3}\,. \tag{B.68}$$

Similarly, we use the L^2-L^2 duality to estimate the L^2 norm of $\mathrm{den}[N_2^{---}(\phi)]$. Let $f \in L^2$. Using the non-abelian Hölder's inequality $1 = \frac{1}{2}+\frac{1}{6}+\frac{1}{3}$, (5.5), and (5.6), we see that

$$|\mathrm{Tr}(fR_-\phi R_-\phi R_-)| \lesssim \|fR_-\|_{I^2}\|\phi R_-\|_{I^6}\|\phi R_-\|_{I^3}\,. \tag{B.69}$$

Using (B.65), Kato-Seiler-Simon's inequality (4.12), and Hardy-Littlewood's inequality (4.16), equation (B.69) shows

$$|\mathrm{Tr}(fR_-\phi R_-\phi R_-)| \lesssim \|f\|_{L^2}\|\nabla\phi\|_{L^2}^{4/3}\|\phi R_-\|_{L^2}^{2/3}\,. \tag{B.70}$$

By the L^2-L^2 and H^1-H^{-1} duality, we see that

$$\|\,\mathrm{den}[N_2^{---}(\phi)]\|_{L^2} \lesssim C_{1,\beta}\|\nabla\phi\|_{L^2}^{4/3}\|\phi\|_{L^2}^{2/3} \tag{B.71}$$

$$\|\,\mathrm{den}[N_2^{--+}(\phi)]\|_{\dot H^{-1}} \lesssim C_{2,\beta}\|\nabla\phi\|_{L^2}^{1/3}\|\phi\|_{L^2}^{5/3} \tag{B.72}$$

Equations (B.38) and (B.38) are proved by inequalities (B.46), (B.50), (B.56), (B.63), (B.71), and (B.72). The proof for Lemma 51 is now complete. □

Now we estimate the higher order N_k's in the expression (B.27) for the nonlinearity $N(\phi)$.

Lemma 52. *Let Assumptions [A1] - [A4] hold and let N_k be given by* (B.28)*, then*

$$\|\,\mathrm{den}[N_k(\phi)]\|_{L^2} \lesssim \|\nabla\phi\|_{L^2}^{k} \tag{B.73}$$

for $k \geq 3$.

Proof. By (5.5) and (5.6), it suffices to estimate $\mathrm{den}[R(\phi R)^k]$ where $R = r_{\mathrm{per}}(z)$ is given in (5.8). Using Lemma 9, we see that

$$\|\,\mathrm{den}[R(\phi R)^k]\|_{L^2} \lesssim \|(1-\Delta)^{4/3+\epsilon} R(\phi R)^k\|_{I^2} \tag{B.74}$$

$$\lesssim \|(\phi R)^k\|_{I^2} \tag{B.75}$$

Using Hölder's inequality with $\frac{1}{2} = \frac{1}{6} + \frac{1}{6} + \frac{1}{6} +$ another k terms of $\frac{1}{\infty}$, (B.75) becomes

$$\|\,\mathrm{den}[R(\phi R)^k]\|_{L^2} \leq \|\phi R\|_{I^6}^3 \|\phi R\|_{\infty}^{k-3} \tag{B.76}$$

$$\leq \|\phi R\|_{I^6}^k, \tag{B.77}$$

where the last line follows since $\|\cdot\|_\infty \leq \|\cdot\|_{I^p}$ for $p \leq \infty$. Combining with Kato-Seiler-Simon's inequality (4.12) and Hardy-Littlewood's inequality (4.16), (B.77) implies (B.73). □

Lemma 53. *Let Assumptions [A1] - [A4] hold and let N_k be given by* (B.28)*, then*

$$\|\,\mathrm{den}[N_k(\phi)]\|_{\dot{H}^{-1}} \lesssim \|\nabla\phi\|_{L^2}^k + C_{k,\beta}\|\nabla\phi\|_{L^2}^k \|\phi\|_{L^2} \tag{B.78}$$

for $k = 3, 4$, where $C_{3,\beta}$ and $C_{4,\beta}$ has explicit forms in (B.36) *and* (B.37) *respectively. Moreover, for $k \geq 5$,*

$$\|\,\mathrm{den}[N_k(\phi)]\|_{\dot{H}^{-1}} \lesssim \|\nabla\phi\|_{L^2}^k \tag{B.79}$$

Proof. The case where $k \geq 5$ follows by the same argument as in Lemma 52. The case where $k = 3, 4$ follows the same argument as Lemma 51 by dividing $N_k(\phi)$ into P_- and P_+ parts. □

Now, we complete the Proof of Proposition 48. Lemmas 52 and 53 show that if $\|\phi\|_{L^2} < \infty$ and $\|\nabla\phi\|_{L^2} = o(1)$, then

$$N(\phi) = \sum_{k\geq 2} \mathrm{den}[N_k(\phi)] \tag{B.80}$$

where N_k is given in (B.28). For ϕ_1 and ϕ_2, we see that

$$N(\phi_1) - N(\phi_2) = \sum_{k\geq 2} \mathrm{den}[N_k(\phi_1) - N_k(\phi_2)]\,. \tag{B.81}$$

Note that $N_k(\phi)$ is an k-th order monomial in ϕ:

$$N_k(\phi) = \mathrm{den} \oint (r_{\mathrm{per}}(z)\phi)^k r_{\mathrm{per}}(z). \tag{B.82}$$

We can expand $N_k(\phi_1) - N_k(\phi_2)$ in the following telescoping form

$$x^k - y^k \tag{B.83}$$

$$= x^{k-1}(x-y) + x^{k-2}(x-y)y + \cdots + (x-y)y^k\,. \tag{B.84}$$

The proof of Proposition 49 is complete by applying Lemmas 51, 52, and 53 on each term in the expansion of $N_k(\phi_1) - N_k(\phi_2)$ given in (B.84). □

Proof of Proposition 48. By (5.35), N_δ and the unscaled nonlinearity $N = N_{\delta=1}$ are related via

$$N_\delta(\varphi) = \delta^{-3/2} U_\delta N(\phi) \tag{B.85}$$

where U_δ is given in (4.43) and

$$\phi = \delta^{-1/2} U_\delta^* \varphi. \tag{B.86}$$

We first observe that

$$\begin{aligned}
&\|N_\delta(\varphi_1) - N_\delta(\varphi_2)\|_{L^2} \\
&\quad \lesssim \delta^{-1/2}(\|\varphi_1\|_{\dot H^1} + \|\varphi_2\|_{\dot H^1})\|\varphi_1 - \varphi_2\|_{\dot H^1} \\
&\quad + \delta^{-7/6} C_{1,\beta}(\|\varphi_1\|_{\dot H^1}^{1/3}\|\varphi_1\|_{L^2}^{2/3} + \|\varphi_2\|_{\dot H^1}^{1/3}\|\varphi_2\|_{L^2}^{2/3}) \\
&\qquad \times \|\varphi_1 - \varphi_2\|_{\dot H^1}, \qquad\qquad (B.87)\\
&\|N_\delta(\varphi_1) - N_\delta(\varphi_2)\|_{\dot H^{-1}} \\
&\quad \lesssim \delta^{1/2}(\|\varphi_1\|_{\dot H^1} + \|\varphi_2\|_{\dot H^1})\|\varphi_1 - \varphi_2\|_{\dot H^1} \\
&\quad + \delta^{-7/6} C_{2,\beta}(\|\varphi_1\|_{\dot H^1}^{1/3}\|\varphi_1\|_{L^2}^{2/3} + \|\varphi_2\|_{\dot H^1}^{1/3}\|\varphi_2\|_{L^2}^{2/3}) \\
&\qquad \times \|\varphi_1 - \varphi_2\|_{L^2} \\
&\quad + C_{3,\beta}(\|\varphi_1\|_{\dot H^1}\|\varphi_1\|_{L^2} + \|\varphi_2\|_{\dot H^1}\|\varphi_2\|_{L^2}) \\
&\qquad \times \|\varphi_1 - \varphi_2\|_{\dot H^1}\,. \qquad\qquad (B.88)
\end{aligned}$$

where the constants $C_{i,\beta}$ are given explicitly in (B.34) - (B.37). We rewrite each term $\|\varphi_2\|_{L^2}$ in (B.87) and (B.88) as $\|\varphi_2\|_{L^2} = \delta\|V\|_{L^1_{\rm per}}^{-1/2}(\delta^{-1}\|V\|_{L^1_{\rm per}}^{1/2}\|\varphi_2\|_{L^2})$. Using the definition of the $B_{s,\delta}$-norm in (5.49), we rewrite (B.87) and (B.88) as

$$\begin{aligned}
&\|N_\delta(\varphi_1) - N_\delta(\varphi_2)\|_{L^2} \\
&\lesssim \delta^{-1/2}(\|\varphi_1\|_{\dot H^1} + \|\varphi_2\|_{\dot H^1})\|\varphi_1 - \varphi_2\|_{\dot H^1} \\
&\quad + \delta^{-7/6+2/3} C_{1,\beta}\|V\|_{L^1_{\rm per}}^{-2/6}(\|\varphi_1\|_{B_{s,\delta}} + \|\varphi_2\|_{B_{s,\delta}}) \\
&\qquad \times \|\varphi_1 - \varphi_2\|_{\dot H^1}, \qquad\qquad (B.89)\\
&\|N_\delta(\varphi_1) - N_\delta(\varphi_2)\|_{\dot H^{-1}} \\
&\lesssim \delta^{1/2}(\|\varphi_1\|_{\dot H^1} + \|\varphi_2\|_{\dot H^1})\|\varphi_1 - \varphi_2\|_{\dot H^1} \\
&\quad + \delta^{-7/6+5/3} C_{2,\beta}\|V\|_{L^1_{\rm per}}^{-5/6}(\|\varphi_1\|_{B_{s,\delta}} + \|\varphi_2\|_{B_{s,\delta}}) \\
&\qquad\quad \times \|\varphi_1 - \varphi_2\|_{B_{s,\delta}} \\
&\quad + \delta C_{3,\beta}\|V\|_{L^1_{\rm per}}^{-1/2}(\|\varphi_1\|_{B_{s,\delta}}^2 + \|\varphi_2\|_{B_{s,\delta}}^2) \\
&\qquad \times \|\varphi_1 - \varphi_2\|_{\dot H^1}\,. \qquad\qquad (B.90)
\end{aligned}$$

By the gap assumption [A3], equations (B.21) and (B.22) follow from (B.89) and (B.90) modulo bounding the coefficients $C_{k,\beta}\|V\|_{L^1_{\rm per}}^{-s}$ for $k = 1, ..., 4$ and $s \le 5/6$. The latter estimates are proved in Corollary 57 below. □

Appendix C

Bounds on V

In this section, we prove bounds on $C_{j,\beta}$ and V with the exchange-correlation term xc included (see (3.9); also see (5.50) for the case without xc).

We estimate the constants $C_{j,\beta}$, $j = 1, 2, 3, 4$, given in (B.34), (B.35), (B.36), and (B.37) below, respectively.

Lemma 54. *Let Assumptions [A1] - [A6] hold. Then*

$$C_{j,\beta} \lesssim C_\beta e^{-\eta(\mathbb{R}^3)\beta} \tag{C.1}$$

where C_β is universal among $C_{j,\beta}$ and is at most polynomial in β and $\eta(\mathbb{R}^3)$ is given in (3.6).

Proof. We show the case for $C_{1,\beta}$ as all other cases are similar. By definition (B.36), we estimate

$$\oint \mathrm{Tr}[f R P_\pm g R P_\pm h P_\pm] \tag{C.2}$$

where $R = r_{\mathrm{per}}(z)$ is given in (5.8), $P_\pm$ is given in (B.29), $f, h \in L^2(\mathbb{R}^3)$, $g \in \dot{H}^1(\mathbb{R}^3)$, and the choice of $P_\pm$ is fixed for the entire expression.

We consider the case for P_- only as the case for P_+ is similar. We first note that if $\beta = \infty$ and we replace f_{FD} by the indicator function $\chi_{(-\infty,0)}$, then $C_{j,\infty} = 0$ for all j by the Cauchy integral formula. Thus, in the P_- case,

$$\oint \mathrm{Tr}[fRP_-gRP_-hP_-] \tag{C.3}$$

$$= \frac{1}{2\pi i}\int_{\Gamma_1} (f_{\mathrm{FD}}(z)-1)\mathrm{Tr}[fRP_-gRP_-hP_-] \tag{C.4}$$

where Γ_1 is the contour given below the formula for P_- in (B.31). By the existence of gap $\eta(\mathbb{R}^3)$ (see Assumption [A3]) and the explicit form of the Fermi-Diract distribution f_{FD} in (1.40), we see that

$$|f_{FD}(\beta(z-\mu)) - 1| \lesssim C_\beta e^{-\eta(\mathbb{R}^3)\beta} \tag{C.5}$$

for z in a contour Γ_1 and C_β is at most polynomial in β. Applying the proof of Case 3 of Lemma 51 to (C.4) and using the fact $\|(z-h_{\mathrm{per},})^{-1}\|_\infty \lesssim 1$ for $z \in \Gamma_1$, (C.1) is proved. □

Since $f'_{\mathrm{FD}} < 0$, the explicit form (3.9) of V implies that $V > 0$:

Lemma 55. *Let Assumptions [A1] - [A6] hold, then* $V > 0$.

Lower bound.

Lemma 56. *Let Assumptions [A1] - [A6] hold, then*

$$\|V\|_{L^1_{\mathrm{per}}} \gtrsim \beta e^{-\beta\eta(\Omega)} \tag{C.6}$$

where $\eta(\Omega)$ *is given in* (3.7).

Proof. By Lemma 55, $V > 0$ and so $\|V\|_{L^1_{\mathrm{per}}} = \int_\Omega V$, where Ω is a fundamental domain of $\mathcal{L}$ (see Section 3.1). By definition (3.9) of V, $\int_\Omega V = -\beta \mathrm{Tr}_{L^2_{\mathrm{per}}} f'_{FD}(\beta(h_{\mathrm{per,xc},0} - \mu))$ where $h_{\mathrm{per,xc},0}$ is given in (3.3). Recall that $\eta(\Omega)$ is the smallest distance between $\mu = \mu_{\mathrm{per}}$ and the spectrum of $h_{\mathrm{per,xc},0}$ (see (3.7)). Consequently,

$$\begin{aligned}\|V\|_{L^1_{\mathrm{per}}} =& -\beta \mathrm{Tr}_{L^2_{\mathrm{per}}(\mathbb{R}^3)} f'_{FD}(\beta(h_{\mathrm{per,xc},0}-\mu)) && \text{(C.7)}\\ \geq& -\beta f'_{FD}(\beta\eta(\Omega)) && \text{(C.8)}\\ =&\beta\frac{e^{\beta\eta(\Omega)}}{(1+e^{\beta\eta(\Omega)})^2}. && \text{(C.9)}\end{aligned}$$

Since $\delta \ll 1$, [A4] implies that $1 \ll \beta$. Combining this with (C.9), we arrive at (C.6). □

We state two immediate corollaries of Lemmas 54 and 56 relating $C_{j,\beta}$ for $j = 1, ..., 4$ (see (B.34) - (B.37)) and V.

Corollary 57. *Let Assumptions [A1] - [A6] hold. For $j = 1, 2, 3, 4$ and C_β at most polynomial in β,*

$$C_{j,\beta}\|V\|^{-5/6}_{L^1_{\mathrm{per}}} \lesssim C_\beta e^{-\eta\beta}, \tag{C.10}$$

where η is given in in the paragraph right above Assumption [A3].

Corollary 58. *Let Assumptions [A1] - [A6] hold. Let $s, t > 0$ and $e \leq 5/6$ be fixed, there exists $C_{s,t,e}$ such that for $\beta = C_{s,t,e}|\ln(\delta)|$,*

$$\delta^{-s} C_{j,\beta}\|V\|^{-e}_{L^1_{\mathrm{per}}} \lesssim \delta^t \tag{C.11}$$

for $j = 1, 2, 3$.

Upper bound.

Lemma 59. *Let Assumptions [A1] - [A6] hold. Let $1 \leq p \leq \infty$. Then*

$$\|V\|_{L^p_{\mathrm{per}}} \lesssim C_\beta e^{-\eta(\Omega)\beta} \tag{C.12}$$

where C_β is polynomial in β and $\eta(\Omega)$ is give in (3.7) (also see Assumption [A3]).

Proof. We do the case for $p = 1$ and $p = \infty$, and conclude the lemma by interpolation.

As in the proof of Lemma 54, we see that

$$\|V\|_{L^1_{\text{per}}} = -\beta \mathrm{Tr}_{L^2_{\text{per}}} f'_{FD}(\beta(h_{\text{per,xc},0} - \mu)). \tag{C.13}$$

where $h_{\text{per,xc},0}$ is given in (3.3). By [A6], [A1], and Theorem 6, the potential $\phi_{\text{per}} + \mathrm{xc}(\rho_{\text{per}})$ is infinitesimally bounded with respect to $-\Delta$. Thus, $h_{\text{per,xc},0}$ has only discrete spectrum on $L^2_{\text{per}}(\mathbb{R}^3)$ and

$$\|V\|_{L^1_{\text{per}}} = \sum_{\lambda \in \sigma(h_{\text{per,xc},0})} \frac{\beta e^{\beta(\lambda-\mu)}}{(1+e^{\beta(\lambda-\mu)})^2} \tag{C.14}$$

$$= \sum_{\mu > \lambda \in \sigma(h_{\text{per,xc},0})} \frac{\beta e^{\beta(\lambda-\mu)}}{(1+e^{\beta(\lambda-\mu)})^2} \tag{C.15}$$

$$+ \sum_{\mu < \lambda \in \sigma(h_{\text{per,xc},0})} \frac{\beta}{(e^{-\frac{1}{2}\beta(\lambda-\mu)} + e^{\frac{1}{2}\beta(\lambda-\mu)})^2} \tag{C.16}$$

Factoring a factor of $e^{-\beta\eta(\Omega)}$ from (C.16), we get

$$\begin{aligned} \|V\|_{L^1_{\text{per}}} = & e^{-\beta\eta(\Omega)} \Bigg(\sum_{\mu > \lambda \in \sigma(h_{\text{per,xc},0})} \frac{\beta e^{\beta(\lambda-\mu+\eta(\Omega))}}{(1+e^{\beta(\lambda-\mu)})^2} \\ & + \sum_{\mu < \lambda \in \sigma(h_{\text{per,xc},0})} \frac{\beta}{(e^{-\frac{1}{2}\beta(\lambda-\mu+\eta(\Omega))} + e^{\frac{1}{2}\beta(\lambda-\mu+\eta(\Omega))})^2} \Bigg). \end{aligned} \tag{C.17}$$

Since the potential $\phi_{\text{per}} + \mathrm{xc}(\rho_{\text{per}})$ is infinitesimally bounded with respect to $-\Delta$, the eigenvalues of $h_{\text{per},0}$ goes to infinite at a similar rate as those of $-\Delta$ (on $L^2_{\text{per}}(\mathbb{R}^3)$). Thus, for λ close to μ, the terms in the bracket in (C.17) are of order $O(C_\beta)$, where C_β is at most polynomial in β. For λ large, we can approximate each term in the sum (C.17) by the eigenvalues of $-\Delta$ and conclude that the sum is summable with a $O(C_\beta)$ sum. This proves the lemma for $p = 1$.

Let $W^{4,1}_{\text{per}}$ be the usual Sobolev space associated to L^1_{per} involving up to 4 derivatives. For the case $p = \infty$, we use the Sobolev inequality

$$\|f\|_\infty \lesssim \|f\|_{W^{4,1}_{\text{per}}} \tag{C.18}$$

for $f \in W^{4,1}_{\text{per}}$, where Thus, it suffices for us to estimate $\|\nabla^4 V\|_{L^1_{\text{per}}}$. To this end, we note that

$$\nabla \operatorname{den}(A) = \operatorname{den}([\nabla, A]) \tag{C.19}$$

for an operator A on $L^2_{\text{per}}(\mathbb{R}^3)$. Thus, it suffices that we estimate the trace 1-norm of $\beta \nabla^s f'_{FD}(\beta(h_{\text{per},0} - \mu))\nabla^{4-s}$ on $L^2_{\text{per}}(\mathbb{R}^3)$ for $s = 0, ..., 4$. Since the potential $\phi_{\text{per}} + \text{xc}(\rho_{\text{per}})$ is infinitesimally bounded with respect to $-\Delta$, it suffices for us to estimate $\beta |h_{\text{per},0}|^s f'_{FD}(\beta(h_{\text{per},0} - \mu))|h_{\text{per},0}|^{4-s}$. This can be done the same way as the case for $p = 1$ by summing eigenvalues of $h_{\text{per},0}$ and the lemma is proved. $\square$

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