



On Derivation of the Poisson–Boltzmann Equation

Ilias Chenn¹ · I. M. Sigal²

Received: 11 February 2020 / Accepted: 9 May 2020 / Published online: 29 May 2020
© Springer Science+Business Media, LLC, part of Springer Nature 2020

Abstract

Starting from the microscopic reduced Hartree–Fock equation, we derive the macroscopic linearized Poisson–Boltzmann equation for the electrostatic potential associated with the electron density.

Keywords Density functional theory · Kohn–Sham equation · Microscopic limit · Partial differential equations of quantum physics · Poisson–Boltzmann equation · Electrostatics

1 Introduction

1.1 The Reduced Hartree–Fock Equation

The success of the Hartree–Fock and density functional theories in revealing the electronic structure of matter warrants their use as a starting point in the derivation of emergent macroscopic properties of quantum matter.

Here, one of the central problems is the derivation of macroscopic Maxwell’s equations in dielectrics. The first attack on such a derivation was made in the pioneering works of Cancès, Lewin and Stoltz and E and Lu and their collaborators [5–9, 15–17, 17]. These works deal with the reduced Hartree–Fock equation (REHF)¹ and the Kohn–Sham equation (KSE) of the density functional theory (DFT) at zero temperature. The first treatment of the positive temperature REHF was given by Levitt [23] (see also [13]).

In this paper, we consider the REHF at positive temperature, which is also a simplified DFT equation, and derive from it the linearized effective Poisson–Boltzmann equation of electrostatics, widely used in molecular and structural biology (see e.g. [19]).

For a positive temperature T and with the electron charge set to $e = -1$, REHF can be written in terms of the one-particle negative charge (or probability) density $\rho(x)$ of the

¹ The REHF obtained from the Hartree–Fock equation (HFE) by omitting the exchange term, see below.

Communicated by Ivan Corwin.

To Joel with friendship and admiration.

✉ I. M. Sigal
im.sigal@utoronto.ca

¹ Dept of Mathematics, MIT, Cambridge, MA, USA

² Dept of Mathematics, Univ of Toronto, Toronto, Canada

electron (or generally any Fermi) gas, as

$$\rho = \text{den}[f_T(h_\rho - \mu)], \tag{1.1}$$

where $\text{den} : A \rightarrow \rho_A$ is 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), $f_T(\lambda)$ is the Fermi–Dirac distribution,

$$f_T(\lambda) := f_{FD}(\lambda/T), \quad f_{FD}(\lambda) = \frac{1}{e^{\lambda} + 1} \tag{1.2}$$

(due to the Fermi–Dirac statistic), μ is the chemical potential and h_ρ is a self-adjoint one-particle Hamiltonian depending on the density ρ (self-consistency). Since h_ρ is self-adjoint the r.h.s. of (1.1) is well defined. Assuming the electrons are subject to an external potential due to a positive charge distribution κ (say, due to positive ions), h_ρ is given by

$$h_\rho := -\Delta - v * (\kappa - \rho), \tag{1.3}$$

where v is an inter-particle pair potential. It is taken to be the electrostatic potential, as specified below.

Let $L^2_{\text{loc}} \equiv L^2_{\text{loc}}(\mathbb{R}^d)$ denote the space of locally square integrable functions. We fix a lattice $\mathcal{L} \subset \mathbb{R}^d$ and let L^2_{per} be the space of L^2_{loc} , periodic w.r.t. \mathcal{L} functions. Finally, let $(L^2_{\text{per}})^\perp$ be the orthogonal complement of the constant functions in L^2_{per} . In what follows, we assume $\rho - \kappa \in L^2 + (L^2_{\text{per}})^\perp$ and v is the electrostatic potential, $v(x) = \frac{1}{4\pi|x|}$ in 3D, or, generally,

$$v * f = (-\Delta)^{-1} f,$$

for $f \in L^2 + (L^2_{\text{per}})^\perp$, so that Δ^{-1} is well-defined.² For ρ 's and κ 's specified above, the operator h_ρ is self-adjoint.

The positive temperature, reduced Hartree–Fock equation (1.1) will be abbreviated, with the view to readability, as the TREHF.

For $T = 0$, function (1.2) becomes the characteristic function of the interval $(-\infty, 0)$ and Eq. (1.1) becomes just the REHF.

1.2 Electrostatic Potential

Due to the choice $v * f = (-\Delta)^{-1} f$, the electrostatic potential $\phi = v * (\kappa - \rho)$ satisfies the Poisson equation

$$-\Delta\phi = (\kappa - \rho). \tag{1.4}$$

Plugging ρ from (1.1) into this equation and taking $v * (\kappa - \rho) = \phi$ in (1.3), we find the equation for ϕ

$$-\Delta\phi = (\kappa - \text{den}[f_T(h^\phi - \mu)]), \tag{1.5}$$

² The decomposition $L^2 + L^2_{\text{per}}$ is unique: if $f \in L^2 + L^2_{\text{per}}$, then the periodic part, f_{per} , of f is given by the Fourier coefficients

$$\hat{f}_{\text{per}}(k) := \lim_{n \rightarrow \infty} \frac{1}{|\Lambda_n|} (2\pi)^{-d/2} \int_{\Lambda_n} e^{ik \cdot x} f(x) dx, \quad k \in \mathcal{L}^*,$$

where $\Lambda_n := \cup_{\lambda \in \mathcal{L}_n} (\Omega + \lambda)$, with $\mathcal{L}_n := \mathcal{L} \cap [-n, n]^d$ and Ω an arbitrary fundamental cell of \mathcal{L} , and \mathcal{L}^* is the reciprocal lattice. Hence $L^2 + L^2_{\text{per}}$ is a Hilbert space with the inner product which is sum of the inner products in L^2 and L^2_{per} . The operator Δ on $L^2 + L^2_{\text{per}}$ is self-adjoint on the natural domain (i.e. $H^2 + H^2_{\text{per}}$) and is invertible on the subspace $L^2 + (L^2_{\text{per}})^\perp$.

where

$$h^\phi = -\Delta - \phi. \tag{1.6}$$

We can recover ρ from ϕ via Eq. (1.4) or the equation

$$\rho = \text{den}[f_T(h^\phi - \mu)]. \tag{1.7}$$

Let H^s and H^s_{per} be the Sobolev spaces corresponding to L^2 and L^2_{per} . If $\kappa, \rho \in L^2 + L^2_{\text{per}}$, $\phi \in H^2 + H^2_{\text{per}}$ and ϕ and $\rho - \kappa$ satisfy (1.4), then

$$\int_{\Omega} \rho_{\text{per}} = \int_{\Omega} \kappa_{\text{per}}, \tag{1.8}$$

where Ω is an arbitrary fundamental cell of \mathcal{L} and the subindex ‘per’ denotes the periodic part of the corresponding function ($\in L^2 + L^2_{\text{per}}$). Indeed, let $\Lambda_n := \cup_{\lambda \in \mathcal{L}_n} (\Omega + \lambda)$, where $\mathcal{L}_n := \mathcal{L} \cap [-n, n]^d$. Integrating (1.4) over the domain Λ_n and using the Stokes’ theorem, we find

$$\int_{\partial\Lambda_n} \nabla\phi = \int_{\Lambda_n} (\kappa - \rho).$$

Since $\lim_{n \rightarrow \infty} \frac{1}{|\Lambda_n|} \int_{\partial\Lambda_n} \nabla\phi = 0$ and $\lim_{n \rightarrow \infty} \frac{1}{|\Lambda_n|} \int_{\Lambda_n} (\kappa - \rho) = \int_{\Omega} (\rho_{\gamma} - \kappa)_{\text{per}}$, the last relation gives (1.8).

Equation (1.8) shows that $\rho - \kappa \in L^2 + (L^2_{\text{per}})^{\perp}$, i.e. it satisfies the conditions mentioned in the paragraph after (1.3).

Equation (1.8) determines the chemical potential μ and expresses the conservation of the charge per fundamental cell of \mathcal{L} . It is considered as the solvability condition and should be added to (1.1) in the periodic case.

In what follows we associate with a solution ρ of (1.1) the electrostatic potential

$$\phi_{\rho} = (-\Delta)^{-1}(\kappa - \rho), \tag{1.9}$$

and with a solution ϕ of Eq. (1.5), the charge density ρ according to (1.4), or (1.7).

1.3 Relation to the TEHF and KSE

The key positive temperature HFE is given by

$$\gamma = f_T(h_{\gamma} - \mu), \tag{1.10}$$

where $f_T(\lambda)$ is as above and, for an external charge distribution κ ,

$$h_{\gamma} := -\Delta - v * (\kappa - \rho_{\gamma}) + ex(\gamma). \tag{1.11}$$

Here, recall, $\rho_{\gamma}(x) := \gamma(x, x)$ and $v * f = (-\Delta)^{-1}f$, and $ex(\gamma)$ (the exchange term) is the operator with the integral kernel $ex(\gamma)(x, y) := -v(x - y)\gamma(x, y)$, where $\gamma(x, y)$ is the integral kernel of γ . Observing that $h_{\gamma}|_{ex(\gamma)=0} = h_{\rho_{\gamma}}$, where h_{ρ} is given in (1.3), one sees that (1.10) with $ex(\gamma) = 0$ implies the equation

$$\gamma = f_T(h_{\rho_{\gamma}} - \mu). \tag{1.12}$$

Equation (1.12) is equivalent to Eq. (1.1). Indeed, applying the map den to Eq. (1.12) gives (1.1). In the opposite direction, if ρ solves (1.1), then the density operator

$$\gamma = f_T(h_{\rho} - \mu), \tag{1.13}$$

acting on $L^2(\mathbb{R}^d)$, solves (1.12). Thus, (1.12) is the TREHF in terms of the density operator γ .

By replacing $ex(\gamma)$ in (1.11) by a local exchange-correlation term $xc(\rho)$ and then applying, as above, the map den to the resulting equation, one obtains the natural extension of the original Kohn–Sham equation to positive temperatures:

$$\rho = \text{den}[f_T(h_\rho^{\text{KS}} - \mu)], \tag{1.14}$$

$$h_\rho^{\text{KS}} := -\Delta - v * (\kappa - \rho) + xc(\rho). \tag{1.15}$$

1.4 The Origin of the TEHF/TREHF Equations

As the TEHF and TREHF arise in the same way, in order to avoid repetitions, we consider here only the later.

Equation (1.12) originates from the static version

$$[h_{\rho_\gamma}, \gamma] = 0 \tag{1.16}$$

of the time dependent RHF equation (see e.g. [12] for a review)

$$\partial_t \gamma = i[h_{\rho_\gamma}, \gamma]. \tag{1.17}$$

Indeed, ignoring symmetries and accidental divergence, γ solves (1.16) if and only if γ solves $\gamma = f((h_{\rho_\gamma} - \mu)/T)$ for some reasonable function f . (The parameters T and μ are of no significance at this stage; they are introduced for future reference.)

The selection of f is done on physics grounds, either bringing the system in question in contact with a thermal reservoir at temperature T and the chemical potential μ , or passing to the thermodynamic limit. This leads to Eq. (1.12).

As we discuss below, Eq. (1.12) is the Euler-Lagrange equation for the natural free energy.

Remark If the particles in question were bosons, then f_{FD} would be replaced by the Bose–Einstein distribution

$$f_{BE}(\lambda) = \frac{1}{e^\lambda - 1}. \tag{1.18}$$

1.5 Results

We are interested in the dielectric response in a medium subjected to a local deformation of the crystalline structure. To formulate our results we introduce some notation and definition.

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

$$L^2_{\text{per}} \equiv L^2_{\text{per}}(\mathbb{R}^3) = \{f \in L^2_{\text{loc}}(\mathbb{R}^3) : f \text{ is } \mathcal{L}\text{-periodic}\}, \tag{1.19}$$

with the inner product $\langle f, g \rangle = \int_{\Omega} \bar{f}g$ and the norm $\|f\|_{L^2_{\text{per}}}^2 = \int_{\Omega} |f|^2$ for some arbitrary fundamental domain Ω of \mathcal{L} . We denote by $H^s_{\text{per}} \equiv H^s_{\text{per}}(\mathbb{R}^3)$ and $\|\cdot\|_{H^s_{\text{per}}}$ the associated Sobolev spaces and their norms, while the standard Sobolev spaces and their norms are denoted by $H^s \equiv H^s(\mathbb{R}^3)$ and $\|\cdot\|_{H^s}$.

Crystals We consider a background charge distribution, $\kappa(y) \equiv \kappa_{\text{per}}(y)$, periodic with respect to the lattice \mathcal{L} (crystal). Here y stands for the microscopic coordinate.

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

$$\kappa_{\text{per}}(y) = \sum_{l \in \mathcal{L}} \kappa_a(y - l), \tag{1.20}$$

where κ_a denotes an ionic (“atomic”) charge distribution.

Dielectrics Next, we describe a model of the (crystalline) dielectric.

Definition 1.1 We say that an \mathcal{L} -periodic background charge density $\kappa_{\text{per}} \in L^2_{\text{per}}$ is dielectric, if TREHF (1.1), with $\kappa = \kappa_{\text{per}}$, has an \mathcal{L} -periodic solution $(\rho_{\text{per}}, \mu_{\text{per}})$, with the following properties:

- (a) the periodic one-particle Schrödinger operator

$$h_{\text{per}} := h^{\phi_{\text{per}}} = -\Delta - \phi_{\text{per}}, \text{ with} \tag{1.21}$$

$$\phi_{\text{per}} := 4\pi(-\Delta)^{-1}(\kappa_{\text{per}} - \rho_{\text{per}}), \tag{1.22}$$

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

- (b) μ_{per} is in this gap;
- (c) $\phi_{\text{per}} \in H^2_{\text{per}}$ and $\|\phi_{\text{per}}\|_{H^2_{\text{per}}} \|\mu_{\text{per}}\| \leq \Delta_{\text{per}}$, independently of T .

An existence result for the dielectrics is discussed in Remarks 6 and 7 after the next theorem. In particular, Proposition 1.3 shows that the set of dielectric charge densities κ_{per} is robust. Moreover, (1.5) can be reformulated so that only ϕ_{per} and μ_{per} , but not κ_{per} , enter it explicitly, see (1.44). So these are the only inputs of our analysis

Dielectric response We consider a macroscopically deformed microscopic crystal charge distribution,

$$\kappa_{\delta}(y) = \kappa_{\text{per}}(y) + \delta^3 \kappa'(\delta y), \tag{1.23}$$

where δ is a small parameter which stands for the ratio of microscopic and macroscopic scale and $\kappa'(x) \in L^2$ is a small local perturbation living on the macroscopic scale. By y and $x = \delta y$, we denote the microscopic and macroscopic coordinates, respectively. Thus, the microscopic scale is $y \sim 1$ and $x \sim \delta$ and the macroscopic one, $y \sim 1/\delta$ and $x \sim 1$.

We formulate the conditions for our main result. We introduce the homogeneous Sobolev spaces

$$\dot{H}^s \equiv \dot{H}^s(\mathbb{R}^3) = \{f \text{ measurable on } \mathbb{R}^3 : \|f\|_{\dot{H}^s} < \infty\} \tag{1.24}$$

for $s \geq 0$ with the associated norm

$$\|f\|_{\dot{H}^s}^2 = \int |(-\Delta)^{s/2} f(k)|^2. \tag{1.25}$$

[A1] (Dielectricity) κ_{per} is dielectric.

Let h_{per} and $h_{\text{per},0}$ denote operators given by expression (1.21) acting on $L^2(\mathbb{R}^3)$ and $L^2_{\text{per}}(\mathbb{R}^3)$, respectively. These operators are self-adjoint and the latter has a purely discrete spectrum. By Assumptions [A1], μ_{per} is in a gap of h_{per} . For notational convenience, we rescale our problem so that

$$\eta := \text{dist}(\mu_{\text{per}}, \sigma(h_{\text{per}})) = 1. \tag{1.26}$$

It follows the Bloch–Floquet decomposition results in Sect. 2.4 below that the gaps of h_{per} are contained in the resolvent set of $h_{\text{per},0}$, so that

$$\eta_0 := \text{dist}(\mu_{\text{per}}, \sigma(h_{\text{per},0})) \geq 1. \tag{1.27}$$

[A2] (Perturbation κ')

$$\kappa' \in H^1 \cap \dot{H}^{-1}.$$

In what follows, the inequalities $A \lesssim B$ and $A \gtrsim B$ mean that there are constants C and c independent of T and δ , s.t. $A \leq CB$ and $A \geq cB$ and similarly for $A \ll B$ and $A \gg B$. Our main result is

Theorem 1.2 *Let Assumptions [A1]–[A2] hold and let $(\phi_{\text{per}}, \mu_{\text{per}})$ be the electrostatic and chemical potentials associated with κ_{per} (entering [A1]) as per Definition 1.1.*

There is $\alpha = \alpha(\Delta_{\text{per}}) > 0$ sufficiently small, s.t., if

[A3] (Regime) *The parameters $T > 0$ and $\delta > 0$ satisfy*

$$c_T := T^{-1} e^{-\eta_0/T} \leq \alpha, \quad c_T^{-8/9} \delta \leq \alpha, \tag{1.28}$$

then the following statements are true

1. *Electrostatic TREHF (1.5), with $\kappa = \kappa_\delta$ given in (1.23) and $\mu = \mu_{\text{per}}$, has a unique solution $\phi_\delta \in H^2_{\text{per}} + H^1$;*
2. *The potential $\phi_\delta(y)$ is of the form*

$$\phi_\delta(y) = \phi_{\text{per}}(y) + \delta\psi(\delta y) + \varphi_{\text{rem}}(\delta y), \tag{1.29}$$

where $\varphi_{\text{rem}}(x) \in H^1$ and obeys the estimates (with $\dot{H}^0 = L^2$)

$$\|\varphi_{\text{rem}}\|_{\dot{H}^i} \ll \alpha^{\frac{1}{4} - \frac{1}{2}i} (c_T^{-1/2} \delta)^{2-i}, \tag{1.30}$$

with α given in (1.28), and $\psi(x) \in H^1$ and satisfies the equation

$$(\nu - \nabla \cdot \epsilon \nabla)\psi = \kappa', \tag{1.31}$$

with a positive number $\nu > 0$ and a constant real, symmetric 3×3 matrix, $\epsilon \geq 1 - O(c_T^2)$;

3. $\epsilon \equiv \epsilon(T)$ and $\nu \equiv \nu(T, \delta)$ are given explicitly by (1.35)–(1.37) and (1.32)–(1.33), below.

We discuss Assumptions [A1] and [A3] in Remarks 6 and 10 and the statements of the theorem, in Remarks 1–4, below.

1.6 Discussion

- (1) Theorem 1.2(1) and Eq. (1.9) connecting the charge density ρ with ϕ imply that RHF equation (1.1), with (1.23) and $\mu = \mu_{\text{per}}$, has a unique solution $\rho_\delta \in L^2_{\text{per}} + \dot{H}^{-1}$.
- (2) The quantity $\nu \equiv \nu(T, \delta)$ is defined as

$$\nu = \delta^{-2} |\Omega|^{-1} (m + O(c_T^2)), \tag{1.32}$$

$$m = -\text{Tr}_\Omega [f'_T(h_{\text{per},0} - \mu)] > 0. \tag{1.33}$$

Lemmas B.1 and B.2 of Appendix B imply the estimates

$$0 < c_T \lesssim m \lesssim c_T. \tag{1.34}$$

By (1.34) and (1.28), m is the leading term in (1.32) and $\nu \gg \delta^{-7/8}$.

(3) The 3×3 matrix, ϵ , in (1.31) is given explicitly by

$$\epsilon := \mathbf{1} + \epsilon' - \epsilon'', \tag{1.35}$$

$$\epsilon' = -\frac{1}{|\Omega|} \text{Tr}_{L^2_{\text{per}}} \oint r^2_{\text{per},0}(z)(-i\nabla)r_{\text{per},0}(z)(-i\nabla)r_{\text{per},0}(z), \tag{1.36}$$

$$\epsilon'' = \frac{1}{|\Omega|} \langle \rho', \bar{K}_0^{-1} \rho' \rangle_{L^2_{\text{per}}}, \tag{1.37}$$

where $r_{\text{per},0}(z) := (z - h_{\text{per},0})^{-1}$ and $h_{\text{per},0}$ denotes the restriction of $h_{\text{per}} := h^{\phi_{\text{per}}} = -\Delta + \phi_{\text{per}}$ to L^2_{per} , \bar{K}_0 is the operator defined in (4.11), and

$$\rho' = 2 \text{den} \oint r^2_{\text{per},0}(z)(-i\nabla)r_{\text{per},0}(z). \tag{1.38}$$

(4) Equations (1.31), (1.32) and (1.34) imply that

$$\|\psi\|_{\dot{H}^i} = O([\delta|\Omega|^{1/2}m^{-1/2}]^{2-i}), \quad i = 0, 1,$$

and therefore, by (1.28), (1.30) and (1.34), we have

$$\|\phi_{\text{rem}}\|_{L^2} \ll \alpha^{1/4}(m^{-1/2}\delta)^2 \ll \|\psi\|_{L^2}.$$

Hence ψ is a subleading term in (1.29) in the L^2 -norm.

(5) (1.31) is the linearized Poisson–Boltzmann equation used extensively in physical chemistry and molecular biology (see e.g. [19]). ϵ is an effective permittivity matrix and $\sqrt{\nu}$ and $1/\sqrt{\nu}$ are the Debye–Hückel parameter and the Debye length, respectively.

The screening term ν in (1.31) is due to the electrons at the tail of the Fermi–Dirac distribution being at the conduction band. (In the macroscopic regime, the Fermi–Dirac distribution becomes the (Maxwell-) Boltzmann distribution.)

(6) (Existence of crystalline dielectrics) We say that the potential ϕ is gapped if the Schrödinger operator $-\Delta - \phi$ has a gap in its continuous spectrum.

Proposition 1.3 *For any \mathcal{L} -periodic, gapped potential $\phi_{\text{per}} \in H^k_{\text{per}}$, $k \geq 2$, and any real number μ_{per} in a gap of $h_{\text{per}} := -\Delta - \phi_{\text{per}}$, there is $\kappa_{\text{per}} \in H^{k-2}_{\text{per}}$ such that Eq. (1.1), with $\kappa = \kappa_{\text{per}}$, has the solution $(\rho = \rho_{\text{per}} \in H^{k-2}_{\text{per}}, \mu = \mu_{\text{per}})$ with the associated (according to (1.4)) electrostatic potential exactly ϕ_{per} . Moreover, the pair $(\phi_{\text{per}}, \mu_{\text{per}})$ satisfies the electrostatic Eq. (1.5) with this κ_{per} .*

Proof Let ϕ_{per} be such that $h_{\text{per}} := -\Delta - \phi_{\text{per}}$ has a gap. We choose μ_{per} to be in this gap and define (see (1.6)–(1.7))

$$\rho_{\text{per}} := \text{den}[f_T(h_{\text{per}} - \mu_{\text{per}})]. \tag{1.39}$$

Next, we define

$$\kappa_{\text{per}} := -\Delta\phi_{\text{per}} + \rho_{\text{per}}. \tag{1.40}$$

Then, it is straightforward to check that $(\rho_{\text{per}}, \mu_{\text{per}})$ is a solution of Eq. (1.1) with background potential κ_{per} . By construction, h_{per} has a gap and μ_{per} is in this gap. \square

One can extend Proposition 1.3 to construct pairs $(h_{\text{per}} = -\Delta - \phi_{\text{per}}, \mu_{\text{per}})$ having any desired property **P**. Following Proposition 1.3, we construct $\rho_{\text{per}}, \phi_{\text{per}}$, and κ_{per} via (1.39) and (1.40) in this order. Then $(\rho_{\text{per}}, \mu_{\text{per}})$ is a solution of Eq. (1.1) with background potential κ_{per} . By construction, h_{per} has property **P**.

The proposition above shows that for any positive η and T , we can find $\kappa_{\text{per}} \in H_{\text{per}}^{k-2}$ such that the solution of Eq. (1.1) with $\kappa = \kappa_{\text{per}}$ and T gives the gap η .

(7) (General dielectrics) We say that a background charge density κ is dielectric if Eq. (1.1) with background charge distribution κ has a solution (ρ, μ) , with ρ in an appropriate space, say, $H_{\text{loc}}^2 \cap L^\infty$, and having the following properties:

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

$$h^\phi := -\Delta - \phi, \text{ with } \phi := 4\pi(-\Delta)^{-1}(\kappa - \rho), \tag{1.41}$$

acting on L^2 , is self-adjoint and has a gap in its spectrum;

(b) μ is in this gap.

By the remark at the end of the previous item we have

Proposition 1.4 (Existence of general dielectrics) *For any gapped potential $\phi \in H_{\text{loc}}^2 \cap L^\infty$ and any number μ in a gap of $h^\phi := -\Delta - \phi$, there is $\kappa \in L_{\text{loc}}^2 \cap L^\infty$ s.t. Eq. (1.1), with these $\kappa \in L_{\text{loc}}^2 \cap L^\infty$ and μ , has the solution ρ , whose the electrostatic potential (according to (1.4)) is ϕ .*

(8) (Existence of ideal crystals) The existence of periodic solutions to Eq. (1.1) (equilibrium crystalline structures exists at $T > 0$) is shown in the following:

Theorem 1.5 *Let $d = 3$ and $\kappa_{\text{per}} \in H_{\text{per}}^2$. Then Eq. (1.1), with the \mathcal{L} -periodic background charge density $\kappa = \kappa_{\text{per}}$ has a solution $(\rho_{\text{per}}, \mu_{\text{per}})$, with ρ_{per} periodic and satisfying $\sqrt{\rho_{\text{per}}} \in H_{\text{per}}^1$.*

We give references to the proof of this theorem below.

- (9) In the limit $T \rightarrow 0$, our expression for the dielectric constant ϵ agrees with [7] (see Appendix A below).
- (10) (Physical dimensions) The physical cell size of common crystals is on the order of 10^{-10} ([35]). This gives $\delta \sim 10^{-10}$. The gap size, η_0 , is on the order $1eV$ [35]. Since the Boltzmann constant, k_B , is of the order $10^{-4}eV/K$, this gives $\eta_0/k_B \sim 10^4 K$. Thus, though we do not compute actual constants in our estimate, we expect that the allowed values of δ and T are within physically interesting ranges.
- (11) (Energy) The evolution (1.17) conserves the number of particles $N_X(\gamma) := \text{Tr}_X(\gamma)$ and the energy

$$E_X(\gamma) := \text{Tr}_X((-\Delta)\gamma) + \frac{1}{2} \int_X \sigma_\gamma v * \sigma_\gamma, \tag{1.42}$$

where X is either \mathbb{R}^d or a fundamental cell Ω of \mathcal{L} , with Tr_X defined accordingly, and $\sigma_\gamma := \kappa - \rho_\gamma$.

Equation (1.12) is the Euler–Lagrange equation for the free energy functional

$$F_T(\gamma) := E_X(\gamma) - TS_X(\gamma) - \mu N_X(\gamma), \tag{1.43}$$

where $S_X(\gamma) = -\text{Tr}_\Omega(\gamma \ln \gamma + (\mathbf{1} - \gamma) \ln(\mathbf{1} - \gamma))$ is the entropy.

To obtain the HF (free) energy functional, one should add to (1.42) ((1.43)) the HF exchange energy term $E_X(\gamma) := \frac{1}{2} \int_X \int_X |v(x - y)\gamma(x, y)|^2$.

Literature The relation of the HF theory to the exact quantum many-body problem was established rigorously in [26].

For $T = 0$, the existence theory for the RHFE and HFE was developed in [1, 11, 21, 26, 29], see [22, 25, 28], for reviews. For the Hartree–Fock equation (1.10) with periodic $\kappa = \kappa_{\text{per}}$, the existence of periodic solutions from certain trace classes was obtained in [10] and [11].

Results for $T = 0$, similar and related to Theorem 1.2, were proven in [5–9, 15–17].

For the case where $T > 0$, F. Nier [32] proved the existence and uniqueness of the TRHF (1.1) via variational techniques. Later, Prodan and Nordlander [33] 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 $\phi_{\text{per}} + \text{xc}(\rho_{\text{per}})$, where $\text{xc}(\rho)$ is a local exchange–correlation term, see (1.15), is small as well. (As was pointed by A. Levitt, a result for small $\kappa = \kappa_{\text{per}}$ would not work in Theorem 1.2 above as Assumption [A1] fails for it.)

The results given in Theorem 1.5 is taken from [13]. Papers [1, 10, 11, 13] use variational techniques and did not provide uniqueness results. A. Levitt [23] proved the screening of small defects for the TRHFE.

Approach As in [23], our starting point is Eq. (1.5) for the electrostatic potential ϕ . We also use some important ideas from [8]. However, our approach to proving Theorem 1.2 is fairly novel. Rather than employing variations-based techniques, we use the Lyapunov–Schmidt reduction, which also allows us to estimate the remainders.

The starting equation of our analysis can be formulated as follows. Let $(\phi_{\text{per}}(x), \mu_{\text{per}})$ be the solution of (1.5), with $\kappa(x) = \kappa_{\text{per}}(x)$, and let κ_δ be given in (1.23). Define ψ by the equality

$$\phi = \phi_{\text{per}} + \psi.$$

Plugging this decomposition into (1.5), with $\kappa = \kappa_\delta$ and $\mu = \mu_{\text{per}}$, and using that $h^\phi = h^{\phi_{\text{per}}} - \psi$, we arrive at the equation for ψ :

$$-\Delta\psi = (\kappa'_\delta - \text{den}[g_{\phi'_{\text{per}}}(\psi)]), \tag{1.44}$$

where $\phi'_{\text{per}} := \phi_{\text{per}} + \mu_{\text{per}}$, $g_{\phi'_{\text{per}}}(\psi) := f_T(h^{\phi'_{\text{per}}} - \psi) - f_T(h^{\phi'_{\text{per}}})$ and $\kappa'_\delta(y) := \delta^3\kappa'(\delta y)$.

This is a nonlinear and nonlocal Poisson equation for ψ . We see that only $\phi'_{\text{per}} := \phi_{\text{per}} + \mu_{\text{per}}$, but not κ_{per} , enters Eq. (1.44) explicitly.

Though we deal with the simplest microscopic model—the reduced HF equation—our techniques are fairly robust and would work for the full-fledged DFT. Also, we favoured rough estimates to more precise but lengthier ones which produce better bounds on β in (1.28), see Appendix D below.

The paper is organized as follows. After presenting preliminary material on charge density estimates and the Bloch–Floquet decomposition in Sect. 2, we prove Theorem 1.2 in Sects. 3–5. Section 3 contains the main steps of the proof of Theorem 1.2. Section 5 covers fairly straightforward technical estimates of the nonlinearity.

2 Densities and Bloch–Floquet Decomposition

2.1 Locally Trace Class Operators

Let $C_c \equiv C_c(\mathbb{R}^3)$ denote the space of compactly supported continuous functions on \mathbb{R}^3 . An operator A on L^2 is said to be locally trace class if fA and Af are trace class for all $f \in C_c$. (For the proofs below, it suffices to require that fA is trace class.)

Let \mathcal{L} be a Bravais lattice on \mathbb{R}^3 and Ω a fundamental domain of \mathcal{L} as in Sect. 1.5. 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

$$T_s : f(x) \mapsto f(x - s). \tag{2.1}$$

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

$$L^p_{\text{per}} \equiv L^p_{\text{per}}(\mathbb{R}^3) = \{f \in L^p_{\text{loc}}(\mathbb{R}^3) : f \text{ is } \mathcal{L}\text{-periodic}\}, \tag{2.2}$$

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

We say that a bounded operator A on L^2 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 (2.1).

Let S^p be the standard p -Schatten space of bounded operators on L^2 with the p -Schatten norm

$$\|A\|_{S^p}^p := \text{Tr}_{L^2}((A^*A)^{p/2}). \tag{2.3}$$

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

$$\|A\|_{S^p_{\text{per}}}^p := \text{Tr}_{\Omega}((A^*A)^{p/2}) := \frac{1}{|\Omega|} \text{Tr}_{L^2}(\chi_{\Omega}(A^*A)^{p/2}\chi_{\Omega}). \tag{2.4}$$

We remark that the S^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.

2.2 Densities

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

$$\int \text{den}(A)f = \text{Tr}(fA), \tag{2.5}$$

for every $f \in C_c$. If $\text{Tr}(fA)$ is continuous in f in the C_c -topology, then the Riesz representation theorem shows that (2.5), for every $f \in C_c$, define $\text{den}[A]$ uniquely. In our case, we will frequently stipulate stronger regularity assumptions on A , implying that $\text{den}[A]$ is actually in a reasonable function space. (e.g. Lemma 2.1 below).

If an operator A has an (distributional) integral kernel, $A(x, y)$, with the diagonal, $A(x, x)$, being a regular countably additive complex Borel measure, then

$$\text{den}(A)(x) = A(x, x). \tag{2.6}$$

Finally, den is a linear map on locally trace class operators with the property that for any $f \in C_c$,

$$\text{den}(fA) = f \text{den}(A). \tag{2.7}$$

Lemma 2.1 *Let A be a locally trace class operator on L^2 and $\epsilon > 0$. We have the following statements.*

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

$$\|\text{den}[A]\|_{L^2} \lesssim \|(1 - \Delta)^{3/4+\epsilon} A\|_{S^2}, \tag{2.8}$$

$$\|\text{den}[A]\|_{L^2_{\text{per}}} \lesssim |\Omega|^{1/2} \|(1 - \Delta)^{3/4+\epsilon} A\|_{S^2_{\text{per}}} \tag{2.9}$$

(2) *If $(1 - \Delta)^{1/4+\epsilon} A \in S^{6/5}$, then $\text{den}[A] \in \dot{H}^{-1}$ (where \dot{H}^s is defined in (1.24)). Moreover,*

$$\|\text{den}[A]\|_{\dot{H}^{-1}} \lesssim \|(1 - \Delta)^{1/4+\epsilon} A\|_{S^{6/5}} \tag{2.10}$$

Proof We prove (2.9) and (2.10) only; (2.8) is similar and easier. We begin with (2.9). 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 $L^2_{\text{per}}-L^2_{\text{per}}$ duality, relation (2.5), $\text{den}[A] \in L^2_{\text{per}}$ and (2.9) holds if and only if

$$|\text{Tr}_{\Omega}(fA)| \lesssim |\Omega|^{1/2} \|f\|_{L^2_{\text{per}}} \|(1 - \Delta)^{3/4+\epsilon} A\|_{S^2_{\text{per}}} \tag{2.11}$$

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,

$$\frac{1}{|\Omega|} |\text{Tr}_{\Omega}(fA)| = \frac{1}{|\Omega|} |\text{Tr}(\chi_{\Omega} f A \chi_{\Omega})| \tag{2.12}$$

$$\lesssim \|A(1 - \Delta)^{3/4+\epsilon}\|_{S^2_{\text{per}}} \|(1 - \Delta)^{-3/4-\epsilon} f\|_{S^2_{\text{per}}}. \tag{2.13}$$

By the Kato–Seiler–Simon inequality

$$\|f(x)g(-i\nabla)\|_{S^p} \lesssim \|f\|_{L^p} \|g\|_{L^p} \tag{2.14}$$

for $2 \leq p < \infty$ (see [36]; one can also replace S^p and L^p by their periodic versions S^p_{per} and L^p_{per} , respectively.), we obtain (2.11). Thus, (2.9) is proved.

Now we prove (2.10) as above. By the $\dot{H}^1-\dot{H}^{-1}$ duality, it suffices to show that

$$|\text{Tr}(fA)| \lesssim \|f\|_{\dot{H}^1} \|(1 - \Delta)^{1/4+\epsilon} A\|_{S^{6/5}} \tag{2.15}$$

for all $f \in \dot{H}^1 \cap C_c$ and for $\epsilon > 0$. So, we estimate $|\text{Tr}(fA)|$. By the non-abelian Hölder inequality with $1 = \frac{1}{6} + \frac{1}{6/5}$ ([36]),

$$|\text{Tr}(fA)| \lesssim \|f(1 - \Delta)^{-1/4-\epsilon}\|_{S^6} \|(1 - \Delta)^{1/4+\epsilon} A\|_{S^{6/5}}. \tag{2.16}$$

The Kato–Seiler–Simon inequality (2.14) shows

$$|\text{Tr}(fA)| \lesssim \|f\|_{L^6} \|(1 - \Delta)^{1/4+\epsilon} A\|_{S^{6/5}}. \tag{2.17}$$

Now, applying the Gagliardo–Nirenberg–Sobolev inequality (for $d = 3$; see [24])

$$\|f\|_{L^6} \lesssim \|\nabla f\|_{L^2} \tag{2.18}$$

to $\|f\|_{L^6}$ in (2.17), we obtain (2.15). The proof of Lemma 2.1 is completed by the $\dot{H}^1-\dot{H}^{-1}$ duality and the fact that $\dot{H}^1 \cap C_c$ is dense in \dot{H}^1 . □

2.3 Bloch–Floquet Decomposition

Let \mathcal{L}^* denote the lattice reciprocal to \mathcal{L} , with the reciprocity relation between bases for \mathcal{L} and \mathcal{L}^* given by $\omega_i \cdot \omega_j^* = 2\pi \delta_{ij}$. Define the (fiber integral) space

$$\mathcal{H}_{\mathcal{L}}^{\oplus} = \{f \in L^2_{\text{loc}}(\mathbb{R}^3_k \times \mathbb{R}^3_x) : T_s^x f = f\} \tag{2.19}$$

$$\text{and } T_r^k f = e^{-ir \cdot x} f, \quad \forall s \in \mathcal{L}, \forall r \in \mathcal{L}^*, \tag{2.20}$$

where T_s^k is the translation in the k -variable by s and T_r^x is the translation in the x -variable by r (see (2.1)). We write $f = f_k(x) \in \mathcal{H}_{\mathcal{L}}^{\oplus}$ as

$$f = \int_{\mathbb{R}^3/\mathcal{L}^*}^{\oplus} f_k d\hat{k} = \int_{\Omega^*}^{\oplus} f_k d\hat{k}, \tag{2.21}$$

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

$$U_{\text{BF}} f := \int_{\Omega^*}^{\oplus} d\hat{k} f_k, \tag{2.22}$$

$$f_k(x) := \sum_{t \in \mathcal{L}} e^{-ik(x+t)} f(x+t) \tag{2.23}$$

and the inverse Bloch–Floquet transform

$$U_{\text{BF}}^{-1} \left(\int_{\Omega^*}^{\oplus} d\hat{k} f_k \right) (x) := \int_{\Omega^*} d\hat{k} e^{ikx} f_k(x), \quad \forall x \in \mathbb{R}^3. \tag{2.24}$$

Lemma 2.2 *We have, for any $f \in L^2$,*

$$\int_{\Omega} f_k(x) dx = \hat{f}(k) \tag{2.25}$$

Proof By (2.23) and a change of variable, we see that

$$\int f_k(x) dx := \int_{\Omega} \sum_{t \in \mathcal{L}} e^{-ik(x+t)} f(x+t) dx \tag{2.26}$$

$$= \sum_{t \in \mathcal{L}} \int_{t+\Omega} e^{-ikx} f(x) dx \tag{2.27}$$

$$= \int e^{-ikx} f(x) dx. \tag{2.28}$$

Equation (2.25) 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 2.3 *Let $f \in L^2$ and f_k be its k -th fiber \mathcal{L} -Bloch–Floquet decomposition. Then for any $S \subset \Omega^*$,*

$$\chi_S(-i\nabla) f = U_{\text{BF}}^{-1} \int_S^{\oplus} d\hat{k} \langle f_k \rangle_{\Omega}. \tag{2.29}$$

Proof Let $f \in L^2$ with the k -th fiber f_k . Then Lemma 2.2 shows that

$$\langle f_k \rangle_\Omega = |\Omega|^{-1} \hat{f}(k). \tag{2.30}$$

Using the definition of the inverse Bloch transform in (2.24) and (2.30), we see that

$$\begin{aligned} U_{\text{BF}}^{-1} \left(\int_S^\oplus d\hat{k} \langle f_k \rangle_\Omega \right) &= \int_{\Omega^*} d\hat{k} e^{i\hat{k}x} \langle f_k \rangle_{\Omega_\delta} \\ &= \int_S d\hat{k} |\Omega|^{-1} e^{i\hat{k}x} \hat{f}(k) \end{aligned} \tag{2.31}$$

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

$$U_{\text{BF}}^{-1} \int_S^\oplus d\hat{k} \langle f_k \rangle_\Omega = \int_S dk e^{ikx} \hat{f}(k) = \chi_S(-i\nabla) f, \tag{2.32}$$

which gives (2.29). □

Let $P_r = \chi_{B(r)}(-i\nabla)$ where $B(r)$ is the ball of radius r centered at the origin (see (3.37)). Lemmas 2.2 and 2.3 imply

Corollary 2.4 *Let $f \in L^2$ and $B(r) \subset \Omega^*$, then*

$$(P_r f)_k = |\Omega|^{-1} \hat{f}(k) \chi_{B(r)}(k). \tag{2.33}$$

Any \mathcal{L} -periodic operator A has a Bloch–Floquet decomposition [34] in the sense that

$$A = U_{\text{BF}}^{-1} \int_{\Omega^*}^\oplus d\hat{k} A_k U_{\text{BF}}, \tag{2.34}$$

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

$$\int_{\Omega^*}^\oplus d\hat{k} A_k \cdot \int_{\Omega^*}^\oplus d\hat{k} f_k = \int_{\Omega^*}^\oplus d\hat{k} A_k f_k. \tag{2.35}$$

Definitions (2.34) and (2.35) implies the following relations for any \mathcal{L} -periodic operators A and B

$$(Af)_k = A_k f_k, \tag{2.36}$$

$$(AB)_k = A_k B_k, \tag{2.37}$$

$$\|A\| = \sup_{k \in \Omega^*} \|A_k\|. \tag{2.38}$$

Furthermore, we have

Lemma 2.5 *Let A be an \mathcal{L} -periodic operator and A_k , its k -fibers in its Bloch–Floquet decomposition. Then*

$$A_k = e^{-ixk} A_0 e^{ixk}.$$

Proof We compute $(Af)_k$. Let T_s denote the translation operator (2.1). Let A_0 denote the 0-th fiber of A in its Bloch–Floquet decomposition. By (2.23) and the periodicity of A ,

$$(Af)_k = \sum_{t \in \mathcal{L}} e^{-ik(x+t)} T_{-t} Af = \sum_{t \in \mathcal{L}} e^{-ikx} A e^{-ikt} T_{-t} f \tag{2.39}$$

$$= e^{-ikx} A_0 e^{ikx} \sum_{t \in \mathcal{L}} e^{-ik(x+t)} T_{-t} f \tag{2.40}$$

$$= e^{-ikx} A_0 e^{ikx} f_k. \tag{2.41}$$

□

Now, we have the following result.

Lemma 2.6 *Let A be an \mathcal{L} -periodic operator and A_k , its k -fibers in its Bloch–Floquet decomposition and let r be such that $B(r) \subset \Omega^*$. Then*

$$P_r A P_r = b(-i\nabla) P_r \tag{2.42}$$

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 2.3 with $S = B(r)$ and $f = A P_r \varphi$ (so that $\chi_S(-i\nabla) = P_r$) to obtain

$$P_r A P_r \varphi = U_{\text{BF}}^{-1} \int_{\Omega^*}^{\oplus} d\hat{k} \langle (A P_r \varphi)_k \rangle_\Omega. \tag{2.43}$$

By Corollary 2.4 and Eq. (2.43), we find

$$P_r A P_r \varphi = |\Omega|^{-1} U_{\text{BF}}^{-1} \int_{B(r)}^{\oplus} d\hat{k} \langle A_k \mathbf{1} \rangle_\Omega \hat{\varphi}(k), \tag{2.44}$$

where $1 \in L^2_{\text{per},\delta}$ is the constant function equal to 1. Using the definition (2.24) of the inverse Bloch–Floquet transform and that $d\hat{k} = |\Omega|^{-1} dk$, we deduce (2.48). □

2.4 Passing to the Macroscopic Variables

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

$$U_\delta : f(x) \mapsto \delta^{-3/2} f(\delta^{-1}x) \tag{2.45}$$

mapping from the microscopic to the macroscopic scale. A change of variable in (2.5) gives the following

Lemma 2.7 *For any operator A on L^2 , we have*

$$\delta^{-3/2} U_\delta \text{den}[A] = \text{den}[U_\delta A U_\delta^*]. \tag{2.46}$$

Finally, note that

$$A \text{ is } \mathcal{L}\text{-periodic iff } U_\delta A U_\delta^* \text{ be } \mathcal{L}_\delta\text{-periodic.} \tag{2.47}$$

Lemma 2.6 implies

Lemma 2.8 *Let A be an \mathcal{L} -periodic operator and A_k , its k -fibers in its Bloch–Floquet decomposition and let r be such that $B(\delta r) \subset \Omega^*$. Then*

$$P_r U_\delta A U_\delta^* P_r = b(-i\delta\nabla) P_r \tag{2.48}$$

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

Proof By $U_\delta^* P_r U_\delta = P_{\delta r}$ and Lemma 2.6, we have

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

Relations $U_\delta P_{\delta r} U_\delta^* = P_r$ and $U_\delta b(-i\nabla) U_\delta^* = b(-i\delta\nabla)$ yield (2.48). □

3 Dielectric Response: Proof of Theorem 1.2

In this section, we prove Theorem 1.2 modulo several technical (though important) statements proved in Sects. 4 and 5.

3.1 Linearized Map

Our starting point is Eq. (1.5), which we reproduce here

$$-\Delta\phi = (\kappa - \text{den}[f_T(h^\phi - \mu)]), \tag{3.1}$$

where, recall, $f_T(\lambda)$ is given in (1.2) and, recall,

$$h^\phi := -\Delta - \phi. \tag{3.2}$$

We consider (3.1) on the function space $\phi \in H^2_{\text{per}} + \dot{H}^1$. 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 linearization of the map on the r.h.s. of (3.1)

$$M := d_\phi \text{den}[f_T(h^\phi - \mu)]|_{\phi=\phi_{\text{per}}}. \tag{3.3}$$

To derive basic properties of M , we find an explicit formula for it. Recalling the relation $f_T(\lambda) := f_{FD}(\lambda/T)$, see (1.2), and assuming that ϕ is close to ϕ_{per} , we write $f_T(h^\phi - \mu)$ using the Cauchy-integral formula

$$f_T(h^\phi - \mu) = \frac{1}{2\pi i} \int_\Gamma dz f_T(z - \mu)(z - h^\phi)^{-1} \tag{3.4}$$

where Γ is a positively oriented contour around the spectrum of h^ϕ not containing the poles of f_T which are located at $\mu + i\pi(2k + 1)T$, $k \in \mathbb{Z}$ (see Fig. 2 below), in which ϵ satisfies

$$\epsilon < T\pi \quad \text{and} \quad -1 < \cos(\mu\epsilon). \tag{3.5}$$

Here we use that h^ϕ is bounded from below and, due to the definition $f_T(\lambda) = \frac{1}{e^{\lambda/T} + 1}$ (see (1.2)) and the relation $|\text{Im}z| \leq \pi/4T$,

$$|f_T(z - \mu)| \lesssim \min(1, e^{-(\text{Re}z - \mu)/T}) \tag{3.6}$$

assuring the convergence of the integral. (Note that we do not use that h^ϕ has a gap and that μ is in the gap.)

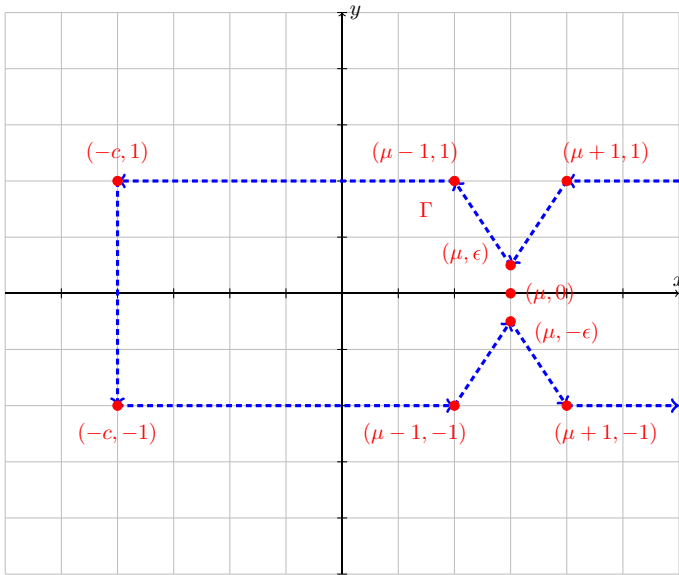


Fig. 1 The contour Γ . It depends on ϵ satisfying (3.5)

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

$$\oint := \frac{1}{2\pi i} \int_{\Gamma} dz f_T(z - \mu) \tag{3.7}$$

where Γ is the contour given in Fig. 1, with the positive orientation.

Recall the notation for the \mathcal{L} -periodic Hamiltonian and introduce one for the \mathcal{L} -periodic resolvent:

$$h_{\text{per}} := h^{\phi_{\text{per}}} = -\Delta - \phi^{\text{per}}, \quad r_{\text{per}}(z) = (z - h_{\text{per}})^{-1}. \tag{3.8}$$

By Theorem 1.5, the electrostatic potential, $\phi_{\text{per}}(y)$ associated with the solution $\rho_{\text{per}}(y)$ (c.f. (1.9)) satisfies

$$\phi_{\text{per}} \in H^2_{\text{per}}. \tag{3.9}$$

Hence the operator h_{per} is self-adjoint and the operator functions above are well-defined. Moreover, under Assumption [A1],

$$\sup_{z \in \Gamma} \|(z - h_{\text{per}})^{-1}\|_{\infty} = O(1). \tag{3.10}$$

Finally, for any operator h , we denote $h^L : \alpha \rightarrow h\alpha$ and $h^R : \alpha \rightarrow \alpha h$.

The next proposition gives an explicit form for M and states its properties (also see [7]).

Proposition 3.1 *Let Assumption [A1] hold. Then*

(1) *The operator M has the following explicit representation*

$$Mf = -\operatorname{den} \left[\oint r_{\text{per}}(z) f r_{\text{per}}(z) \right] \tag{3.11}$$

$$= -\frac{1}{2} \operatorname{den} \left[\frac{\tanh(\frac{1}{2T}(h_{\text{per}}^L - \mu)) - \tanh(\frac{1}{2T}(h_{\text{per}}^R - \mu))}{h_{\text{per}}^L - h_{\text{per}}^R} f \right], \tag{3.12}$$

where $f \in L^2$ on the right hand side is considered as a multiplication operator.

(2) *The operator M is bounded, self-adjoint, positive on L^2 and \mathcal{L} -periodic (c.f. Sect. 2.2) and satisfies*

$$\|M\| \lesssim 1. \tag{3.13}$$

Proof of Proposition 3.1 In this proof, we omit the subscript “per” in h_{per} and $r_{\text{per}}(z)$. We begin with item (1). Equation (3.11) follows from definition (3.3), the Cauchy formula (3.4) and a simple differentiation of the resolvent.

Now, we use (3.11) to derive (3.12). By the definition of h^L and h^R and the second resolvent identity, we have, for any operator α ,

$$\begin{aligned} (z - h)^{-1} \alpha (z - h)^{-1} &= (z - h^L)^{-1} (z - h^R)^{-1} \alpha \\ &= (h^L - h^R)^{-1} ((z - h^L)^{-1} - (z - h^R)^{-1}) \alpha. \end{aligned} \tag{3.14}$$

Using the Cauchy integral formula and the definition (3.7) and the choice of the contour Γ i(see Fig. 1), we observe that

$$\begin{aligned} \oint (z - h)^{-1} \alpha (z - h)^{-1} &= (h^L - h^R)^{-1} \\ &\times \frac{1}{2\pi i} \int_{\Gamma} dz f_T(z - \mu) ((z - h^L)^{-1} - (z - h^R)^{-1}) \alpha \\ &= (h^L - h^R)^{-1} (f_T(h^L - \mu) - f_T(h^R - \mu)) \alpha. \end{aligned} \tag{3.15}$$

Now, by definition (1.2), $f_T(\lambda) := \frac{1}{e^{\lambda/T} + 1}$ and therefore $f_T(\lambda) = \frac{1}{2}(1 + \tanh(\lambda/2T))$. This relation, together with (3.15), gives

$$\begin{aligned} \oint (z - h)^{-1} \alpha (z - h)^{-1} &= \frac{1}{2} \frac{\tanh(\frac{1}{2T}(h^L - \mu)) - \tanh(\frac{1}{2T}(h^R - \mu))}{h^L - h^R} \alpha. \end{aligned} \tag{3.16}$$

This, together with (3.11), gives (3.12). Item (1) is now proved.

Now we prove item (2). Since $h = h_{\text{per}}$ is self-adjoint and bounded below, we can pick $c > 0$ sufficiently large, s.t. $h \geq -c + 1$. Then, in particular, $h + c$ is invertible and, for each function $f \in L^2(\mathbb{R}^3)$, we define the operator

$$\alpha_f := (c + h)^{-1/2} f (c + h)^{-1/2}. \tag{3.17}$$

The Kato–Seiler–Simon inequality (2.14) shows that α_f is Hilbert–Schmidt and

$$\|\alpha_f\|_{S^2} \lesssim \|f\|_{L^2} \tag{3.18}$$

(the S^2 norm is given in (2.3)). Using (3.11), together with (2.5), we write $\langle f, Mg \rangle$

$= -\oint \text{Tr}(\bar{f}r(z)gr(z))$, which can be transformed to

$$\langle f, Mg \rangle = -\oint \text{Tr}(\alpha_f^*(c+h)r(z)\alpha_g r(z)(c+h)). \tag{3.19}$$

Moreover, by (3.16), we have that

$$\langle f, Mg \rangle = \text{Tr}(\alpha_f^*G(h^L, h^R)\alpha_g), \tag{3.20}$$

$$G(x, y) := -\frac{1}{2} \frac{\tanh(\frac{1}{2T}(x-\mu)) - \tanh(\frac{1}{2T}(y-\mu))}{(x+c)^{-1} - (y+c)^{-1}}. \tag{3.21}$$

Since the function $G : \mathbb{R}^2 \rightarrow \mathbb{R}$ is bounded on the set $x, y \geq -c + 1$, we see that M is bounded due to (3.18) and (3.20).

Moreover, we can also see from expressions (3.20) - (3.21) that M is symmetric since G is real and h^L and h^R are self-adjoint in the space S^2 . Since M is bounded, it is self-adjoint. Since the function G in (3.21) is positive for $x, y \geq -c + 1$, Eq. (3.20) and spectral theorem on S^2 show that $\langle f, Mf \rangle = \text{Tr}(\alpha_f^*G(h^L, h^R)\alpha_f) > 0$ for any nonzero $f \in L^2(\mathbb{R}^3)$. This shows that M is positive.

Finally, formula (3.11) and the fact $h = h_{\text{per}}$ and $r = r_{\text{per}}(z)$ are \mathcal{L} -periodic show that M is \mathcal{L} -periodic.

To prove bound (3.13), we use (3.11) and (2.8) to find

$$\|Mf\|_{L^2} \lesssim \|(1-\Delta)\oint r(z)fr(z)\|_{S^2} \tag{3.22}$$

$$\lesssim \left| \oint \|(1-\Delta)r(z)\|^2 \|f(1-\Delta)^{-1}\|_{S^2} \right|. \tag{3.23}$$

Now, writing $-\Delta = h - z + \phi_{\text{per}} + z$, for $z \in \Gamma$, and using the uniform boundedness of $\|\phi_{\text{per}}\|_{H^2}$ which follows from Assumption [A1], we derive the estimate

$$\|(1-\Delta)r(z)\| \lesssim 1, \tag{3.24}$$

which, together with (3.23) and the Kato-Seiler-Simon inequality (2.14), gives bound (3.13). The proof of Proposition 3.1 is now complete. \square

3.2 Scaling and Splitting

This step is to pass from the microscopic coordinate y to the macroscopic one, $x = \delta y$ passing to the macroscopic quantities (with superscripts δ) which are related the microscopic quantities (with subscripts δ) as

$$\kappa^\delta = \delta^{-3/2}U_\delta\kappa_\delta, \quad \phi^\delta(x) = \delta^{1/2}(U_\delta\phi_\delta)(x) = \delta^{-1}\phi_\delta(\delta^{-1}x), \tag{3.25}$$

$$\kappa_{\text{per}}^\delta(x) := \delta^{-3}\kappa_{\text{per}}(\delta^{-1}x) = (\delta^{-3/2}U_\delta\kappa_{\text{per}})(x), \tag{3.26}$$

where $U_\delta : f(x) \mapsto \delta^{-3/2}f(\delta^{-1}x)$, the $L^2(\mathbb{R}^3)$ -unitary scaling map, see (2.45) (note that the L^1 -norm, hence total charge, is preserved under this scaling). Let

$$\kappa^\delta(x) = \kappa_{\text{per}}^\delta(x) + \kappa'(x) \tag{3.27}$$

be the macroscopic perturbed background potential. Accordingly, we rescale equation (3.1) by applying $\delta^{-3/2}U_\delta$ to it. Using Lemma 2.7 and relations $U_\delta f_T(h^\phi - \mu)U_\delta^* = f_T(U_\delta h^\phi U_\delta^* - \mu)$ and

$$U_\delta h^\phi U_\delta^* = -\delta^2 \Delta - \delta \phi^\delta,$$

we arrive at the rescaled electrostatic potential equation

$$-\Delta \phi^\delta = \kappa^\delta - F_\delta(\phi^\delta), \tag{3.28}$$

$$F_\delta(\phi) = \text{den}[f_T(-\delta^2 \Delta - \delta \phi - \mu)]. \tag{3.29}$$

We will consider (3.28) on the space $H_{\text{per}}^2 + \dot{H}^1$.

Let $\phi_{\text{per}}^\delta = \delta^{1/2} U_\delta \phi_{\text{per}}$, where ϕ_{per} is the periodic potential associated to the periodic solution $(\rho_{\text{per}}, \mu_{\text{per}})$ of (1.1) with periodic background charge κ_{per} given in Theorem 1.5. We split the solution ϕ^δ into the big part ϕ_{per}^δ and the fluctuation

$$\varphi \equiv \phi^\delta := \phi^\delta - \phi_{\text{per}}^\delta. \tag{3.30}$$

We rewrite Eq. (3.28) by expanding the r.h.s. around ϕ_{per}^δ to obtain

$$K_\delta \varphi = \kappa' + N_\delta(\varphi) \tag{3.31}$$

where N_δ is defined by this expression and

$$K_\delta = -\Delta + M_\delta, \text{ with } M_\delta = d_\phi F_\delta(\phi_{\text{per}}^\delta). \tag{3.32}$$

Note that the inputs into this equation are $\phi_{\text{per}}, \mu = \mu_{\text{per}}$ and κ' (cf. (1.44)).

As was mentioned in the introduction, we prove Theorem 1.2 by decomposing φ in (3.30) in small and large momentum parts (c.f. [8]). 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 (1.1) by applying $\delta^{-3/2} U_\delta$ to it and rescaled the microscopic potentials via (3.25), it follows that

$$F_\delta = \delta^{-3/2} U_\delta \circ F \circ (\delta^{-1/2} U_\delta^*) \tag{3.33}$$

where $F = F_{\delta=1}$. Thus, by the definition of M_δ in (3.32) and the fact it is linear, it can be written as

$$M_\delta = \delta^{-2} U_\delta M U_\delta^*, \tag{3.34}$$

where $M := M_{\delta=1}$ and is given by (3.3).

Recall that an operator A on $L^2(\mathbb{R}^3)$ is said to be \mathcal{L} -periodic if and only if it commutes with the translations T_s (see (2.1)) by all lattice elements $s \in \mathcal{L}$. As an immediate consequence of Proposition 3.1, representation (3.11), and the rescaling (3.34), we have the following result

Proposition 3.2 *Let Assumption [A1] hold. Then M_δ is \mathcal{L}_δ -periodic, positive (so that $K_\delta = -\Delta + M_\delta > -\Delta$), bounded on L^2 with an $O(\delta^{-2})$ bound, and has the following representation*

$$M_\delta \varphi = -\delta \text{den} \left[\oint r_{\text{per}}^\delta(z) \varphi r_{\text{per}}^\delta(z) \right], \tag{3.35}$$

where the resolvent operator $r_{\text{per}}^\delta(z)$ acting on $L^2(\mathbb{R}^3)$ is given by

$$r_{\text{per}}^\delta(z) = (z - h_{\text{per}}^\delta)^{-1}, \quad h_{\text{per}}^\delta = -\delta^2 \Delta - \delta \phi_{\text{per}}^\delta. \tag{3.36}$$

3.3 Lyapunov–Schmidt Decomposition

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}_δ^* as in Sect. 2.4. We recall the definition of the orthogonal projection onto low momenta (as [8])

$$P_r = \chi_{B(r)}(-i\nabla), \tag{3.37}$$

where $B(r)$ is the ball of radius r centred at the origin. With m given in (1.33) and estimated in (1.34), we choose r such that $B(r) \subset \Omega_\delta^*$ and

$$a := \delta r = O(1) \text{ small, but } a^4 \gg m, \tag{3.38}$$

is independent of δ and T (or m) and is fixed. Below, we use the convention that \lesssim is independent of r, δ and T . Let

$$\bar{P}_r = 1 - P_r \tag{3.39}$$

be the orthogonal projection onto the large momenta. We decompose

$$\varphi = \varphi_s + \varphi_l, \tag{3.40}$$

where $\varphi_s = P_r\varphi$ and $\varphi_l = \bar{P}_r\varphi$. Here s stands for small momentum and l stands for large momenta. We split (3.31) as

$$P_r K_\delta(\varphi_s + \varphi_l) = P_r \kappa' + P_r N_\delta(\varphi), \tag{3.41}$$

$$\bar{P}_r K_\delta(\varphi_s + \varphi_l) = \bar{P}_r \kappa' + \bar{P}_r N_\delta(\varphi). \tag{3.42}$$

We solve (3.42) for φ_l in the ball

$$B_{l,\delta} := \{\varphi \in \bar{P}_r H^1 : \|\varphi\|_{\dot{H}^1} \leq c_l\}, \tag{3.43}$$

while keeping φ_s fixed in the (deformed) ball

$$B_{s,\delta} := \{\varphi \in P_r H^1 : \|\varphi\|_\delta \leq c_s\}, \tag{3.44}$$

with the norm $\|\varphi\|_\delta$ given by

$$\|\varphi\|_\delta^2 := \sum_0^1 \zeta^{2(i-1)} \|\nabla^i \varphi\|_{L^2}^2, \quad \zeta := \delta m^{-1/2}. \tag{3.45}$$

The constants c_s and c_l above (should not be confused with the estimating function c_T which appeared in Theorem 1.2) are chosen to satisfy the conditions

$$\zeta \ll c_s \ll c_l \ll \theta^{-3/2} \zeta, \tag{3.46}$$

where $\theta := m^{-8/9} \delta$ and, recall, $\zeta := \delta m^{-1/2}$.

The latter condition can be satisfied, provided

$$\theta := m^{-8/9} \delta \ll 1. \tag{3.47}$$

Due to estimate (1.34), this is equivalent to condition (1.28).

We see that, while our model is parametrized by δ and β satisfying (1.28), our method is determined by the parameters a, c_s and c_l , satisfying (3.38) and (3.46).

The subleading term, ψ , in (1.29) just fits into $B_{s,\delta}$: $\|\psi\|_\delta \sim \zeta \ll c_s$. Finally, we note that since $\nabla^{-1} \bar{P}_r \leq r^{-1} \bar{P}_r$, $\nabla^{-1} := \nabla \Delta^{-1}$, $r = a/\delta$, we have

$$\|\varphi\|_{L^2} \lesssim m^{1/2} \zeta \|\varphi\|_{\dot{H}^1}, \quad \|\varphi\|_\delta \lesssim \|\varphi\|_{\dot{H}^1}, \quad \forall \varphi \in \text{Ran } \bar{P}_r. \tag{3.48}$$

Equation (3.48) shows that, if $m^{1/2} \zeta = \delta \ll c_s/c_l$, then, in the L^2 -norm, $B_{l,\delta}$ is much smaller than $B_{s,\delta}$.

In the proofs below, we will use the convention $\|\cdot\|_{\dot{H}^0} \equiv \|\cdot\|_{L^2}$ and the estimates of the nonlinearity N_δ (defined implicitly through (3.31)) proved in Proposition 5.2 in Sect. 5 below, under Assumption [A1]:

$$\begin{aligned} & \|N_\delta(\varphi_1) - N_\delta(\varphi_2)\|_{L^2} \\ & \lesssim m^{-\frac{1}{3}} \delta^{-1/2} (\|\varphi_1\|_\delta + \|\varphi_2\|_\delta) \|\varphi_1 - \varphi_2\|_\delta. \end{aligned} \tag{3.49}$$

Proposition 3.3 *Let Assumptions [A1]–[A3] hold. Assume $\varphi_s \in B_{s,\delta}$ and that (3.38) holds. Then Eq. (3.42) on $B_{l,\delta}$ has a unique solution $\varphi_l = \varphi_l(\varphi_s) \in B_{l,\delta}$.*

Proof of Proposition 3.3 We use that, by Proposition 3.2, $\bar{K}_\delta := \bar{P}_r K_\delta \bar{P}_r$ is invertible on the range of \bar{P}_r (see (3.39)) to convert (3.42) into a fixed point problem

$$\varphi_l = \Phi_l(\varphi_l) = \Phi'_l + \Phi''_l(\varphi_l), \tag{3.50}$$

where

$$\Phi'_l := \bar{K}_\delta^{-1} (-M_\delta \varphi_s + \bar{P}_r \kappa'), \tag{3.51}$$

$$\Phi''_l(\varphi_l) := \bar{K}_\delta^{-1} \bar{P}_r N_\delta(\varphi_s + \varphi_l). \tag{3.52}$$

Given φ_s , this is a fixed point problem for φ_l . We will solve this problem in the ball $B_{l,\delta}$ defined in (3.43). Let $\dot{H}^0 \equiv L^2$. We begin with the following simple but key lemma

Lemma 3.4 *Let Assumption [A1] hold and let $c_T := T^{-1} e^{-\eta_0/T} \lesssim 1$ (which is weaker than Assumption [A3]). Then, for $f \in L^2(\mathbb{R}^3)$,*

$$\|\bar{K}_\delta^{-1} f\|_{\dot{H}^{k-i}} \lesssim r^{-2+k} \|f\|_{\dot{H}^{-i}}, \quad i \leq k, \quad k = 0, 1 \tag{3.53}$$

$$\|\bar{K}_\delta^{-1} M_\delta P_r f\|_{L^2} \lesssim \|f\|_{L^2}, \tag{3.54}$$

$$\|\bar{K}_\delta^{-1} M_\delta P_r f\|_{\dot{H}^1} \lesssim \|f\|_\delta. \tag{3.55}$$

Proof of Lemma 3.4 Since $-\Delta \bar{P}_r \geq r^2 \bar{P}_r$, we have the inequality $r^2 \|f\|^2 \lesssim \langle f, \bar{K}_\delta f \rangle \leq \|f\| \|\bar{K}_\delta f\|$, which gives $r^2 \|f\| \lesssim \|\bar{K}_\delta f\|$, which implies (3.53) for $k = i = 0$.

Since $\bar{K}_\delta \bar{P}_r \geq -\Delta \bar{P}_r$, we have $\|\bar{P}_r f\|_{\dot{H}^1}^2 \lesssim \langle f, \bar{K}_\delta f \rangle \leq \|\bar{P}_r f\| \|\bar{K}_\delta f\|$. This inequality and $\|\bar{P}_r f\| = \|\nabla^{-1} \bar{P}_r \nabla f\| \leq r^{-1} \|\nabla f\|$, where

$$\nabla^{-1} := \nabla(-\Delta)^{-1}, \tag{3.56}$$

give $\|\bar{P}_r f\|_{\dot{H}^1} \lesssim r^{-1} \|\bar{K}_\delta f\|$, which implies (3.53) for $k = 1$.

Inequality (3.53), with $i = 0$, and the bound $\|M_\delta\| \lesssim \delta^{-2}$, proven in Proposition 3.2, yield

$$\|\bar{K}_\delta^{-1} M_\delta P_r f\|_{\dot{H}^k} \lesssim r^k \|f\|_{L^2}, \tag{3.57}$$

for $k = 0, 1$, which for $k = 0$ implies (3.54).

Finally, we prove more subtle (3.55). Using ∇^{-1} from (3.56), we write $\nabla \bar{K}_\delta^{-1} M_\delta f = \nabla \bar{K}_\delta^{-1} \nabla \cdot (\nabla^{-1} M_\delta) f$. Proposition 3.2 shows that $\nabla \bar{K}_\delta^{-1} \nabla \leq 1$. It follows

$$\|\nabla \bar{K}_\delta^{-1} M_\delta f\|_{L^2} \lesssim \|\bar{P}_r \nabla^{-1} M_\delta f\|_{L^2}. \tag{3.58}$$

This bound and Proposition C.4 of Appendix C imply (3.55). □

Definition (3.51) and Eqs. (3.55) and (3.53), with $k = 1, i = 0$, show that

$$\|\Phi'_l\|_{\dot{H}^1} \lesssim \|\varphi_s\|_\delta + r^{-1} \|\kappa'\|_{L^2}. \tag{3.59}$$

For the nonlinear term, $\bar{\Phi}''_l(\varphi_l) := K_\delta^{-1} \bar{P}_r N_\delta(\varphi_s + \varphi_l)$ (see (3.52)), Eqs. (3.53), with $k = 1, i = 0$, (5.1) and the inequality $\|\varphi_l\|_{s,\delta} \lesssim \|\varphi_l\|_{\dot{H}^1}$ (see (3.48)) give

$$\|\bar{\Phi}''_l(\varphi_l)\|_{\dot{H}^1} \lesssim r^{-1} m^{-\frac{1}{3}} \delta^{-1/2} (\|\varphi_s\|_\delta + \|\varphi_l\|_{\dot{H}^1})^2. \tag{3.60}$$

Since $\|\varphi_s\|_\delta \leq c_s$ and $\|\varphi_l\|_\delta \leq c_l$ for $\varphi_s \in B_{l,\delta}$ and $\varphi_s \in B_{s,\delta}$ (see (3.44) and (3.43)) and, due to our assumption (3.46), we have

$$\delta \|\kappa'\|_{L^2} + c_s + \delta^{1/2} m^{-1/3} (c_s + c_l)^2 \ll c_l, \tag{3.61}$$

(3.59)–(3.61) show that Φ_l maps $B_{l,\delta}$ into itself.

Once more, by Eqs. (3.48), (3.53), with $k = 1, i = 0$, (3.49) and (3.55), we see that Φ_l satisfies

$$\begin{aligned} &\|\Phi_l(\varphi_1) - \Phi_l(\varphi_2)\|_{\dot{H}^1} \\ &\lesssim r^{-1} m^{-\frac{1}{3}} \delta^{-1/2} (\|\varphi_1\|_\delta + \|\varphi_2\|_\delta) \|\varphi_1 - \varphi_2\|_\delta \end{aligned} \tag{3.62}$$

and therefore, since $r = a/\delta$, is a contraction on $B_{l,\delta}$ for $m^{-\frac{1}{3}} \delta^{1/2} c_l \ll 1$, which follows from (3.46). Proposition 3.3 now follows by applying the fixed point theorem on $B_{l,\delta}$. □

Let $\varphi_l = \varphi_l(\varphi_s)$ be the solution to Eq. (3.42) given in Proposition 3.3 with $\varphi_s \in B_{s,\delta}$. Later on we will need a Lipschitz estimate on the solution, $\varphi_l(\varphi_s) \in B_{l,\delta}$.

Lemma 3.5 *If $\varphi, \psi \in B_{s,\delta}$, then the solution, $\varphi_l(\varphi_s) \in B_{l,\delta}$, to (3.42) given in Proposition 3.3 satisfies the estimate*

$$\|\varphi_l(\varphi) - \varphi_l(\psi)\|_{\dot{H}^1} \lesssim \|\varphi - \psi\|_\delta. \tag{3.63}$$

Proof Since $\varphi_l(\varphi), \varphi_l(\psi)$ satisfy (3.42) (and therefore (3.50)), we see that

$$\begin{aligned} \varphi_l(\varphi) - \varphi_l(\psi) &= -\bar{K}_\delta^{-1} M_\delta(\varphi - \psi) \\ &\quad + \bar{K}_\delta^{-1} \bar{P}_r (N_\delta(\varphi + \varphi_l(\varphi)) - N_\delta(\psi + \varphi_l(\psi))). \end{aligned} \tag{3.64}$$

Using Eqs. (3.64), (3.53), with $k = 1, i = 0$, and (3.55) and nonlinear estimate (3.49) and going through the same arguments as in the proof of Proposition 3.3, we show (3.63). □

We substitute $\varphi_l = \Phi_l(\varphi_l)$ (see (3.50)), with $\Phi_l(\varphi_l)$ given by (3.50)–(3.52) into Eq. (3.41) and note that $P_r K_\delta \bar{P}_r = P_r M_\delta \bar{P}_r$ to arrive at the following equation

$$\ell \varphi_s = Q \kappa' + Q N(\varphi(\varphi_s)), \tag{3.65}$$

where $\varphi(\varphi_s) = \varphi_s + \varphi_l(\varphi_s)$ with $\varphi_l(\varphi_s)$ being the solution of (3.42), and

$$\ell := P_r K_\delta P_r - P_r M_\delta \bar{K}_\delta^{-1} M_\delta P_r, \tag{3.66}$$

$$Q := P_r - P_r M_\delta \bar{K}_\delta^{-1}. \tag{3.67}$$

Note that ℓ is the Feshbach–Schur map of $K_\delta := -\Delta + M_\delta$ with projection P_r .

In Sect. 3.4 below, we prove the following

Proposition 3.6 *Under Assumption [A1], Eq. (3.65) has a unique solution $\varphi_s \in B_{s,\delta}$.*

As a consequence of Propositions 3.3 and 3.6 and Eqs. (3.40) and (3.48), Eq. (3.31) has the unique solution $\varphi = \varphi_s + \varphi_l \in H^1(\mathbb{R}^3)$, with the estimate

$$\|\varphi\|_\delta \leq c_s + c_l.$$

This proves the existence and uniqueness of the solution $\phi_\delta \in (H^2_{\text{per}} + H^1)(\mathbb{R}^3)$ of (3.28) (and therefore of (1.5)) with κ given in (1.23). This completes the proof of Theorem 1.2(1). □

Now, we address Theorem 1.2(2). Below, we let $\beta = T^{-1}$, so that

$$c_T = \beta e^{-\beta\eta_0} =: s_\beta.$$

We begin with a result, proven in Sect. 4, which gives a detailed description of the operator ℓ .

Proposition 3.7 *On ran P_r , the operator ℓ in (3.66) is a smooth, real, even function of $-i\nabla$ and it has the expansion*

$$\ell = \nu - \nabla\epsilon\nabla + O(\delta^2(-i\nabla)^4) \tag{3.68}$$

where $\nu = \delta^{-2}|\Omega|^{-1}(m + O(s_\beta^2))$, with m given in (1.33), and ϵ is a matrix given explicitly in (1.35)–(1.37) and satisfies the estimate

$$\epsilon \geq \mathbf{1} - O(s_\beta^2). \tag{3.69}$$

By Proposition 3.7 the leading order term in ℓ is given by

$$\ell_0 := \nu - \nabla\epsilon\nabla, \tag{3.70}$$

where $\nu = \delta^{-2}|\Omega|(m + O(s_\beta^2))$, with m given in (1.33), $\epsilon \geq \mathbf{1} - O(s_\beta^2)$.

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

$$\ell_0\psi = \kappa' \tag{3.71}$$

(since $\nu > 0$ and $\epsilon > 0$, this solution exists) and write

$$\varphi_s = P_r\psi + \psi_1 \tag{3.72}$$

where ψ_1 is defined by this expression. In Sect. 3.5 below to prove the following

Proposition 3.8 *Under Assumption [A1], $\psi_1 \in B_{s,\delta}$ obeys the estimate*

$$\|\psi_1\|_\delta \lesssim (m^{1/2} + \theta^{1/2})\zeta. \tag{3.73}$$

Due to (3.40) and (3.72), the solution φ of Eq. (3.31) can be written as

$$\varphi = P_r\psi + \psi_1 + \varphi_l \tag{3.74}$$

with $\psi_1 \in B_{s,\delta}$, satisfying estimate (3.73), and $\varphi_l \in B_{l,\delta}$.

To complete the proof of item (2) of Theorem 1.2, we notice that (3.30), (3.74) and the relation $P_r\psi = \psi - \bar{P}_r\psi$ imply (1.29) with

$$\varphi_{\text{rem}} = \psi_1 - \bar{P}_r\psi + \varphi_l. \tag{3.75}$$

Thus it remains to estimate the remainders above (see (1.30)).

Equation (3.73) controls ψ_1 . To control the term $-\bar{P}_r\psi$, we use (3.56) and $\ell_0^{-1}\bar{P}_r \leq r^{-2}$ to obtain, for $i = 0, 1$,

$$\begin{aligned} \|\bar{P}_r\psi\|_{\dot{H}^i} &= \|\nabla^i \bar{P}_r \ell_0^{-1} \kappa'\|_{L^2} = \|\ell_0^{-1} \bar{P}_r \nabla^i \kappa'\|_{L^2} \\ &\lesssim r^{-2} \|\kappa'\|_{\dot{H}^i}. \end{aligned} \tag{3.76}$$

Since, by condition (1.28), $(m^{1/2} + \theta^{1/2})\zeta^{2-i} \gg \delta^2$, Eqs. (3.73) and (3.76), together with (3.75), show that

$$\|\psi_1 - \bar{P}_r\psi\|_\delta \lesssim (m^{1/2} + \theta^{1/2})\zeta. \tag{3.77}$$

By Proposition 3.3, φ_l is in the range of \bar{P}_r and bounded as $\|\varphi_l\|_{\dot{H}^1} \lesssim c_l$. Hence, using (3.48) and taking $c_l = \omega^{-1/4}\zeta$, $\omega := \max(\theta^2, m) \ll 1$ (satisfying (3.46)) and using that $r^{-1}\omega\zeta = \omega m^{1/2}\zeta^2 \ll m^{1/4}\zeta^2$, gives

$$\|\varphi_l\|_{L^2} \ll m^{1/4}\zeta^2, \quad \|\varphi_l\|_{\dot{H}^1} \lesssim \omega^{-1/4}\zeta. \tag{3.78}$$

By (1.34), Eqs. (3.77) and (3.78) imply part (2) of Theorem 1.2.

Finally, part (3) of Theorem 1.2 follows from Proposition 3.7 and Eqs. (3.70) and (3.71). \square

3.4 Small Quasi-momenta: Proof of Proposition 3.6

Our starting point is Eq. (3.65). By Proposition 3.7, the operator ℓ given in (3.66) is invertible. Hence we can rewrite (3.65) as the fixed point problem:

$$\varphi_s = \Phi_s(\varphi_s), \quad \Phi_s(\varphi_s) := -\ell^{-1}Q(\kappa - N(\varphi(\varphi_s))), \tag{3.79}$$

where $\varphi(\varphi_s) = \varphi_s + \varphi_l(\varphi_s)$ with $\varphi_l(\varphi_s)$ being the solution of (3.42), and Q is given in (3.67).

First, we estimate the operator $\ell^{-1}Q$ in Φ_s . Recall, m is given in (1.33).

Lemma 3.9 *Assume (3.38) and, recall, $\zeta := \delta m^{-1/2}$. Then*

$$\|\ell^{-1}Qf\|_\delta \lesssim \zeta \|f\|_{L^2}. \tag{3.80}$$

Proof By the choice $a := \delta r = O(1)$ (see (3.38)), we have that that

$$O(\delta^2(-i\nabla)^4) = O(a^2(-i\nabla)^2) \text{ on } \text{Ran } P_r.$$

By Proposition 3.7, we have that $\nu = \delta^{-2}|\Omega|^{-1}(m + O(s_\beta^2))$, which, together with the lower bound in (1.34), implies

$$\nu \gtrsim \delta^{-2}|\Omega|^{-1}m = |\Omega|^{-1}\zeta^{-2}. \tag{3.81}$$

These two facts and Eq. (3.68) imply $\nabla^k \ell^{-1} \lesssim \zeta^{2-k}$, $k = 0, 1, 2$, which gives

$$\|\nabla^k \ell^{-1}\| \lesssim \zeta^{2-k}, \quad k = 0, 1, 2, \tag{3.82}$$

for the L^2 -operator norm. Furthermore, we claim the bound

$$\|\nabla^k \ell^{-1} P_r M_\delta \bar{K}_\delta^{-1}\| \lesssim \zeta^{2-k} m^{1/2}. \tag{3.83}$$

Indeed, decomposing M_δ according to (C. 2)–(C. 4) of Proposition C.1 and using bound Eqs. (3.82), we find

$$\begin{aligned} & \|\nabla^k \ell^{-1} P_r M_\delta \nabla^{-1} \bar{P}_r\| \\ & \leq \|\nabla^k \ell^{-1} P_r M'_\delta P_r\| + \|\nabla^k \ell^{-1} \nabla P_r \nabla^{-1} M''_\delta \nabla^{-1} \bar{P}_r\| \\ & \lesssim \zeta^{2-k} \delta^{-1} m^{1/2} + \zeta^{1-k}, \end{aligned} \tag{3.84}$$

where $\|\cdot\|$ is the operator norm in L^2 . Since $\zeta := \delta m^{-1/2}$, this implies

$$\|\nabla^k \ell^{-1} P_r M_\delta \nabla^{-1} \bar{P}_r f\|_{L^2} \lesssim a^{-1} \zeta^{1-k} \|f\|_{L^2}. \tag{3.85}$$

Equation (3.53), with $k = 1, i = 0$, and (3.85), together with the insertion of $\mathbf{1} = \nabla^{-1} \nabla = \Delta^{-1} \nabla \nabla$ between M_δ and \bar{K}_δ^{-1} , imply (3.83).

Using (3.82) and (3.83) and recalling the definition $Q := P_r - P_r M_\delta \bar{K}_\delta^{-1}$ (see (3.67)), we find that

$$\|\nabla^k \ell^{-1} Q\| \lesssim \zeta^{2-k}, \quad k = 0, 1, 2, \tag{3.86}$$

which, due to the definition of the norm $\|f\|_\delta \simeq \sum_0^1 \zeta^{k-1} \|\nabla^k \varphi\|_{L^2}$ in (3.45), implies Lemma 3.9. □

Lemma 3.9 and nonlinear estimate (5.1), together with $\zeta \delta^{-1/2} = m^{-1/2} \delta^{1/2}$, imply that, under Assumption [A1],

$$\begin{aligned} & \|\ell^{-1} Q[N_\delta(\varphi) - N_\delta(\psi)]\|_\delta \\ & \lesssim m^{-5/6} \delta^{1/2} (\|\varphi\|_\delta + \|\psi\|_\delta) \|\varphi - \psi\|_\delta. \end{aligned} \tag{3.87}$$

Equation (3.79), Lemma 3.5 and estimate (3.87) imply, for $\varphi, \psi \in B_{s,\delta}$,

$$\|\Phi_s(\varphi_s)\|_\delta \lesssim \zeta \|\kappa'\|_{L^2} + m^{-5/6} \delta^{1/2} c_s^2, \tag{3.88}$$

$$\|\Phi_s(\varphi_s) - \Phi_s(\varphi'_s)\|_\delta \lesssim m^{-5/6} \delta^{1/2} c_s \|\varphi_s - \varphi'_s\|_\delta. \tag{3.89}$$

These inequalities, together with the inequality $m^{5/6} \delta^{-1/2} = \theta^{-3/2} \zeta \gg c_s \gg \zeta$, which follows from assumption (3.46), yield that $\Phi_s(\varphi_s)$ is a contraction on $B_{s,\delta}$ and therefore has a unique fixed point. This proves Proposition 3.6. □

3.5 Proof of Proposition 3.8

In view of Proposition 3.7, we write

$$\ell = \ell_0 + \ell', \tag{3.90}$$

where ℓ_0 is defined (3.70), and ℓ' is defined by this expression. By Proposition 3.7, $\ell' = O(\delta^2 (-i\nabla)^4)$ on the range of P_r .

Inserting (3.72) into Eq. (3.65) and using (3.90) and the relations $\ell P_r \psi = P_r \kappa' + \ell' P_r \psi$ and $-P_r \kappa' + Q \kappa' = -P_r M_\delta \bar{K}_\delta^{-1} \kappa'$, we obtain the equivalent equation for ψ_1 :

$$\ell \psi_1 = -\ell' P_r \psi - P_r M_\delta \bar{K}_\delta^{-1} \kappa' + Q N_\delta(\tilde{\varphi}), \tag{3.91}$$

$$\tilde{\varphi} = \tilde{\varphi}(\psi_1) := P_r \psi + \psi_1 + \varphi_l (P_r \psi + \psi_1), \tag{3.92}$$

with $\varphi_l = \varphi_l(f)$ the solution to Eq. (3.42) given by Proposition 3.3 with φ_s replaced by $f \in B_{s,\delta}$.

By Proposition 3.7, the operators ℓ and ℓ_0 are invertible. We invert ℓ_0 (see (3.70)) in (3.71) to obtain

$$\psi := \ell_0^{-1} \kappa'. \tag{3.93}$$

Furthermore, we invert ℓ (see (3.66)) in Eq. (3.91) and use (3.95) to find

$$\psi_1 = \Phi_1(\psi_1) = \Phi'_1 + \Phi''_1(\tilde{\varphi}), \tag{3.94}$$

where $\tilde{\varphi}$ is given in (3.92), and, with Q given in (3.67),

$$\Phi'_1 := -\ell^{-1}[\ell' \ell_0^{-1} \kappa' + P_r M_\delta \bar{K}_\delta^{-1} \kappa'], \tag{3.95}$$

$$\Phi''_1(\tilde{\varphi}) := \ell^{-1} Q N(\tilde{\varphi}). \tag{3.96}$$

(3.94) is a fixed point equation for ψ_1 . However, we do not have to solve it since we have already proved the existence of ψ_1 . We use (3.94) to estimate ψ_1 .

Next, by Proposition 3.7, Eq. (3.81) and the relation $O(\delta^2(-i\nabla)^4) = O(a^2(-i\nabla)^2)$ on $\text{Ran } P_r$ (see the definition of P_r in (3.37)), valid due to the choice $a := \delta r = O(1)$ (see (3.38)), we have that the operators ℓ, ℓ_0, ℓ' given in (3.66), (3.70), and (3.90), respectively, satisfy

$$|\ell'| \lesssim \delta^2(-i\nabla)^4, \tag{3.97}$$

$$\ell_0 \gtrsim -\Delta + \zeta^{-2}, \tag{3.98}$$

$$\ell \gtrsim -\Delta + \zeta^{-2}, \tag{3.99}$$

where, recall, $\zeta := m^{-1/2} \delta$, with m given in (1.33), (cf. (3.82)).

Using (3.97)–(3.99) and the fact ℓ, ℓ_0, ℓ' are self-adjoint and are functions of $-i\nabla$ and therefore mutually commute, and using (3.83), we find that

$$\|\Phi'_1\|_{\dot{H}^i} \lesssim \delta^2 \|\kappa'\|_{H^i} + m^{1/2} \zeta^{2-i} \|\kappa'\|_{L^2}, \quad i = 0, 1. \tag{3.100}$$

By the choice of the $B_{s,\delta}$ norm (see (3.45)) and since $\delta^2 \ll m^{1/2} \zeta^{2-i}$ (by (3.46), or (1.28)), we see that

$$\|\Phi'_1\|_\delta \lesssim m^{1/2} \zeta \|\kappa'\|_{L^2}. \tag{3.101}$$

Now, we turn our attention to the map $\Phi(\tilde{\varphi}) := \ell^{-1} Q N(\tilde{\varphi})$ (see (3.96)). The definition of $\Phi(\tilde{\varphi})$ and Eq. (3.87) give

$$\|\Phi''_1(\tilde{\varphi})\|_\delta \lesssim m^{-5/6} \delta^{1/2} \|\tilde{\varphi}\|_\delta^2. \tag{3.102}$$

Next, we estimate $\tilde{\varphi} = \tilde{\varphi}(\psi_1) := P_r \psi + \psi_1 + \varphi_l(P_r \psi + \psi_1) = \varphi_s + \varphi_l$ (see (3.92)). By Propositions 3.3 and 3.6, $\|\varphi_l\|_\delta \leq c_l$ and $\|P_r \psi + \psi_1\|_\delta \lesssim c_s$ and therefore $\|\tilde{\varphi}\|_\delta \lesssim c_s + c_l$. This, together with (3.102) and condition (3.46) and inequality (3.48), yields

$$\|\Phi''_1(\tilde{\varphi})\|_\delta \lesssim m^{-5/6} \delta^{1/2} c_l^2. \tag{3.103}$$

Equations (3.101) and (3.103) and the relation $m^{-5/6} \delta^{1/2} = \theta^{3/2} \zeta^{-1}$ imply

$$\|\Phi_1(\psi_1)\|_\delta \lesssim m^{1/2} \zeta \|\kappa'\|_{L^2} + \theta^{3/2} \zeta^{-1} c_l^2. \tag{3.104}$$

By condition (3.46) and our choice $c_l = \omega \zeta$, $\omega := \min(\theta^{-1/2}, m^{-1/4})$, we see that (3.104) implies

$$\|\Phi_1(\psi_1)\|_\delta \lesssim (a^{-2} m^{1/2} + \theta^{1/2}) \zeta.$$

Since $\psi_1 = \Phi_1(\psi_1)$ and, the above estimate gives (3.73), proving Proposition 3.8. □

4 Analysis of the Operator ℓ . Proof of Proposition 3.7

The goal of this section is to prove Proposition 3.7. The proof follows readily from Lemmas 4.1, 4.3 and 4.4 below. Throughout this section, we suppose Assumption [A1] holds, without mentioning this explicitly.

Let M_k and \bar{K}_k be the k -th Bloch–Floquet fibers of $M \equiv M_{\delta=1}$ and $\bar{K} \equiv \bar{K}_{\delta=1}$ (see (2.34), not to be confused with M_δ and \bar{K}_δ). Since, by Proposition 3.2, \bar{K} is invertible, then so is \bar{K}_k and $\bar{K}_k^{-1} = (\bar{K}^{-1})_k$ (see (2.37)). We have

Lemma 4.1 *The operator ℓ , defined in (3.66), is of the form*

$$\ell = \delta^{-2} b(-i\delta\nabla) P_r, \tag{4.1}$$

where $b(k)$ is a smooth, even function of $-i\delta\nabla$ given explicitly as:

$$b(k) = |\Omega|^{-1} \langle 1, (|k|^2 + M_k - M_k \bar{K}_k^{-1} M_k) 1 \rangle_{L^2_{\text{per}}}. \tag{4.2}$$

Proof Since M_δ is \mathcal{L}_δ -periodic by Proposition 3.2, Eq. (3.66) implies that so is ℓ . Moreover, (3.66) and (3.34) yield

$$\begin{aligned} \ell &= P_r [\delta^{-2} U_\delta (-\Delta + M) U_\delta^*] P_r - P_r [\delta^{-2} U_\delta M U_\delta^*] \\ &\quad \times \bar{P}_r [\delta^{-2} U_\delta (-\Delta + M) U_\delta^*]^{-1} \bar{P}_r [\delta^{-2} U_\delta M U_\delta^*] P_r, \end{aligned}$$

where, recall, $M \equiv M_\delta|_{\delta=1}$, which implies that

$$\ell = \delta^{-2} U_\delta \ell|_{\delta=1} U_\delta^*. \tag{4.3}$$

The last two properties and Lemma 2.8 show that ℓ is a function of $-i\delta\nabla$ of the form (4.1), where $b(k) = \langle (\ell|_{\delta=1})_k 1 \rangle_\Omega$, with $(\ell|_{\delta=1})_k$ being the Bloch–Floquet fibres of $\ell|_{\delta=1}$ and 1 standing for the constant function, $1 \in L^2_{\text{per}}(\mathbb{R}^3)$. Using Eqs. (2.37), (3.66) and $\Delta_k \mathbf{1} = 0$, we find explicit form (4.2) of $b(k)$.

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

Proposition 4.2 *The operator M has a Bloch–Floquet decomposition (2.34) whose k -fiber, M_k , acting on L^2_{per} is given by*

$$M_k f = - \text{den} \left[\oint r_{\text{per},0}(z) f r_{\text{per},k}(z) \right] \tag{4.4}$$

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

$$r_{\text{per},k}(z) = (z - h_{\text{per},k})^{-1}, \tag{4.5}$$

$$h_{\text{per},k} = (-i\nabla - k)^2 - \phi_{\text{per}}. \tag{4.6}$$

Proof of Proposition 4.2 Let T_S be given in (2.1) and $\varphi \in L^2$. 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 (2.23) and Eq. (3.11), we obtain

$$\begin{aligned} (M\varphi)_k(x) &= - \sum_{t \in \mathcal{L}} e^{-ik(x+t)} \oint T_{-t} \text{den} [r_{\text{per}}(z) \varphi r_{\text{per}}(z)] \\ &= - \sum_{t \in \mathcal{L}} e^{-ik(x+t)} \oint \text{den} [T_t^* r_{\text{per}}(z) \varphi r_{\text{per}}(z) T_t]. \end{aligned} \tag{4.7}$$

Since $r_{\text{per}}(z)$ is \mathcal{L} -periodic, (4.7) shows

$$(M\varphi)_k(x) = - \sum_{t \in \mathcal{L}} e^{-2\pi i k(x+t)} \oint \text{den} [r_{\text{per}}(z)(T_{-t}\varphi)r_{\text{per}}(z)]. \tag{4.8}$$

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 (4.8). We obtain

$$(M\varphi)_k(x) = -e^{-ikx} \oint \text{den} \left[r_{\text{per}}(z) \sum_{t \in \mathcal{L}} e^{-ikt} (T_{-t}\varphi)r_{\text{per}}(z) \right]. \tag{4.9}$$

This and the definition of the Bloch–Floquet decomposition of φ , (2.23), imply

$$(M\varphi)_k(x) = - \oint \text{den} \left[r_{\text{per}}(z)\varphi_k e^{ikx} r_{\text{per}}(z) e^{-ikx} \right]. \tag{4.10}$$

Since $e^{ikx}(-i\nabla)e^{-ikx} = -i\nabla - k$, and therefore $e^{ikx}r_{\text{per}}(z)e^{-ikx} = r_{\text{per},k}(z)$, this gives (4.4). \square

Since the resolvents $r_{\text{per},k}(z)$ are smooth in k (see (4.5)–(4.6)), then, by (4.4), M_k is also smooth in k . Hence, by (4.2), $b(k)$ is smooth in k .

Since the operator $M_k - M_k \bar{K}_k^{-1} M_k$ in (4.2) is self-adjoint, the function $b(k)$ is real. By Lemma 4.2 and the properties $\bar{r}_{\text{per},k}(z) := \mathcal{C}r_{\text{per},k}(z)\mathcal{C} = r_{\text{per},-k}(\bar{z})$, where \mathcal{C} is the complex conjugation, and the contour of integration in (4.4) is symmetric w.r.to the reflection $z \rightarrow \bar{z}$, we have $b(k) = \bar{b}(k) = b(-k)$, i.e. $b(k)$ is even. \square

Let $K_0 = K_{k=0}$ denote the 0-fiber of K , acting on $L^2_{\text{per}}(\mathbb{R}^3)$. 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

$$\bar{K}_0 := \bar{\Pi}_0 K_0 \bar{\Pi}_0. \tag{4.11}$$

Recall the abbreviation $s_\beta := \beta e^{-\eta_0\beta}$. With this notation, we have

Lemma 4.3 *Let m be given in (1.33). The function $b(k)$ given in (4.2) satisfies*

$$b(k) = |\Omega|^{-1}(m + O(s_\beta^2)) + k \cdot \epsilon k + k \cdot O(s_\beta)k + O(|k|^4), \tag{4.12}$$

where m is a scalar given by (1.33) and ϵ is a real matrix given by (1.35)–(1.37).

Proof of Lemma 4.3 First, we use (4.2) to write $b(k)$ as

$$b(k) = b_1(k) - b_2(k), \tag{4.13}$$

$$b_1(k) := |k|^2 + |\Omega|^{-1} \langle 1, M_k 1 \rangle_{L^2_{\text{per}}}, \tag{4.14}$$

$$b_2(k) := |\Omega|^{-1} \langle 1, M_k \bar{K}_k^{-1} M_k 1 \rangle_{L^2_{\text{per}}}. \tag{4.15}$$

We begin with $b_1(k)$. We claim that

$$b_1(k) = |\Omega|^{-1} m + \epsilon'_1 |k|^2 + k \cdot (1 + \epsilon')k + O(|k|^4), \tag{4.16}$$

where m and ϵ' are given in (1.33) and (1.36), respectively, and ϵ'_1 is a real, symmetric matrix satisfying $\epsilon'_1 = O(s_\beta)$, contributing to the third term on the r.h.s. of (4.12).

Using definition of b_1 in (4.14) and Proposition 4.2, we see that

$$b_1(k) = -|\Omega|^{-1} \langle 1, \text{den} \oint r_{\text{per},0}(z) 1 r_{\text{per},k}(z) \rangle_{L^2(\Omega)} \tag{4.17}$$

$$= -|\Omega|^{-1} \text{Tr}_\Omega \oint r_{\text{per},0}(z) r_{\text{per},k}(z), \tag{4.18}$$

where 1 is the constant function $1 \in L^2_{\text{per}}$ and Ω is an arbitrary fundamental cell of \mathcal{L} . To begin with, using the Cauchy-formula for derivatives, we obtain

$$b_1(0) = -|\Omega|^{-1} \text{Tr}_\Omega \oint r_{\text{per},0}^2(z) = |\Omega|^{-1} m. \tag{4.19}$$

Next, recall that $h_{\text{per},k} = (-i\nabla - k)^2 - \phi_{\text{per}}$ (see (4.6)). We have, by the resolvent identity, that

$$r_{\text{per},k}(z) - r_{\text{per},0}(z) = r_{\text{per},k}(z) [2(-i\nabla) \cdot k - |k|^2] r_{\text{per},0}(z). \tag{4.20}$$

Applying this identity to (4.18) and using that $b_1(k)$ is even, we obtain (4.16), with $\epsilon'_1 := -|\Omega|^{-1} \text{Tr}_{L^2_{\text{per}}} \oint r_{\text{per},0}^3(z)$ and ϵ' given by (1.36).

Using the Cauchy-integral formula, we rewrite ϵ'_1 as

$$\epsilon'_1 = -\frac{1}{2} \text{Tr}_{L^2_{\text{per}}} f''_T(h_{\text{per}} - \mu). \tag{4.21}$$

Then following the proof of Lemma B.2 with f'_{FD} replaced by f''_{FD} , we show that $\epsilon'_1 = O(s_\beta)$. This proves (4.16).

Next, we prove the expansion

$$b_2(k) = k \cdot \epsilon'' k + k \cdot \epsilon''_1 k + O(|k|^4) + O(s_\beta^2), \tag{4.22}$$

where ϵ'' is given in (1.37), ϵ''_1 is a real matrix satisfying $\epsilon''_1 = O(s_\beta)$ (contributing to the third term on the r.h.s. of (4.12)). First, we recall from (4.15)

$$b_2(k) = |\Omega|^{-1} \langle 1, (M \bar{K}^{-1} M)_k 1 \rangle_{L^2_{\text{per}}} \tag{4.23}$$

$$= |\Omega|^{-1} \langle M_k 1, \bar{K}_k^{-1} M_k 1 \rangle_{L^2_{\text{per}}}, \tag{4.24}$$

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

$$\rho_k = (\bar{P}_a)_k M_k 1 \in L^2_{\text{per}}, \tag{4.25}$$

where L^2_{per} is given in (1.19), a is given in (3.38), and P_a is defined in (3.37), we find

$$b_2(k) = |\Omega|^{-1} \langle \rho_k, \bar{K}_k^{-1} \rho_k \rangle_{L^2_{\text{per}}}. \tag{4.26}$$

Now, we expand ρ_k in k . By (4.4), we have $M_{k=0} 1 = -\text{den} \left[\oint r_{\text{per},0}^2(z) \right]$. Next, recall $\oint := \frac{1}{2\pi i} \int_\Gamma dz f_T(z - \mu)$ (see (3.7)) to obtain

$$M_{k=0} 1 = -\text{den} f'_T(h_{\text{per},0} - \mu). \tag{4.27}$$

Since $f'_{FD} \leq 0$, we have $M_{k=0}\mathbf{1} > 0$. Introduce the function

$$V(x) = -\operatorname{den} [f'_T(h_{\text{per},0} - \mu)](x) \geq 0. \tag{4.28}$$

By definition (4.25) and Eqs. (4.4), (4.27) and (4.28), we have

$$\rho_k = (\bar{P}_a)_k V + \rho'_k, \tag{4.29}$$

$$\rho'_k := (\bar{P}_a)_k \operatorname{den} \oint r^2_{\text{per},0}(z)(2(-i\nabla)k + k^2)r_{\text{per},k}(z). \tag{4.30}$$

Inserting the decomposition (4.29) into (4.26) gives

$$|\Omega|b_2(k) = \langle V, \bar{K}_k^{-1} V \rangle + 2\operatorname{Re}\langle V, \bar{K}_k^{-1} \rho'_k \rangle + \langle \rho'_k, \bar{K}_k^{-1} \rho'_k \rangle. \tag{4.31}$$

We expand the third term on the r.h.s. on (4.31). First, we give a rough bound. For $z \in \Gamma$, we claim the estimates

$$\begin{aligned} \|(1 - \Delta)^\alpha r_{\text{per},k}(z)\| &\leq \|(1 - \Delta)^\alpha r_{\text{per}}(z)\| \lesssim d^{\alpha-1} \lesssim 1, \end{aligned} \tag{4.32}$$

for $\alpha = 0, 1/2$, where $d \equiv d(z) := \operatorname{dist}(z, \sigma(h_{\text{per}})) \geq \frac{1}{4}$. The first estimate follows from (2.38). The second estimate is straightforward for $\alpha = 0, 1$, which by interpolation, gives it for all $\alpha \in [0, 1]$. For $\alpha = 1/2$, it can be also proven directly as $\|(-\Delta)^{1/2} f\|^2 = \langle f, (h_{\text{per}} - z + \phi_{\text{per}} + z)f \rangle$. Taking $f = r_{\text{per}}(z)u$, we arrive at the second estimate in (4.32) for $\alpha = 1/2$.

By the second resolvent identity (4.20) and estimates (4.32), we have the expansion

$$r_{\text{per},k}(z) = r_{\text{per},0}(z) + O(|k|d^{-3/2} + |k|^2d^{-2}).$$

Using this expansion in (4.30), we find

$$\rho'_k = \rho' \cdot k + O(|k|^2),$$

where ρ' is given in (1.38). Using the latter relation, the relation $\bar{K}_k^{-1} = \bar{K}_0^{-1} + O(k)$ and the fact that, since on L^2_{per} the spectrum of $-i\nabla$ is discrete, $(\bar{P}_a)_{k=0} = (\bar{P}_{a=0})_{k=0}$ for a is sufficiently small, we obtain

$$|\Omega|^{-1} \langle \rho'_k, \bar{K}_k^{-1} \rho'_k \rangle = -k\epsilon''k + O(k^4), \tag{4.33}$$

for ϵ'' is given in (1.37), where the power of the remainder comes from the fact $b_2(k)$ is even which is shown by the same argument that was used in demonstration that $b(k)$ is even. Equations (4.31) and (4.33) show that

$$b_2(k) = b_2(0) - k\epsilon''k + O(k^4) + \operatorname{Rem}, \tag{4.34}$$

$$\operatorname{Rem} := \langle V, [\bar{K}_k^{-1} - \bar{K}_0^{-1}]V \rangle + 2\operatorname{Re}\langle V, \bar{K}_k^{-1} \rho'_k \rangle, \tag{4.35}$$

with $b_2(0) := |\Omega|^{-1} \langle V, \bar{K}_k^{-1} V \rangle$. To estimate $b_2(0)$ and the terms in (4.35), we use Eq. (3.53) and the relation $\|\bar{K}^{-1}\| = \sup_k \|\bar{K}_k^{-1}\|$ (see (2.38)) to obtain

$$\|\bar{K}_k^{-1}\| \lesssim 1.$$

We use this bound, Lemma B.2, (4.30) and the fact that $b_2(k)$ is even in k , to obtain

$$\begin{aligned} |\Omega||\text{Rem}| &\lesssim (\|V\|_{L^2_{\text{per}}}^2 + \|V\|_{L^2_{\text{per}}})|k|^2 \\ &= O(s_\beta|k|^2), \end{aligned} \tag{4.36}$$

$$|\Omega|b_2(0) = O(\|V\|_{L^2_{\text{per}}}^2) = O(s_\beta^2). \tag{4.37}$$

We identify the first, third and fourth terms on the r.h.s. of (4.34) with the fourth, third and second terms in (4.22), respectively. Equations (4.34)–(4.36) imply (4.22).

Equations (4.13), (4.16), and (4.22) yield equation (4.12), with $\epsilon'_1 + \epsilon'_1$ making up the third term on the r.h.s. of (4.12). This completes the proof of Lemma 4.3. \square

Lemma 4.4 *The 3×3 matrix ϵ entering (4.2) is symmetric and satisfies*

$$\epsilon \geq \mathbf{1} - O(s_\beta^2). \tag{4.38}$$

Proof We prove this lemma using the Feshbach–Schur map. Let $P = P_s$ (see (3.37)) for some real number $s > 0$, unrelated to r and satisfying $B(\delta s) \subset \Omega^*$. For any projection P and operator H on $L^2(\mathbb{R}^3)$, the Feshbach–Schur map $F_P(H)$ is defined as

$$F_P(H) := PHP - PH\bar{P}\bar{H}^{-1}\bar{P}HP, \tag{4.39}$$

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 [20]

$$-\lambda \notin \sigma(H) \iff -\lambda \notin \sigma(F_P(H + \lambda) - \lambda P). \tag{4.40}$$

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

$$H \geq 0 \iff F_P(H + \lambda) - \lambda P \geq 0. \tag{4.41}$$

With the Laplacian Δ , we define

$$K_{c,\delta} = K_\delta + c\Delta. \tag{4.42}$$

Since $M_\delta > 0$ by Proposition 3.1, we have that $K_{c,\delta} > 0$ for all $c \in [0, 1)$. Consequently, (4.41) shows that, for any $\lambda > 0$,

$$F_P(K_{c,\delta} + \lambda) - \lambda P \geq 0. \tag{4.43}$$

Using definition (4.39) and the resolvent identity, we obtain

$$F_P(K_{c,\delta} + \lambda) - \lambda P \tag{4.44}$$

$$= PK_{c,\delta}P - PM_\delta(\bar{K}_{c,\delta} + \lambda\bar{P})^{-1}M_\delta P \tag{4.45}$$

$$= F_P(K_{c,\delta}) + \lambda PM_\delta\bar{K}_{c,\delta}^{-1}(\bar{K}_{c,\delta} + \lambda\bar{P})^{-1}M_\delta P \tag{4.46}$$

$$\begin{aligned} &= F_P(K_{c,\delta}) + \lambda PM_\delta\bar{K}_{c,\delta}^{-2}M_\delta P \\ &\quad - \lambda^2 PM_\delta(\bar{K}_{c,\delta})^{-2}(\bar{K}_{c,\delta} + \lambda\bar{P})^{-1}M_\delta P. \end{aligned} \tag{4.47}$$

By the choice of $P = P_s$ (see (3.37)), we see that $\bar{K}_{c,\delta} \gtrsim s^2$. Since $M_\delta \lesssim \delta^{-2}$, we see that the last term in (4.47) is bounded by $O(\lambda^2\delta^{-4}s^{-6})$. Thus, (4.44) - (4.47) implies

$$F_P(K_{c,\delta} + \lambda) - \lambda P = F_P(K_{c,\delta}) + \lambda W + O(\lambda^2\delta^{-4}s^{-6})P, \tag{4.48}$$

where $W := PM_\delta(\bar{K}_{c,\delta})^{-2}M_\delta P$. To estimate W , we proceed as in the proof of Lemma 4.1. First, since M_δ is \mathcal{L}_δ -periodic by Proposition 3.2, W is \mathcal{L}_δ -periodic. Moreover, the definition $W := PM_\delta(\bar{K}_{c,\delta})^{-2}M_\delta P$ and (3.34) yield

$$\begin{aligned} W &= P_s(\delta^{-2}U_\delta M_1 U_\delta^*)\bar{P}_s[\delta^{-2}U_\delta(-\Delta + M_1)U_\delta^*]^{-2}\bar{P}_s(\delta^{-2}U_\delta M_1 U_\delta^*)P_s \\ &= P_{\delta s}M_1\bar{P}_{\delta s}\bar{K}_1^{-1}\bar{P}_{\delta s}M_1P_{\delta s}, \end{aligned}$$

which implies that

$$W = U_\delta W|_{\delta=1}U_\delta^*. \tag{4.49}$$

($(\bar{K}_{c,\delta})^{-1}$ entering W in the second power eats up δ^{-2} compared to (4.3).) Since $B(\delta s) \subset \Omega^*$, the last two properties and Lemma 2.8 show that W is a function of $-i\delta\nabla$ of the form

$$W = w(-i\delta\nabla)P, \tag{4.50}$$

where $w(k) = \langle W_k 1 \rangle_\Omega$, with W_k being the Bloch–Floquet fibers of W and 1 standing for the constant function, $1 \in L^2_{\text{per}}(\mathbb{R}^3)$. Using Eq. (2.37), we find, as in (4.1)–(4.2), the explicit form of $w(k)$:

$$w(k) = |\Omega|^{-1} \langle 1, M_k \bar{K}_k^{-2} M_k 1 \rangle_{L^2_{\text{per}}}, \tag{4.51}$$

where M_k and \bar{K}_k are the k -th Bloch–Floquet fibres of $M_{\delta=1}$ and $\bar{K}_{\delta=1}$.

Since the operator $M_k \bar{K}_k^{-2} M_k$ in (4.2) is self-adjoint, the function $w(k)$ is real. Arguing as with $b(k)$ in the proof of Lemma 4.1, we conclude that $w(k)$ is even and smooth. Furthermore, as with $b_2(k)$ in the proof of Lemma 4.3, we expand $w(k)$ in k to the fourth order to obtain

$$W = O(s^2_\beta) - \delta^2 \nabla \epsilon_3 \nabla P + O(\delta^4 (-i\nabla)^4 P), \tag{4.52}$$

$$\epsilon_3 := |\Omega|^{-1} \langle \rho', \bar{K}_{c,0}^{-2} \rho' \rangle_{L^2_{\text{per}}} > 0, \tag{4.53}$$

where ρ' is given in (1.38), $K_{c,0} \equiv K_{c,\delta=1,k=0}$ is the 0-th fiber of $K_{c,\delta=1}$, and $\bar{K}_{c,0} = \bar{\Pi}_0 K_{c,0} \bar{\Pi}_0$. Here $\bar{\Pi}_0 = 1 - \Pi_0$ and Π_0 is the projection in L^2_{per} onto constants. The inverse $\bar{K}_{c,0}^{-2}$ is taken on the range of $\bar{\Pi}_0$. Equations (4.48) and (4.52) imply that

$$\begin{aligned} F_P(K_{c,\delta} + \lambda) - \lambda P &= F_P(K_{c,\delta}) + O(s^2_\beta) - \lambda \delta^2 \nabla \epsilon_3 \nabla P \\ &\quad + O(\delta^4 (-i\nabla)^4 P) + O(\lambda \delta^{-4} s^{-6} P). \end{aligned} \tag{4.54}$$

Now, we use definition (4.42) to expand the term $F_P(K_{c,\delta})$ in (4.54) in c . A simple computation shows that

$$F_P(K_{c,\delta}) = F_P(K_\delta) + c\Delta P \tag{4.55}$$

$$- \sum_{n \geq 1} c^n PM_\delta(\bar{K}_\delta^{-1}(-\Delta))^n \bar{K}_\delta^{-1}M_\delta P. \tag{4.56}$$

Since $\bar{K}_\delta \geq 0$, (4.56) is negative, we conclude

$$F_P(K_{c,\delta}) \leq F_P(K_\delta) + c\Delta P. \tag{4.57}$$

Since $F_P(K_\delta) = \ell$ for $r = s$ (see (3.66)), we see, by Lemma 4.3, that

$$F_P(K_\delta) = -\nabla \epsilon \nabla P + O(\delta^2 (-i\nabla)^4 P), \tag{4.58}$$

with ϵ defined there. We use that $O(\delta^4(-i\nabla)^4 P) = O(\tilde{a}^2(-i\nabla)^2 P)$, where $\tilde{a} := \delta s$ (which is unrelated to the a in (3.38)) and (4.57) and (4.58) to obtain

$$F_P(K_{c,\delta}) \leq -\nabla(\epsilon - c + O(\tilde{a}^2))\nabla P. \tag{4.59}$$

Setting $\epsilon_4 := O(\tilde{a}^2) + \lambda\delta^2\epsilon_3$, we see that Eqs. (4.54), (4.43) and (4.59) imply

$$\begin{aligned} &-\nabla(\epsilon + \epsilon_4 - c)\nabla P + O(\lambda\delta^{-4}s^{-6})P + O(s_\beta^2)P \\ &\geq F_P(K_{c,\delta} + \lambda) - \lambda P \geq 0. \end{aligned} \tag{4.60}$$

Inequality (4.60) holds for all $s \in (0, \delta^{-1})$. Taking $s = \delta^{-3/4}$, we find

$$-\nabla\epsilon\nabla P \geq [(c - O(\delta^{1/2}))\Delta - O(\lambda\delta^{1/2}) - O(s_\beta^2)]P_\delta,$$

where $P_\delta := P_{s=\delta^{-3/4}}$. Since this holds for every $\delta > 0$, since $P \equiv P_s$ converges strongly to $\mathbf{1}$, as $s \rightarrow \infty$, and since the expression for ϵ given in Lemma 4.3 is independent of δ , we see that

$$-\nabla\epsilon\nabla \geq -c\Delta - O(s_\beta^2),$$

for every $c \in [0, 1)$. Passing to the Fourier transform gives $\xi \cdot \epsilon\xi \geq c|\xi|^2 - O(s_\beta^2)$, $\forall \xi \in \mathbb{R}^3$. For $\xi \in \mathbb{R}^3$, with $|\xi| \geq 1$, this implies $\xi \cdot \epsilon\xi \geq (c - O(s_\beta^2))|\xi|^2$, which is equivalent to (4.38). \square

5 Nonlinear Estimates

Let N_δ be given implicitly by (3.31) and recall the definition of the $B_{s,\delta}$ norm from (3.45). Let $\dot{H}^0 \equiv L^2$. In this section we prove estimates on N_δ .

Proposition 5.1 *Let Assumption [A1] hold. If $\|\varphi_1\|_{B_{s,\delta}}, \|\varphi_2\|_{B_{s,\delta}} = o(\delta^{-1/2})$, then we have the estimate*

$$\begin{aligned} &\|N_\delta(\varphi_1) - N_\delta(\varphi_2)\|_{L^2} \\ &\lesssim m^{-1/3}\delta^{-1/2}(\|\varphi_1\|_{B_{s,\delta}} + \|\varphi_2\|_{B_{s,\delta}})\|\varphi_1 - \varphi_2\|_{\dot{H}^1}. \end{aligned} \tag{5.1}$$

In Appendix D, we prove a more refined estimate. We derive Proposition 5.1 from its version with $\delta = 1$ by rescaling. For $\delta = 1$, we have the following result.

Proposition 5.2 *Let Assumption [A1] hold and either $\|\psi\|_{L^2} = o(1)$ or $\|\nabla\psi\|_{L^2} = o(1)$. Then $N := N_{\delta=1}$ satisfies the estimate*

$$\begin{aligned} \|N(\psi_1) - N(\psi_2)\|_{L^2} &\lesssim \sum_{j=1}^2 \left[(\|\psi_j\|_{\dot{H}^1})\|\psi_1 - \psi_2\|_{\dot{H}^1} \right. \\ &\quad + (\|\psi_j\|_{\dot{H}^1}^{1/3}\|\psi_j\|_{L^2}^{2/3})\|\psi_1 - \psi_2\|_{\dot{H}^1} \\ &\quad \left. + \|\psi_j\|_{\dot{H}^1}\|\psi_1 - \psi_2\|_{\dot{H}^1}^{1/3}\|\psi_1 - \psi_2\|_{L^2}^{2/3} \right]. \end{aligned} \tag{5.2}$$

We first derive Proposition 5.1 from Proposition 5.2 and then prove the latter statement.

Proof of Proposition 5.1 By (3.33), N_δ and the unscaled nonlinearity $N = N_{\delta=1}$ are related via

$$N_\delta(\varphi) = \delta^{-3/2}U_\delta N(\psi), \quad \psi = \delta^{-1/2}U_\delta^* \varphi, \tag{5.3}$$

where U_δ is given in (2.45). Equations (5.2) and (5.3) the relation $\|U_\delta^* \varphi\|_{L^2} = \|\varphi\|_{L^2}$ and the notation $\psi_j = \delta^{-1/2}U_\delta^* \varphi_j$ imply

$$\begin{aligned} \|N_\delta(\varphi_1) - N_\delta(\varphi_2)\|_{L^2} &\lesssim \delta^{-3/2} \sum_{j=1}^2 \left[\|\psi_j\|_{\dot{H}^1} \|\psi_1 - \psi_2\|_{\dot{H}^1} \right. \\ &\quad + \|\psi_j\|_{\dot{H}^1}^{1/3} \|\psi_j\|_{L^2}^{2/3} \|\psi_1 - \psi_2\|_{\dot{H}^1} \\ &\quad \left. + \|\psi_j\|_{\dot{H}^1} \|\psi_1 - \psi_2\|_{\dot{H}^1}^{1/3} \|\psi_1 - \psi_2\|_{L^2}^{2/3} \right]. \end{aligned} \tag{5.4}$$

Furthermore, using the relation $\|\psi_j\|_{\dot{H}^k} = \delta^{-1/2}\|U_\delta^* \varphi_j\|_{\dot{H}^k} = \delta^{k-1/2}\|\varphi\|_{\dot{H}^k}$, we find

$$\begin{aligned} \|N_\delta(\varphi_1) - N_\delta(\varphi_2)\|_{L^2} &\lesssim \delta^{-3/2} \sum_{j=1}^2 \left[\delta \|\varphi_j\|_{\dot{H}^1} \|\varphi_1 - \varphi_2\|_{\dot{H}^1} \right. \\ &\quad + \delta^{1/3} (\|\varphi_j\|_{\dot{H}^1}^{1/3} \|\varphi_j\|_{L^2}^{2/3} \|\varphi_1 - \varphi_2\|_{\dot{H}^1} \\ &\quad \left. + \|\varphi_j\|_{\dot{H}^1} \|\varphi_1 - \varphi_2\|_{\dot{H}^1}^{1/3} \|\varphi_1 - \varphi_2\|_{L^2}^{2/3} \right]. \end{aligned} \tag{5.5}$$

To estimate the terms on the r.h.s. of (5.5) we use the inequality $a^{1/3}b^{2/3} \leq \frac{2}{3}(a + b)$, with $a := \|\varphi\|_{\dot{H}^1}$ and $b := m^{1/2}\delta^{-1}\|\psi\|_{L^2}$, to obtain

$$\|\varphi\|_{\dot{H}^1}^{1/3} \|\psi\|_{L^2}^{2/3} \leq \frac{2}{3}(m^{-1/2}\delta)^{2/3}(\|\varphi\|_{\dot{H}^1} + m^{1/2}\delta^{-1}\|\psi\|_{L^2}).$$

With the definition of the norm $\|\cdot\|_\delta$ in (3.45), this yields $\delta^{1/3}\|\varphi\|_{\dot{H}^1}^{1/3}\|\varphi\|_{L^2}^{2/3}\|\chi\|_{\dot{H}^1} \leq \frac{2}{3}m^{-1/3}\delta\|\varphi\|_\delta\|\chi\|_{\dot{H}^1}$. Since $\|\chi\|_{\dot{H}^1} \leq \|\chi\|_\delta$, this in turn implies

$$\delta^{1/3}\|\varphi\|_{\dot{H}^1}^{1/3}\|\varphi\|_{L^2}^{2/3}\|\chi\|_{\dot{H}^1} \leq \frac{2}{3}m^{-1/3}\delta\|\varphi\|_\delta\|\chi\|_\delta.$$

Applying this inequality to (5.5), we arrive at (5.1). □

Proof of Proposition 5.2 Let h_{per} and $r_{\text{per}}(z)$ be given in (3.8). First we observe that Eqs. (3.28)–(3.32), with $\delta = 1$, read

$$N(\psi) = F(\phi) - F(\phi_{\text{per}}) - d_\varphi F(\phi_{\text{per}})\psi, \tag{5.6}$$

$$F(\phi) = \text{den}[f_T(h^\phi - \mu)], \tag{5.7}$$

where $\psi := \phi - \phi_{\text{per}}$ and, recall, $h^\phi := -\Delta - \phi = h_{\text{per}} - \psi$. Next, using Eqs. (3.4) and (3.7) and expanding $(z - h^\phi)^{-1} = (z - h_{\text{per}} + \psi)^{-1}$ to the second order, we find

$$N(\psi) := \text{den}[\tilde{N}_2(\psi)], \tag{5.8}$$

where

$$\tilde{N}_k(\psi) := \oint (z - h_{\text{per}} + \psi)^{-1} [(-\psi)r_{\text{per}}(z)]^k, \tag{5.9}$$

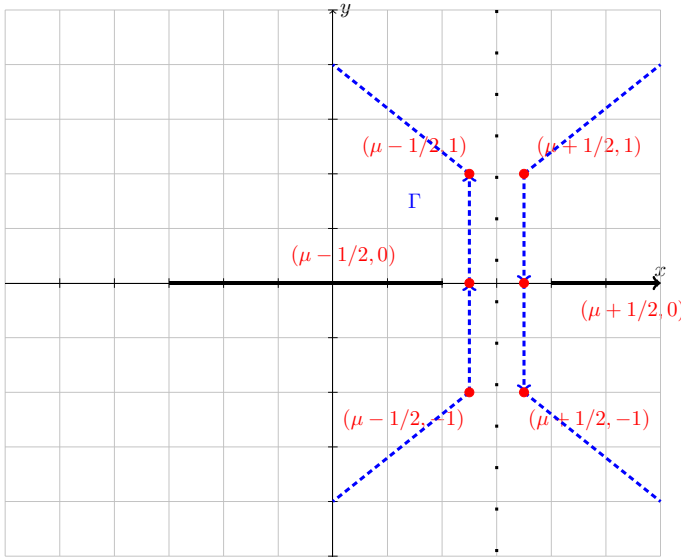


Fig. 2 The deformation of the contour Γ is indicated by the blue dashed line. The spectrum of h_{per} is denoted by solid black line. The poles of $f_T(z - \mu)$ are denoted by the black dots. The number c denotes the lower bound $h_{\text{per}} > -c + 1$

with ϕ given by $\phi := \frac{1}{2\pi i} \int_{\Gamma} dz f_T(z - \mu)$, where Γ is the contour given in Fig. 1 (see (3.7)), equipped with the positive orientation.

We deform the contour Γ given in Fig. 1 into the contour indicated in Fig. 2 by the blue dashed line and consisting of two separate contours traversed counter-clockwise.

By the formal resolvent expansion (without justifying the convergence)

$$(z - h_{\text{per}} + \psi)^{-1} = \sum_{k=2}^{\infty} r_{\text{per}}(z)[(-\psi)r_{\text{per}}(z)]^k, \tag{5.10}$$

we see that $N(\psi)$ can be written as the formal series

$$N(\psi) = \sum_{k=2}^{\infty} \text{den}[N_k(\psi)], \tag{5.11}$$

where

$$N_k(\psi) := \oint r_{\text{per}}(z)[(-\psi)r_{\text{per}}(z)]^k. \tag{5.12}$$

Proposition 5.3 *Let Assumption [A1] hold and let N_2 be given by (5.12). Assume that $\|\nabla\psi\|_{L^2} = o(1)$, then we have the estimate*

$$\|\text{den}[N_k(\psi)]\|_{L^2} \lesssim \|\nabla\psi\|_{L^2}^{4/3} \|\psi\|_{L^2}^{2/3} \|\psi\|_{H^j}^{k-2}, \quad j = 0, 1, \tag{5.13}$$

where the constants associated with \lesssim are independent of β .

Proof Below, we use the notation $r = r_{\text{per}}(z)$, where $r_{\text{per}}(z)$ is given in (3.8), and the estimate (see (4.32))

$$\|(1 - \Delta)^\alpha r\| \lesssim d^{\alpha-1} \lesssim 1, \tag{5.14}$$

for $\alpha \in [0, 1]$ and $z \in \Gamma$, where

$$d \equiv d(z) := \text{dist}(z, \sigma(h_{\text{per}})) \geq \frac{1}{4}. \tag{5.15}$$

We use the L^2 – L^2 duality to estimate the L^2 norm of $\text{den}[N_k(\psi)]$. We have, by (2.5) and definition (5.12),

$$\begin{aligned} \|\text{den}[N_k(\psi)]\|_{L^2} &= \sup_{\|f\|_{L^2}=1} \left| \int f \text{den}[N_k(\psi)] \right| \\ &= \sup_{\|f\|_{L^2}=1} |\text{Tr}[f N_k(\psi)]| \\ &= \sup_{\|f\|_{L^2}=1} \left| \oint \text{Tr}(f r(\psi r)^k) \right|. \end{aligned} \tag{5.16}$$

(In the last two lines, f is considered as a multiplication operator.)

Let $f \in L^2$ and recall the Schatten norm $\|\cdot\|_{S^p}$ defined in (2.3). Using the non-abelian Hölder’s inequality $1 = \frac{1}{2} + \frac{1}{6} + \frac{1}{3} + \frac{1}{\infty}$, we see that, for $k \geq 2$,

$$|\text{Tr}(f r(\psi r)^k)| \lesssim \|f r\|_{S^2} \|\psi r\|_{S^6} \|\psi r\|_{S^3} \|\psi r\|_{S^3}^{k-2}. \tag{5.17}$$

Next, we use the operator trace-class estimate $\|A\|_{S^3}^3 = \text{Tr}(|A|^3) \leq \|A\| \text{Tr}(|A|^2) = \|A\| \|A\|_{S^2}^2 \leq \|A\|_{S^6} \|A\|_{S^2}^2$ to obtain

$$\|A\|_{S^3} \leq \|A\|_{S^6}^{1/3} \|A\|_{S^2}^{2/3}. \tag{5.18}$$

Using this equality to estimate the third factor in (5.17) and the standard relative bounds $\|\psi r\| \lesssim \|\psi\|_{L^2}$ and $\|\psi r\| \lesssim \|\psi\|_{L^6} \lesssim \|\psi\|_{\dot{H}^1}$, we bound the r.h.s. of (5.17) as

$$|\text{Tr}(f r(\psi r)^k)| \lesssim \|f r\|_{S^2} \|\psi r\|_{S^6}^{4/3} \|\psi r\|_{S^2}^{2/3} \|\psi\|_{\dot{H}^1}^{k-2}, \quad i = 0, 1. \tag{5.19}$$

For a typical term on the r.h.s., we have $\|g r\|_{S^p} \leq \|g(1 - \Delta)^{-\alpha_p}\|_{S^p} \|(1 - \Delta)^{\alpha_p} r\|$, with $3/(2p) < \alpha_p < 1$, $p > 3/2$, which, together with Kato–Seiler–Simon’s inequality (2.14) and inequality (5.14), gives

$$\|g r\|_{S^p} \lesssim \|g\|_{L^p} d^{\alpha_p-1}, \quad 3/(2p) < \alpha_p < 1, \quad p > 3/2.$$

Applying this estimate to each of the first three factors on the r.h.s. of (5.19) and using the Gagliardo–Nirenberg–Sobolev inequality (2.18), we find

$$|\text{Tr}(f r(\psi r)^k)| \lesssim d^{-4/3} \|f\|_{L^2} \|\nabla \psi\|_{L^2}^{4/3} \|\psi\|_{L^2}^{2/3} \|\psi\|_{\dot{H}^j}^{k-2}, \tag{5.20}$$

for $j = 0, 1$. Recalling definition (5.15) of $d \equiv d(z)$, we see that the integral on the r.h.s. of (5.16) converges absolutely. Equations (5.20), (5.15), (3.7) and (3.6) give

$$\left| \oint \text{Tr}(f r(\psi r)^k) \right| \lesssim \|f\|_{L^2} \|\nabla \psi\|_{L^2}^{4/3} \|\psi\|_{L^2}^{2/3} \|\psi\|_{\dot{H}^j}^{k-2}, \tag{5.21}$$

for $j = 0, 1$. Equations (5.16) and (5.21) imply (5.13). □

Now, we complete the proof of Proposition 5.2. Proposition 5.3 shows that if $\|\psi\|_{L^2} < \infty$ and either $\|\psi\|_{L^2} = o(1)$ or $\|\psi\|_{\dot{H}^1} = o(1)$, then series (5.11) converges absolutely in L^2 .

Now, using series (5.11), we write

$$N(\psi_1) - N(\psi_2) = \sum_{k \geq 2} \text{den}[N_k(\psi_1) - N_k(\psi_2)]. \tag{5.22}$$

By definition (5.12), $N_k(\psi)$ is an k -th degree monomial in ϕ . Hence, we can expand $N_k(\psi_1) - N_k(\psi_2)$ in the following telescoping form

$$x^k - y^k = x^{k-1}(x - y) + x^{k-2}(x - y)y + \dots + (x - y)y^k. \tag{5.23}$$

The proof of Proposition 5.2 follows by applying appropriate and straightforward extension of Proposition 5.3 to each term in the expansion of $N_k(\psi_1) - N_k(\psi_2)$ given in (5.23). \square

Acknowledgements The authors thank Rupert Frank, Jürg Fröhlich, Gian Michele Graf, Christian Hainzl and Jianfeng Lu for stimulating discussions and to the anonymous referee for many pertinent remarks. The correspondence with Antoine Levitt played a crucial role in steering the research at an important junction. The second author is also grateful to Volker Bach, Sébastien Breteaux, Thomas Chen and Jürg Fröhlich for enjoyable collaboration on related topics. The research on this paper is supported in part by NSERC Grant No.NA7901. The first author is also in part supported by NSERC CGS D graduate scholarship.

Appendix A: $\epsilon(T) \rightarrow \epsilon(0)$ as $T \rightarrow 0$

Lemma A 1 *Let $xc = 0$. Then $\epsilon \equiv \epsilon(T) \rightarrow \epsilon(0)$ as $T \rightarrow 0$, where $\epsilon(0)$ is the dielectric constant for $T = 0$ obtained in [7].*

Proof We see from (1.35) below that $\epsilon(T)$, $T = 1/\beta$, is of the form

$$\epsilon(T) = \frac{1}{2\pi i} \int_{\Gamma} f_T(z - \mu)X(z) \tag{A.1}$$

where $X(z)$ is some holomorphic function on $\mathbb{C} \setminus \mathbb{R}$, independent of β , and remains holomorphic on the real axis where the gap of h_{per} occurs. On \mathbb{R} , we note that $f_{\text{FD}}(\beta x)$ converges to the indicator function $\chi_{(-\infty, 0)}$ as $\beta \rightarrow \infty$. If we take $\beta \rightarrow \infty$, the integral

$$\frac{1}{2\pi i} \int_{\Gamma} f_T(z - \mu)X(z) \tag{A.2}$$

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 [7] 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: Bounds on m and V

In this section, we prove bounds on m and V given (1.33) and (4.28). Note that $m = \|V\|_{L^1_{\text{per}}}$. Since $f'_T < 0$ ($T = 1/\beta$), (4.28) implies that $V > 0$ and therefore, by (4.28), $\|V\|_{L^1_{\text{per}}} = \int_{\Omega} V$, where Ω is a fundamental domain of \mathcal{L} (see Sect. 1.5), which yields

$$m = \int_{\Omega} V = -\text{Tr}_{L^2_{\text{per}}} f'_T(h_{\text{per},0} - \mu), \quad \mu = \mu_{\text{per}}. \tag{B.1}$$

Lemma B.1 *Let Assumption [A1] hold and η_0 be given in (1.27). Then*

$$m = \|V\|_{L^1_{\text{per}}} \geq \frac{1}{4}\beta e^{-\beta\eta_0}, \tag{B.2}$$

where η_0 is given in (1.27).

Proof Using that η_0 is the smallest distance between $\mu = \mu_{\text{per}}$ and the spectrum of $h_{\text{per},0}$ (see (1.27)) and Eq. (B.1) and replacing $\text{Tr}_{L^2_{\text{per}}} f'_T(h_{\text{per},0} - \mu)$ by the contribution of the eigenvalue of $h_{\text{per},0}$ closest to μ , we find

$$m \geq -f'_T(\eta_0) = \beta \frac{e^{\beta\eta_0}}{(1 + e^{\beta\eta_0})^2} \geq \frac{1}{4}\beta e^{-\beta\eta_0}. \tag{B.3}$$

This gives (B.2). □

Lemma B.2 *Let Assumption [A1] hold. Then, for $1 \leq p \leq \infty$,*

$$\|V\|_{L^p_{\text{per}}} \lesssim \beta e^{-\eta_0\beta}. \tag{B.4}$$

Proof We do the case for $p = 1$ and $p = \infty$, and conclude the lemma by interpolation. By Assumption [A1], the potential ϕ_{per} is bounded. Thus, $h_{\text{per},0}$ has only discrete spectrum on $L^2_{\text{per}}(\mathbb{R}^3)$ and

$$\frac{1}{\beta} \|V\|_{L^1_{\text{per}}} = \sum_{\lambda \in \sigma(h_{\text{per},0})} \frac{e^{\beta(\lambda-\mu)}}{(1 + e^{\beta(\lambda-\mu)})^2} \tag{B.5}$$

$$\leq \sum_{\mu > \lambda \in \sigma(h_{\text{per},0})} e^{\beta(\lambda-\mu)} + \sum_{\mu < \lambda \in \sigma(h_{\text{per},0})} e^{-\beta(\lambda-\mu)} \tag{B.6}$$

$$= \sum_{\lambda \in \sigma(h_{\text{per},0})} e^{\beta|\lambda-\mu|}. \tag{B.7}$$

Again, we use that η_0 is the smallest distance between $\mu = \mu_{\text{per}}$ and the spectrum of $h_{\text{per},0}$ (see (1.27)). Peeling the eigenvalue(s) closest to μ and letting $\eta_0 + \xi$ stand for the distance between μ and the rest of the spectrum $\sigma(h_{\text{per},0})$, we find, for some constant c ,

$$\sum_{\lambda \in \sigma(h_{\text{per},0})} e^{\beta|\lambda-\mu|} = c e^{\beta\eta_0} + \sum_{\lambda \in \sigma(h_{\text{per},0}), |\lambda-\mu| \geq \eta_0+\xi} e^{\beta|\lambda-\mu|}. \tag{B.8}$$

We estimate the sum on the r.h.s. by an integral as follows. Since the potential ϕ_{per} is infinitely bounded with respect to $-\Delta$, the eigenvalues of $h_{\text{per},0}$ go to infinity at a similar rate as those of $-\Delta$ (on $L^2_{\text{per}}(\mathbb{R}^3)$), i.e. as n^2 . Thus, assuming that for λ sufficiently large, the n th eigenvalue $\lambda_n \approx n^2$ has the degeneracy of the order $O(n^k)$, $k \geq 0$, we conclude that

$$\begin{aligned} \sum_{\mu < \lambda \in \sigma(h_{\text{per},0})} e^{-\beta(\lambda-\mu)} &\lesssim \int_{x^2 \geq \mu + \eta_0 + \xi} x^k e^{-\beta(x^2-\mu)} dx \\ &= \frac{1}{2} \int_{y \geq \eta_0 + \xi} (y + \mu)^{\frac{k-1}{2}} e^{-\beta y} dy \lesssim \frac{1}{\beta} \mu^{\frac{k-1}{2}} e^{-\beta(\eta_0 + \xi)}. \end{aligned} \tag{B.9}$$

For the first sum in (B.6), we consider separately the cases $\mu \lesssim 1$ and $\mu \gg 1$ and, in the 2nd case, break the sum into the sums over $\lambda \lesssim 1$ and $\lambda \gg 1$. In the first three situations, the

estimate is straightforward and in the last one, we proceed as in (B.9) to obtain

$$\sum_{\mu - \eta_0 - \xi \geq \lambda \in \sigma(h_{\text{per},0})} e^{\beta(\lambda - \mu)} \lesssim \frac{1}{\beta} \mu^{\frac{k-1}{2}} e^{-\beta\eta_0}.$$

This proves the lemma for $p = 1$.

Let $W_{\text{per}}^{4,1}$ 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

$$\|f\|_{\infty} \lesssim \|f\|_{W_{\text{per}}^{4,1}} \tag{B.10}$$

for $f \in W_{\text{per}}^{4,1}$. Thus, it suffices for us to estimate $\|\nabla^j V\|_{L^1_{\text{per}}}$, $j = 0, \dots, 4$. To this end, we note that

$$\nabla \text{den}(A) = \text{den}([\nabla, A]) \tag{B.11}$$

for an operator A on $L^2_{\text{per}}(\mathbb{R}^3)$. Thus, it suffices that we estimate the trace 1-norm of $\nabla^s f'_T(h_{\text{per},0} - \mu)\nabla^{4-s}$ on $L^2_{\text{per}}(\mathbb{R}^3)$ for $s = 0, \dots, 4$. Since the potential ϕ_{per} is bounded together with all its derivatives, we have, for $s = 0, \dots, 4$,

$$\|\nabla^s h^{-s/2}\| \lesssim 1, \tag{B.12}$$

where $h := h_{\text{per},0} + c$, with $c > 0$ s.t. $h_{\text{per},0} + c > 0$. Indeed, to fix ideas, consider one of the terms, say, $\|\nabla^3 h^{-3/2}\|$. We have $\|\nabla^3 f\|^2 \leq \|(-\Delta)^{3/2} f\|^2 = \langle f, (h + \phi_{\text{per}} - c)^3 f \rangle$. Taking $f = h^{-3/2}u$, expanding the binomial $(h + \phi_{\text{per}} - c)^3$ and commuting the operator h in the resulting terms $h^2\phi_{\text{per}}$ and $\phi_{\text{per}}h^2$ to the right and left, respectively, and estimating the resulting commutators, $[h, \phi]$ and $[\phi_{\text{per}}, h] = -[h, \phi_{\text{per}}]$, we arrive at the estimate $\|\nabla^3 h^{-3/2}\| \lesssim 1$ as claimed. (B.12) implies also that $\|h^{-2+s/2}\nabla^{4-s}\| \lesssim 1$, for $j = 0, \dots, 4$. As the result, we have

$$\|\nabla^s f'_T(h_{\text{per},0} - \mu)\nabla^{4-s}\|_{S^1} \lesssim \|g(h_{\text{per},0})\|_{S^1},$$

where $g(x) := -(x + c)^{s/2} f'_T(x - \mu)(x + c)^{2-s/2} \geq 0$. Hence, it suffices to estimate $\|g(h_{\text{per},0})\|_{S^1} = \text{Tr}[g(h_{\text{per},0})]$. The latter 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

Appendix C: Bound on M_{δ}

In an analogy to $L^2_{\text{per}} \equiv L^2_{\text{per}}(\mathbb{R}^3)$ given in (1.19), we let

$$L^2_{\text{per},\delta} \equiv L^2_{\text{per},\delta}(\mathbb{R}^3) := \{f \in L^2_{\text{loc}}(\mathbb{R}^3) : f \text{ is } \mathcal{L}_{\delta}\text{-periodic}\}. \tag{C.1}$$

Moreover, we recall $\nabla^{-1} := \nabla(-\Delta)^{-1}$ (see (3.56)). The main result of this appendix is the following

Proposition C.1 *Let Assumption [A1] hold. Then the operator M_{δ} can be decomposed as*

$$M_{\delta} = M'_{\delta} + M''_{\delta}, \tag{C.2}$$

with the operator M'_{δ} and M''_{δ} satisfying the estimates

$$\|\bar{P}_r \nabla^{-1} M'_{\delta} P_r \varphi\|_{L^2} \lesssim \delta^{-1} \|V\|_{L^2_{\text{per}}} \|P_r \varphi\|_{L^2}, \tag{C.3}$$

$$\|\bar{P}_r \nabla^{-1} M''_{\delta} P_r \nabla^{-1} \varphi\|_{L^2} \lesssim \|P_r \varphi\|_{L^2}. \tag{C.4}$$

Proof of Proposition C.1 Proposition 4.2 and the rescaling relation (3.34) imply the explicit form for the k -fibers of M_δ :

Lemma C.2 *Then M_δ has a Bloch–Floquet decomposition (2.34) with $\mathcal{L} = \mathcal{L}_\delta$, whose k -fiber $M_{\delta,k}$ acting on $L^2_{\text{per},\delta}$ is given by*

$$M_{\delta,k}f = -\delta \operatorname{den} \left[\oint r_{\text{per},0}^\delta(z) f r_{\text{per},k}^\delta(z) \right] \tag{C.5}$$

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

$$r_{\text{per},k}^\delta = (z - h_{\text{per},k}^\delta)^{-1}, \quad h_{\text{per},k}^\delta = \delta^2(-i\nabla - k)^2 + \delta\phi_{\text{per}}^\delta. \tag{C.6}$$

We decompose the operator $M_{\delta,k}$ acting on $L^2_{\text{per},\delta}$ as

$$M_{\delta,k} =: M_{\delta,0} + M''_{\delta,k}, \tag{C.7}$$

where $M_{\delta,0} = M_{\delta,k=0}$ and M'_δ is defined by the expression (C.7). We define operators M'_δ and M''_δ on $L^2(\mathbb{R}^2)$ via

$$M'_\delta := \int_{\Omega_\delta^*}^\oplus d\hat{k} M_{\delta,0}\varphi, \tag{C.8}$$

$$M''_\delta := \int_{\Omega_\delta^*}^\oplus d\hat{k} M''_{\delta,k}\varphi, \tag{C.9}$$

where Ω_δ^* is a fundamental cell of the reciprocal lattice to \mathcal{L}_δ and $d\hat{k} = |\Omega_\delta^*|^{-1}dk$. By Lemma C.2 and definition (C.7), the latter operators satisfy (C.2).

Lemma C.3 M'_δ (see (C.8)) restricted to the range of P_r is a multiplication operator given by

$$(M'_\delta P_r\varphi)(x) = V_\delta(x)(P_r\varphi)(x), \tag{C.10}$$

where

$$V_\delta(x) = -\delta^{-2} \operatorname{den} [f'_T(h_{\text{per},0} - \mu)] (\delta^{-1}x), \tag{C.11}$$

with $h_{\text{per},0}$ given in (4.6) (with $k = 0$).

Proof By (C.5) and definition of M'_δ in (C.8), we see that

$$M'_\delta P_r\varphi = - \int_{\Omega_\delta^*}^\oplus d\hat{k} \delta \operatorname{den} \left[\oint r_{\text{per},0}^\delta(z) (P_r\varphi)_k r_{\text{per},0}^\delta(z) \right]. \tag{C.12}$$

By Corollary 2.4 and the Cauchy integral formula,

$$M'_\delta P_r\varphi = - \int_{\Omega_\delta^*}^\oplus d\hat{k} \delta \operatorname{den} \left[\oint (r_{\text{per},0}^\delta(z))^2 \right] |\Omega_\delta|^{-1} \hat{\varphi}(k) \tag{C.13}$$

$$= - \int_{\Omega_\delta^*}^\oplus d\hat{k} \operatorname{den} [f'_T(h_{\text{per},0}^\delta - \mu)] |\Omega_\delta|^{-1} \hat{\varphi}(k). \tag{C.14}$$

where $r_{\text{per},0}^\delta(z)$ and $h_{\text{per},0}^\delta$ are given in (C. 6). Applying the inverse Bloch–Floquet transform (2.24), (C. 14) implies

$$M'_\delta P_r \varphi = -\delta \operatorname{den}[f'_T(h_{\text{per},0}^\delta - \mu)] \int_{\Omega_\delta^*} d\hat{k} e^{-i\hat{k}x} |\Omega_\delta|^{-1} \hat{\varphi}(k). \tag{C. 15}$$

Since $d\hat{k}$ is normalized by the volume $|\Omega_\delta^*|$ (which is independent of the choice of the cell), (C. 15) shows

$$M'_\delta P_r \varphi = -\delta \operatorname{den} \left[f'_T(h_{\text{per},0}^\delta - \mu) \right] P_r \varphi. \tag{C. 16}$$

By Lemma 2.7 and recalling the definition of U_δ from (2.45), we see that

$$\delta \operatorname{den} \left[f'_T(h_{\text{per},0}^\delta - \mu) \right] = \delta \operatorname{den} \left[U_\delta f'_T(h_{\text{per},0}^\delta - \mu) U_\delta^* \right] \tag{C. 17}$$

$$= \delta^{-2} \operatorname{den} \left[f'_T(h_{\text{per},0}^\delta - \mu) \right] (\delta^{-1}x), \tag{C. 18}$$

where $h_{\text{per},0} = h_{\text{per},0}^{\delta=1}$, which together with (C. 16) gives (C. 10)–(C. 11). □

Proof of (C. 3) Let V_δ be given in (C. 11). Since the Bloch–Floquet decomposition is unitary, we see, by Lemma C.3 and Corollary 2.4, that

$$\|M'_\delta P_r \varphi\|_{L^2}^2 = \|V_\delta P_r \varphi\|_{L^2}^2 = \int_{\Omega_\delta^*} d\hat{k} \|V_\delta \hat{\varphi}(k)\| |\Omega_\delta|^{-1} \| \cdot \|_{L^2_{\text{per},\delta}}^2, \tag{C. 19}$$

where $L^2_{\text{per},\delta}$ is given in (C. 1). Using the fact that $d\hat{k} = |\Omega_\delta^*|^{-1} dk$ and $|\Omega_\delta| = \delta^3 |\Omega|$, (C. 19) implies

$$\|M'_\delta P_r \varphi\|_{L^2}^2 = \delta^{-3} |\Omega| \|V_\delta\|_{L^2_{\text{per},\delta}}^2 \|P_r \varphi\|_{L^2}^2. \tag{C. 20}$$

By a change of variable, we see that $\|V_\delta\|_{L^2_{\text{per},\delta}} = \delta^{-1/2} \|V\|_{L^2_{\text{per}}}$, where V is given by (4.28). Combing with (C. 20), the fact $\bar{P}_r(-i\nabla)^{-1} \lesssim r^{-1}$ (where ∇^{-1} is given in (3.56)) and $r^{-1} = a^{-1}\delta \lesssim \delta$ (see (3.38)) yields Eq. (C. 3). □

Proof of (C. 4) Let M''_δ be given by (C. 9) and $k^{-1} := k/|k|^2$. Let $\varphi \in L^2(\mathbb{R}^3)$. By Corollary 2.4, we have

$$(P_r \nabla^{-1} \varphi)_k = k^{-1} \hat{\varphi}(k) |\Omega_\delta|^{-1} \chi_{B(r)}(k). \tag{C. 21}$$

This gives $M''_\delta P_r \nabla^{-1} \varphi = |\Omega_\delta|^{-1} \int_{B(r)}^\oplus d\hat{k} M''_{\delta,k} k^{-1} \hat{\varphi}(k)$. Since the Bloch–Floquet decomposition is unitary, we see, using (C. 21), that

$$\begin{aligned} \|M''_\delta P_r \nabla^{-1} \varphi\|_{L^2}^2 &= |\Omega_\delta|^{-2} \int_{B_r} d\hat{k} \|M''_{\delta,k} 1\|_{L^2_{\text{per},\delta}}^2 |k|^{-2} |\hat{\varphi}(k)|^2. \end{aligned} \tag{C. 22}$$

Since $d\hat{k} = |\Omega^*|^{-1} dk = |\Omega| dk$ and $|\Omega_\delta| = \delta^3 |\Omega|$, (C. 22) is bounded as

$$\begin{aligned} \|M''_\delta P_r \nabla^{-1} \varphi\|_{L^2}^2 &\lesssim \delta^{-3} \sup_{k \in B_r} \left(\|M''_{\delta,k} 1\|_{L^2_{\text{per},\delta}}^2 |k|^{-2} \right) \|P_r \varphi\|_{L^2}^2, \end{aligned} \tag{C. 23}$$

where $1 \in L^2_{\text{per},\delta}$ is the constant function 1 and $L^2_{\text{per},\delta}$ is given in (C. 1).

By (C. 5) and (C. 7), we have, for $M''_{\delta,k}$ given in (C. 7), that

$$M''_{\delta,k}\varphi = -\delta \operatorname{den} \left[\oint r_{\operatorname{per},0}(z)\varphi(r_{\operatorname{per},k}^\delta(z) - r_{\operatorname{per},0}^\delta(z)) \right]. \tag{C. 24}$$

Since $r_{\operatorname{per},k}^\delta(z) - r_{\operatorname{per},0}^\delta(z) = r_{\operatorname{per},0}^\delta(z)A_k r_{\operatorname{per},k}^\delta(z)$, where $A_k := -2(-i\nabla)\delta k + \delta^2|k|^2$, this gives

$$M''_{\delta,k}\varphi = -\delta \operatorname{den} \oint \left[r_{\operatorname{per}}^\delta(z)\varphi r_{\operatorname{per}}^\delta(z)A_k r_{\operatorname{per},k}^\delta(z) \right]. \tag{C. 25}$$

By the rescaling relation (3.34) and (C. 25), we see that

$$\begin{aligned} \|M''_{\delta,k}1\|_{L^2_{\operatorname{per},\delta}} &= \|U_\delta^* M''_{\delta,k} U_\delta \cdot U_\delta^* 1\|_{L^2_{\operatorname{per}}} = \delta^{3/2-2} \|M''_{1,k}1\|_{L^2_{\operatorname{per}}} \\ &= \delta^{-1/2} \left\| \operatorname{den} \left[\oint r_{\operatorname{per}}^2(z)A_k r_{\operatorname{per},\delta k}(z) \right] \right\|_{L^2_{\operatorname{per}}}. \end{aligned} \tag{C. 26}$$

By (C. 26), notation $A_k := -2(-i\nabla)\delta k + \delta^2|k|^2$ and inequality (4.32), with $\alpha = 0, 1/2$, we obtain, for $|k| \leq r$,

$$\begin{aligned} \|M''_{\delta,k}1\|_{L^2_{\operatorname{per}}} |k|^{-1} &\lesssim \delta^{-1/2+1} + \delta^{-1/2+2}r \\ &= \delta^{1/2} + \delta^{3/2}r. \end{aligned} \tag{C. 27}$$

By (3.38) and (C. 23), Eq. (C. 27) shows that

$$\|M''_\delta P_r \nabla^{-1}\varphi\|_{L^2} \lesssim \delta^{-1}. \tag{C. 28}$$

This bound, the observation that $\|\bar{P}_r \nabla^{-1}\|_\infty \lesssim r^{-1}$ (see (3.37)) and the definition $r = a/\delta \lesssim 1/\delta$ imply Eq. (C. 4). □

This completes the proof of Proposition C.1. □

We use Proposition C.1 to prove the following

Proposition C.4 *Let Assumption [A1] hold and let $\beta e^{-\eta_0\beta} \lesssim 1$ (which is weaker than Assumption [A3]). Then the operator M_δ is bounded as*

$$\|\nabla^{-1} \bar{P}_r M_\delta f\|_{\dot{H}^1} \lesssim \|f\|_\delta. \tag{C. 29}$$

Proof of Proposition C.4 Decomposing M_δ according to (C. 2) and using bounds Eqs. (C. 3) and (C. 4) of Proposition C.1, we see that

$$\begin{aligned} \|\nabla^{-1} \bar{P}_r M_\delta P_r \varphi\|_{L^2} &\leq \|\nabla^{-1} \bar{P}_r M'_\delta P_r \varphi\|_{L^2} + \|\nabla^{-1} \bar{P}_r M''_\delta P_r \varphi\|_{L^2} \\ &\lesssim \delta^{-1} \|V\|_{L^2_{\operatorname{per}}} \|f\|_{L^2} + \|\nabla f\|_{L^2}, \end{aligned} \tag{C. 30}$$

where V is given in (4.28). Using $\|V\|_{L^2_{\operatorname{per}}} \leq \|V\|_{L^\infty}^{1/2} \|V\|_{L^1_{\operatorname{per}}}^{1/2}$ and the definition $m := \|V\|_{L^1_{\operatorname{per}}}$ in (C. 30) gives

$$\|\nabla^{-1} \bar{P}_r M_\delta f\|_{\dot{H}^1} \lesssim \|V\|_{L^\infty}^{1/2} (\delta^{-1} m^{1/2} \|f\|_{L^2}) + \|\nabla f\|_{L^2}. \tag{C. 31}$$

Lemma B.2 and definition (3.45) imply (C. 29). □

Appendix D: Refined Nonlinear Estimates

Let N_δ be given implicitly by (3.31) and recall the definition of the $B_{s,\delta}$ norm from (3.45). Let $\dot{H}^0 \equiv L^2$. In this section we prove estimates on N_δ .

Proposition D.1 *Let Assumption [A1] hold. If $\|\varphi_1\|_{B_{s,\delta}}, \|\varphi_2\|_{B_{s,\delta}} = o(\delta^{-1/2})$, then we have the estimate*

$$\begin{aligned} & \|N_\delta(\varphi_1) - N_\delta(\varphi_2)\|_{L^2} \\ & \lesssim e^{-\beta} m^{-1/3} \delta^{-1/2} (\|\varphi_1\|_{B_{s,\delta}} + \|\varphi_2\|_{B_{s,\delta}}) \|\varphi_1 - \varphi_2\|_{\dot{H}^1}. \end{aligned} \tag{D.1}$$

We derive Proposition D.1 from its version with $\delta = 1$ by rescaling. For $\delta = 1$, we have the following result.

Proposition D.2 *Let Assumption [A1] hold $\|\psi\|_{L^2} = o(1)$. Then $N := N_{\delta=1}$ satisfies the estimate*

$$\begin{aligned} \|N(\psi_1) - N(\psi_2)\|_{L^2} & \lesssim \sum_{j=1}^2 \left[(\|\psi_j\|_{\dot{H}^1}) \|\psi_1 - \psi_2\|_{\dot{H}^1} \right. \\ & \quad + e^{-\beta} (\|\psi_j\|_{\dot{H}^1}^{1/3} \|\psi_j\|_{L^2}^{2/3}) \|\psi_1 - \psi_2\|_{\dot{H}^1} \\ & \quad \left. + \|\psi_j\|_{\dot{H}^1} \|\psi_1 - \psi_2\|_{\dot{H}^1}^{1/3} \|\psi_1 - \psi_2\|_{L^2}^{2/3} \right]. \end{aligned} \tag{D.2}$$

The derivation of Proposition D.1 from Proposition D.2 is same as that of Proposition 5.1 from Proposition 5.2 and we omit it here.

Proof of Proposition D.2 Let h_{per} and $r_{\text{per}}(z)$ be given in (3.8). We use the relations (5.6)–(5.12) in the proof of Proposition 5.2. Following the latter proof we see that it suffices to improve the estimate of $N_k(\psi)$ in Proposition 5.3, to which we proceed. \square

Proposition D.3 *Let Assumption [A1] hold and let N_k be given by (5.12). Assume that $\|\nabla\psi\|_{L^2} = o(1)$, then, for any $k \geq 2$, we have the estimate*

$$\|\text{den}[N_k(\psi)]\|_{L^2} \lesssim \|\nabla\psi\|_{L^2}^k + e^{-\beta} \|\nabla\psi\|_{L^2}^{4/3} \|\psi\|_{L^2}^{2/3} \delta_{k,2}, \tag{D.3}$$

where the constants associated with \lesssim are independent of β and $\delta_{k,2}$ is the Kronecker delta.

Proof We begin with $k = 2$. To improve upon estimate (5.13), we, following [8], use the partition of unity

$$P_1 + P_2 = \mathbf{1}, \text{ with } P_1 := \chi_{h_{\text{per}} < \mu} \text{ and } P_2 := \chi_{h_{\text{per}} \geq \mu}. \tag{D.4}$$

Let $R_i \equiv R_i(z) = r_{\text{per}}(z) P_i$ where $i = 1, 2$, P_i and $r_{\text{per}}(z)$ are given in (D.4) and (3.8). Recalling definition (5.12) of $N_k(\psi)$ and inserting the partition of unity, $P_1 + P_2 = \mathbf{1}$, after each R in the integrand of (5.12), we arrive at

$$N_2(\psi) = \sum_{a,b,c=1,2} N_2^{abc}(\psi), \tag{D.5}$$

where the $N_2^{abc}(\psi)$, for $a, b, c = 1, 2$, denote the operators

$$N_2^{abc}(\psi) = \oint R_a \phi R_b \psi R_c. \tag{D.6}$$

We estimate the terms individually. Below, we use the estimate (see (4.32))

$$\|(1 - \Delta)^\alpha R_i(z)\| \lesssim d^{\alpha-1} \lesssim 1, \quad i = 1, 2, \tag{D.7}$$

for $\alpha \in [0, 1]$ and $z \in \Gamma$, where

$$d \equiv d(z) := \text{dist}(z, \sigma(h_{\text{per}})) \geq \frac{1}{4}. \tag{D.8}$$

Case 1 (121) and (212). We estimate the case for (121), the other case is done similarly. Since $P_1 P_2 = 0$, we write

$$N_2^{(121)}(\psi) = \oint R_1 \psi R_2 P_2 \psi R_1 \tag{D.9}$$

$$= \oint R_1 [P_1, \psi] P_2 R_2 P_2 [\psi, P_1] R_1. \tag{D.10}$$

Applying Lemma 2.1 and Eq. (D.7) to the r.h.s. and using that the operator norm is bounded by the L^2 norm, we find

$$\|\text{den}[N_2^{(121)}(\psi)]\|_{L^2} \lesssim \|(1 - \Delta)^{3/4+\epsilon} N_2^{(121)}(\phi)\|_{S^2} \tag{D.11}$$

$$\lesssim \left| \oint \right| d^{-3} \|[P_1, \psi] P_2\|_{S^2}^2. \tag{D.12}$$

where, recall,

$$\left| \oint \right| := \frac{1}{2\pi} \int_{\Gamma} dz |f_T(z - \mu)|. \tag{D.13}$$

A key observation allowing us to obtain an improved estimate is that the commutators lead to gradient estimates:

Lemma D.4 *Let Assumption [A1] hold, we have the estimate*

$$\|[P_i, \psi]\|_{S^2} \lesssim \|\nabla \psi\|_{L^2}, \quad i = 1, 2. \tag{D.14}$$

Proof of Lemma D.4 Since the identity commutes with any operator and $P_2 = \mathbf{1} - P_1$ (see (D.4)), we prove the lemma for P_1 only. Since h_{per} (see (3.8)) has a gap at μ , the Cauchy integral formula implies

$$P_1 = \frac{1}{2\pi i} \int_{\Gamma_1} (z - h_{\text{per}})^{-1} = \frac{1}{2\pi i} \int_{\Gamma_1} r_{\text{per}}(z) \tag{D.15}$$

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 $h_{\text{per}} > -c + 1$, and the contour is traversed counter-clockwise. We see that

$$[P_1, \psi] = \frac{1}{2\pi i} \int_{\Gamma_1} [r_{\text{per}}(z), \psi] \tag{D.16}$$

$$= \frac{1}{2\pi i} \int_{\Gamma_1} r_{\text{per}}(z) [\nabla \cdot, \nabla \psi] r_{\text{per}}(z) + \frac{1}{2\pi i} \int_{\Gamma_1} r_{\text{per}}(z) (2\nabla \psi \cdot \nabla) r_{\text{per}}(z). \tag{D.17}$$

Lemma D.4 is now proved by an application of the Kato–Seiler–Simon inequality ((2.14)) to (D.17) and noting that Γ_1 is compact and has length $O(1)$. □

Using Lemma D.4 and estimates (3.6) and (D.8) in (D.12) yields that

$$\| \text{den}[N_2^{(121)}(\psi)] \|_{L^2} \lesssim \| \nabla \psi \|_{L^2}^2. \tag{D.18}$$

Case 2: (112), (211), (122), (221) We estimate the case for (112), the other cases are done similarly. Again, since $P_1 P_2 = 0$, we write

$$N_2^{(112)}(\psi) = \oint R_1 \psi R_1 \psi R_2 \tag{D.19}$$

$$= \oint R_1 \psi R_1 [\psi, P_1] R_2. \tag{D.20}$$

Using Lemma 2.1 as in with $N_2^{(121)}(\psi)$ in (D.11), we estimate (D.20) as

$$\| \text{den}[N_2^{(112)}(\psi)] \|_{L^2} \lesssim \left| \oint \right| d^{-1} \| \psi R_1 \| \| [\psi, P_1] R_2 \|_{S^2}. \tag{D.21}$$

where $|\oint|$ is defined in (D.13). By the inequality $\|A\| \leq \|A\|_{L^p}$, for any $p < \infty$ for any operator A on $L^2(\mathbb{R}^3)$, and the Kato–Seiler–Simon inequality (2.14), we find $\| \psi R_1 \| \leq \| \psi R_1 \|_{S^6} \lesssim \| \psi \|_{L^6}$. Using this, together with Lemma D.4, in (D.21), we obtain

$$\| \text{den}[N_2^{(112)}(\psi)] \|_{L^2} \lesssim \left| \oint \right| d^{-2} \| \psi \|_{L^6} \| \nabla \psi \|_{L^2}. \tag{D.22}$$

Combining this with (3.6), (D.8) and Hardy–Littlewood’s inequality (2.18) gives

$$\| \text{den}[N_2^{(112)}(\psi)] \|_{L^2} \lesssim \| \nabla \psi \|_{L^2}^2. \tag{D.23}$$

Case 3 (111) and (222). We use the L^2 – L^2 duality to estimate the L^2 norm of $\text{den}[N_2^{(qqq)}(\psi)]$, $q = 1, 2$. We have, by (2.5) and definition (5.12),

$$\begin{aligned} \| \text{den}[N_2^{(qqq)}(\psi)] \|_{L^2} &= \sup_{\|f\|_{L^2}=1} \left| \int f \text{den}[N_2^{(qqq)}(\psi)] \right| \\ &= \sup_{\|f\|_{L^2}=1} \left| \text{Tr}[f N_2^{(qqq)}(\psi)] \right| \\ &= \sup_{\|f\|_{L^2}=1} \left| \oint \text{Tr}(f R_q \psi R_q \psi R_q) \right|. \end{aligned} \tag{D.24}$$

(In the last two lines, f is considered as a multiplication operator.) To show that the integral on the r.h.s. converges absolutely, we follow the arguments in (5.17)–(5.20) to prove, for $q = 0, 1$,

$$| \text{Tr}(f R_q (\psi R_q)^2) | \lesssim d^{-4/3} \|f\|_{L^2} \| \nabla \psi \|_{L^2}^{4/3} \| \psi \|_{L^2}^{2/3}. \tag{D.25}$$

Due to definition (D.8) of $d \equiv d(z)$, this shows that the integral on the r.h.s. of (D.24) converges absolutely.

Lemma D.5 For $q = 1, 2$, we have

$$\begin{aligned} &\oint \text{Tr}[f R P_q g R P_q h P_q] \\ &= \frac{1}{2\pi i} \int_{\Gamma_q} (f_T(z) - 1) \text{Tr}[f R P_q g R P_q h P_q]. \end{aligned} \tag{D.26}$$

Proof Note that the contour Γ in Fig. 2 is the union of two disjoint contours, $\Gamma = \Gamma_1 \cup \Gamma_2$, with Γ_1 being the closed contour and Γ_1 unbounded one (i.e. the parts of Γ with $\text{Re } z < \mu$ and $\text{Re } z > \mu$). We first note that, by Bloch’s theory,

$$\int_{\Gamma_q} dz \text{Tr}[f R P_q g R P_q h P_q] = \int_{\Gamma_q} dz \int_{(\Omega^*)^3} d\hat{k} d\hat{k}_1 d\hat{k}_2 \tag{D.27}$$

$$\times \text{Tr}_{L^2_{\text{per}}} f_{k-k_1} (R P_q)_{k_1} g_{k_1-k_2} (R P_q)_{k_2} h_{k_2-k} (R P_q)_k. \tag{D.28}$$

Computing the trace in the complete orthonormal basis of eigenvectors $\varphi_{m,k}$ of $(R P_q)_k$ (with eigenvalues $\lambda_{m,k}$) and inserting the complete orthonormal bases of eigenvectors φ_{n,k_1} and φ_{r,k_2} of $(R P_q)_{k_1}$ and $(R P_q)_{k_2}$ (with eigenvalues λ_{n,k_1} and λ_{r,k_2}) into (D.28), we see that

$$\int_{\Gamma_1} \text{Tr}[f R P_q g R P_q h P_q] = \sum_{m,n,r} \int_{(\Omega^*)^3} d\hat{k} d\hat{k}_1 d\hat{k}_2 \tag{D.29}$$

$$\times \langle \varphi_{m,k}, f_{k-k_1} \varphi_{n,k_1} \rangle \langle \varphi_{n,k_1}, g_{k_1-k_2} \varphi_{r,k_2} \rangle \langle \varphi_{r,k_2}, h_{k_2-k} \varphi_{m,k} \rangle \tag{D.30}$$

$$\times \int_{\Gamma_q} dz \frac{1}{(z - \lambda_{m,k})(z - \lambda_{n,k_1})(z - \lambda_{r,k_2})}. \tag{D.31}$$

Since P_1 projects to the spectrum of h_{per} on the left of μ , we see that $\lambda_{m,k}, \lambda_{n,k_1}, \lambda_{r,k_2} < \mu$. In particular, these eigenvalues are in the left closed contour in Fig. 2. Consequently, Cauchy’s integral formula shows that the term in the large bracket in (D.31) is identically zero. Similar argument applies to P_2 . This shows that

$$\frac{1}{2\pi i} \int_{\Gamma_q} \text{Tr}[f R P_q g R P_q h P_q] = 0. \tag{D.32}$$

Thus (D.26) follows. □

Using the explicit form of the Fermi–Dirac distribution f_T in (1.2), we see that

$$|f_T(z - \mu) - 1| = \frac{e^{\beta(\text{Re } z - \mu)}}{|1 + e^{\beta(z - \mu)}|}. \tag{D.33}$$

By condition (1.26) and by the choice of the contour, Γ , in Fig. 2, we see that the if $z \in \Gamma$, then $\text{Re } z$ is at least at the distance ≥ 1 from μ . Hence, for z in a contour Γ , (D.33) implies that

$$|f_T(z - \mu) - 1| \lesssim e^{-\beta}. \tag{D.34}$$

Applying estimates (D.34) and (D.25) to the r.h.s. of (D.26) and recalling the definition (D.8) of $d \equiv d(z) \geq \frac{1}{4}$, we arrive at the inequality

$$\begin{aligned} & \left| \oint \text{Tr}[f R P_q g R P_q h P_q] \right| \\ & \lesssim e^{-\beta} \|f\|_{L^2} \|\nabla \psi\|_{L^2}^{4/3} \|\psi\|_{L^2}^{2/3}. \end{aligned} \tag{D.35}$$

This inequality, together with the relation (D.24), gives

$$\left\| \text{den}[N_2^{(qqq)}(\phi)] \right\|_{L^2} \lesssim e^{-\beta} \|\nabla \phi\|_{L^2}^{4/3} \|\phi\|_{L^2}^{2/3}. \tag{D.36}$$

Inequalities (D.18), (D.23) and (D.36) imply estimate (D.3) for $k = 2$.

Now we estimate N_k for $k > 2$. By (3.6) and (3.10), it suffices to estimate $\text{den}[R(\phi R)^k]$ where $R = r_{\text{per}}(z)$ is given in (3.8). Using Lemma 2.1, we see that

$$\|\text{den}[R(\phi R)^k]\|_{L^2} \lesssim (1 - \Delta)^{4/3+\epsilon} R(\phi R)^k \|_{S^2} \quad (\text{D.37})$$

$$\lesssim \|(\phi R)^k\|_{S^2}. \quad (\text{D.38})$$

Using Hölder's inequality with $\frac{1}{2} = \frac{1}{6} + \frac{1}{6} + \frac{1}{6} +$ another k terms of $\frac{1}{\infty}$, (D.38) becomes

$$\|\text{den}[R(\phi R)^k]\|_{L^2} \leq \|\phi R\|_{S^6}^3 \|\phi R\|^{k-3} \quad (\text{D.39})$$

$$\leq \|\phi R\|_{S^6}^k, \quad (\text{D.40})$$

where the last line follows since $\|\cdot\| \leq \|\cdot\|_{S^p}$ for $p < \infty$. Combining with Kato–Seiler–Simon's inequality (2.14) and Hardy–Littlewood's inequality (2.18), (D.40) implies (D.3) for $k \geq 3$. \square

The rest of the proof of Proposition D.1 proceeds as the proof of in Proposition 5.3. \square

References

- Anantharaman, A., Cancès, E.: Existence of minimizers for Kohn–Sham models in quantum chemistry. *Ann. I. H. Poincaré - AN* **26**, 2425–2455 (2009)
- Bach, V., Breteaux, S., Chen, Th., Fröhlich, J.M., Sigal, I.M.: The time-dependent Hartree–Fock–Bogoliubov equations for bosons. *J. Evol. Equ.* 2020 (to appear). [arXiv:1602.05171v2](https://arxiv.org/abs/1602.05171v2)
- Bach, V., Lieb, E.H., Solovej, J.P.: Generalized Hartree–Fock theory and the Hubbard model. *J. Stat. Phys.* **76**, 3–89 (1994)
- Brislaw, C.: Kernels of trace class operators, *Proceedings AMS* 104. No. 4 (1988)
- Cancès, E., Deleurence, A., Lewin, M.: A new approach to the modeling of local defects in crystals: the reduced Hartree–Fock case. *Commun. Math. Phys.* **281**(1), 129–177 (2008)
- Cancès, E., Deleurence, A., Lewin, M.: Non-perturbative embedding of local defects in crystalline materials. *J. Phys.* **20**, 294213 (2008)
- Cancès, E., Lewin, M.: The dielectric permittivity of crystals in the reduced Hartree–Fock approximation. *Arch. Ration. Mech. Anal.* **197**(1), 139–177 (2010)
- Cancès, E., Lewin, M., Stoltz, G.: *The Microscopic Origin of the Macroscopic Dielectric Permittivity of Crystals*. Lecture Notes in Computational Science and Engineering, vol. 82. Springer (2011)
- Cancès, E., Stoltz, G.: A mathematical formulation of the random phase approximation for crystals. *Ann. I. H. Poincaré - AN* **29**(6), 887–925 (2012)
- Catto, I., Le Bris, C., Lions, P.-L.: On the thermodynamic limit for Hartree–Fock type models. *Ann. I. H. Poincaré - AN* **18**(6), 687–760 (2001)
- Catto, I., Le Bris, C., Lions, P.-L.: On some periodic Hartree type models. *Ann. I. H. Poincaré - AN* **19**(2), 143–190 (2002)
- Chenn, I., Sigal, I.M.: On the Bogolubov–de Gennes equations. [arXiv:1701.06080v2](https://arxiv.org/abs/1701.06080v2) (2019)
- Chenn, I., Sigal, I.M.: On effective PDEs of quantum physics. In: D'Abicco, M., et al. (eds.) *New Tools for Nonlinear PDEs and Application*, Birkhäuser Series. Trends in Mathematics.
- Cycon, H., Froese, R., Kirsch, W., Simon, B.: *Schrödinger Operators (with Applications to Quantum Mechanics and Global Geometry)*. Springer, Berlin (1987)
- E, W., Lu, J.: Electronic structure of smoothly deformed crystals Cauchy–Born Rule for the nonlinear tight-binding model. *Commun. Pure Appl. Math.* **63**(11), 1432–1468 (2010)
- E, W., Lu, J.: The electronic structure of smoothly deformed crystals: Wannier functions and the Cauchy–Born rule. *Arch. Ration. Mech. Anal.* **199**(2), 407–433 (2011)
- E, W., Lu, J.: The Kohn–Sham equation for deformed crystals. *Mem. AMS* (2013)
- E, W., Lu, J., Yang, X.: Effective Maxwell equations from time-dependent density functional theory. *Acta. Math. Sin.-English Ser* **27**, 339–368 (2011)
- Fogolari, F., Brigo, A., Molinari, H.: The Poisson–Boltzmann equation for biomolecular electrostatics: a tool for structural biology. *J. Mol. Recognit.* **15**, 377–392 (2002)
- Gustafson, S.J., Sigal, I.M.: *Mathematical Concepts of Quantum Mechanics*, 2nd edn. Universitext, Springer (2011)

21. Hainzl, Ch., Lewin, M., Seré, E.: Existence of atoms and molecules in the mean-field approximation of no-photon quantum electrodynamics. *Arch. Ration. Mech. Anal.* **192**(3), 453–499 (2009)
22. Le Bris, C., Lions, P.-L.: From atoms to crystals: a mathematical journey. *J. Bull AMS* **42**, 291–363 (2005)
23. Levitt, A.: Screening in the finite-temperature reduced Hartree-Fock model. [arXiv:1810.03342v1](https://arxiv.org/abs/1810.03342v1) (2018)
24. Lieb, E., Loss, M.: *Analysis*, 2nd edn. AMS Press, Providence, RI (2001)
25. Lieb, E.H.: The stability of matter: from atoms to stars. *Bull. AMS* **22**, 1–49 (1990)
26. Lieb, E.H., Simon, B.: The Hartree-Fock theory for Coulomb systems. *Commun. Math. Phys.* **53**(3), 185–194 (1977)
27. Lindblad, G.: Expectations and entropy inequalities for finite quantum systems. *Commun. Math. Phys.* **39**, 111–119 (1974)
28. Lions, P.L.: *Hartree-Fock and Related Equations. Nonlinear Partial Differential Equations and Their Applications. Collège de France Seminar, vol. IX. Pitman Res. Notes Math. Ser. vol. 181, pp. 304–333 (1988)*
29. Lions, P.L.: Solutions of Hartree-Fock equations for Coulomb systems. *Commun. Math. Phys.* **109**, 33–97 (1987)
30. Markowich, P.A., Rein, G., Wolansky, G.: Existence and nonlinear stability of stationary states of the Schrödinger-Poisson system. *J. Stat. Phys.* **106**(5–6), 1221–1239 (2002)
31. Mermin, N.D.: Thermal properties of the inhomogeneous electron gas. *Phys. Rev.* **137**, A1441 (1965)
32. Nier, F.: A variational formulation of Schrödinger-Poisson systems in dimension $d \leq 3$. *Commun. PDEs* **18**(7 and 8), 1125–1147 (1993)
33. Prodan, E., Nordlander, P.: On the Kohn-Sham equations with periodic background potential. *J. Stat. Phys.* **111**(3–4), 967–992 (2003)
34. Reed, M., Simon, B.: *Method of Modern Mathematical Physics IV: Analysis of Operators*. Academic Press, London (1978)
35. Sevik, C., Bulutay, C.: Theoretical study of the insulating oxides and nitrate: SiO_2 , GeO_2 , Al_2O_3 , Si_3N_4 , and Ge_3N_4 . [arXiv:cond-mat/0610176v2](https://arxiv.org/abs/cond-mat/0610176v2) (2008)
36. Simon, B.: *Trace Ideals and Their Applications*, 2nd edn. AMS Press, Providence, RI (2005)

Publisher's Note Springer Nature remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.