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# On an effective equation of the reduced Hartree-Fock theory

**Abstract:** We show that there is a one-to-one correspondence between solutions to the Poisson-landscape equations and the reduced Hartree-Fock equations in the semi-classical limit at low temperature. Moreover, we prove that the difference between the two corresponding solutions is small by providing explicit estimates.

## 1 Introduction

### 1.1 Reduced Hartree-Fock equation

Despite the success of the density functional theory (DFT), its computational difficulties remain a major bottleneck. Filoche and Mayboroda initiated a series of recent works on the landscape function [18], which led to a further simplification of the DFT by introducing the Poisson-landscape (PL) equation [19,37]. The landscape theory and numerical simulations [2–4,19,37,43] suggest that solving the PL equation can be an efficient and accurate replacement of the original DFT. This success undoubtedly demands a rigorous mathematical justification and a theoretical foundation.

DFT originated as a systematic way to study the large many-body quantum system by using a self-consistent 1-body approximation. Parallel to its development, a number of effective theories existed along with DFT; examples include the Hartree-Fock theory, the Bardeen-Cooper-Schrieffer (BCS) theory, and the Thomas-Fermi theory of electrons. While DFT enjoyed a similar energy functional as the more complex Hartree-Fock theory and the BCS theory, inheriting a form of accuracy, it also gravitated toward the Thomas-Fermi theory to study the simpler electron density instead of density matrices. Owing to these characteristics, the Kohn-Sham (KS) energy and the equation of DFT were developed [21,22]. These equations and their related theory have become a mainstay of modern condensed matter physics. Some notable areas of application include semi-conductor design, deformation theory in solid mechanics, and quantum chemistry. In the mean time, a plethora of mathematical studies also ensued, for example, see [17,23,26,27,30–33,35,42].

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The KS equation is a set of functional equations for the electron density $\rho$, which is often simplified to the reduced Hartree-Fock equation (REHF) to illuminate core mathematical properties while maintaining its key features [8–10,13,20,28,29,41]. This is achieved by ignoring the exchange-correlations terms in the KS equation. In the same spirit, we will also consider this simplified REHF in our work and be consistent with the aforementioned landscape theory in [19,37].

Consider a semi-conductor at a positive temperature, $\beta^{-1}$, with a background charge distribution $\kappa$,[1] and a band-offset potential $V$.[2] We choose physical units such that as many physical constants are set to 1 as possible. In this case, the REHF equation states that the material's electron density, $\rho$, is given by

$$\rho = \mathrm{den} f_{\mathrm{FD}}(\beta(-\Delta + V - \phi - \mu)), \tag{1}$$

where $\mu$ is the chemical potential/Fermi energy, $f_{\mathrm{FD}}$ is the Fermi-Dirac distribution

$$f_{\mathrm{FD}}(\lambda) = \frac{1}{1 + e^\lambda}, \tag{2}$$

$\phi$ is the electric potential solving the Poisson equation

$$-\Delta\phi = \kappa - \rho, \tag{3}$$

and den is the density operator defined via

$$(\mathrm{den} A)(x) = A(x, x), \tag{4}$$

where $A$ is an operator on $L^2(\mathbb{R}^3)$ and $A(x, y)$ is the integral kernel of $A$ (see Appendix A for more details). If $A$ has a full set of eigenbasis $\phi_i$ with eigenvalues $\lambda_i$, then den$A$ has the more familiar expression:

$$(\mathrm{den} A)(x) = \sum_i \lambda_i |\phi_i|^2(x). \tag{5}$$

We remark that while equation (1) is an equation for microscopic electronic structures of matter, dopant potentials and band-offsets often vary on another larger mesoscopic scale. A precise formulation of the problem would require a homogenized version of (1) where mesoscopic parameters such as the dielectric operator emerge. However, we will make the possibly unphysical assumption that (1) is already homogenized and the dielectric constant is 1 purely for mathematical simplicity (Remark 1.6).

Moreover, we further restrict ourselves to the semi-classical regime and modify (1) as follows:

$$\rho = \mathrm{den} f_{\mathrm{FD}}(\beta(-\varepsilon^2\Delta + V - \phi - \mu)), \tag{6}$$

where $\varepsilon \ll 1$ is the semi-classical parameter. In addition, in semi-conductor models, the band-offset potential $V$ is piecewise constant (often viewed as a realization of a random potential of Anderson type). We restrict our study to a potential of the form $V = V_{\min} + \delta V_p$, where $V_{\min}$ is a constant, $V_p$ is a piecewise constant function, and $\delta \ll 1$ is a small parameter, i.e., $V$ is a piecewise constant potential being close to a constant $V_{\min}$. (See more precise definition of $V$ in the next subsection.) In this regime, one natural effective equation for (6) is expressed as follows:

$$\rho = \frac{1}{(2\pi\varepsilon)^3} \int_{\mathbb{R}^3} \mathrm{d}p f_{\mathrm{FD}}(\beta(p^2 + V_{\min} + \delta V_p - \phi - \mu)), \tag{7}$$

where $\phi$ solves (3) as mentioned earlier, and $V_{\min}$ and $V_p$ will be specified later. However, the piecewise constant $V$ renders semi-classical analysis potentially ineffective. That is, the error of the difference between the right-hand side of (6) and the right-hand side of (7) cannot be meaningfully controlled. Consequently, a form of regularization is needed. There were previous results in semi-classical analysis

[1] In semiconductor production, such a background charge is usually called a dopant density/doping level.
[2] For simplicity, we only consider the conduction band potential (band edge) $V_{\mathrm{cond}} = V - \phi$. The band-offset potential $V$ is defined to be $V_{\mathrm{cond}} + \phi$. We refer readers to [19] and references therein for more details of these terminologies in semi-conductor models.

dealing with potentials without any assumption on regularity, see, e.g., [29]. The PL equation presents a different regularization method that preserves both the spectrum of the Hamiltonian $H = -\varepsilon^2\Delta + V - \phi$ and the density $\rho$ (more details can be found in the proof of Theorem 1.3). We want to emphasize that the PL equation was proposed as a computational simplification rather than a regularization method for the semi-classical expansion initially, see more discussion in the next subsection.

## 1.2 Landscape theory and the PL equation

In one view, the landscape theory presents a partial diagonalization of the Schrödinger Hamiltonian $H = -\varepsilon^2\Delta + V - \phi$ [4]. In [18], if $H > 0$, the landscape function $u$ is defined as follows:

$$Hu = 1, \tag{8}$$

and the landscape potential $W$ is defined as follows:

$$W = 1/u. \tag{9}$$

Conjugating $H$ by $u$, we obtain

$$u^{-1}Hu = -\varepsilon^2\Delta - 2u^{-1}\varepsilon\nabla u \cdot \varepsilon\nabla + W. \tag{10}$$

We remark here that $u^{-1}Hu$ has the same spectrum as $H$. This forms the basis for isospectral regularization as mentioned at the end of the previous section. Ignoring the drift term in $u^{-1}Hu$, this suggests that we should modify equation (7) as follows:

$$\rho = \frac{1}{(2\pi\varepsilon)^3}\int_{\mathbb{R}^3} dp f_{\mathrm{FD}}(\beta(p^2 + W - \mu)), \tag{11}$$

where

$$W = 1/u, \tag{12}$$

$$(-\varepsilon^2\Delta + V - \phi)u = 1. \tag{13}$$

This equation was proposed as a computational simplification to the REHF and studied in the physical work [19,34,37]. Together with (3), they bear the name PL equation.

Numerical solution to the REHF equation requires an extensive computation of a large number of eigenvalues and eigenfunctions of the Hamiltonian $H$. Although various eigensolvers have been developed for this purpose (for a survey, see [6,40]), such a direct computation remains a challenge in large-scale systems, particularly in high dimensions. In the specific setting of semi-conductor physics with random potentials, the landscape function $u$ alleviates this problem through the approximation that the $i$th lowest eigenvalue $E_i$ of the Hamiltonian $H$ can be numerically predicted by the $i$th smallest local minimum of the landscape potential $W$ (defined in (9)), $W_i$:

$$E_i \approx \left(1 + \frac{d}{4}\right)W_i, \tag{14}$$

where $d$ is the spatial dimension [2]. Following this success, [2] showed further that the number of eigenvalues below $E$, $N_V(E)$, of $H$ can be approximated by

$$N_V(E) \approx \frac{1}{(2\pi\varepsilon)^3}\int_{\mathbb{R}^3\times\Omega} dp dx \mathbf{1}_{\{p^2 + W(x)\leq E\}} \tag{15}$$

numerically. This approximation enjoys a more accurate prediction than the usual Weyl's law on average. We note that the left-hand side of (15) is

$$\int_{\mathbb{R}^3} \rho_{T=0,\mu=E}, \tag{16}$$

where $\rho_{T=0,\mu=E}$ is the electron density at zero temperature with $\mu = E$ (cf. (6)). Consequently, we expect that the solutions to the PL equation (11) are good approximations to the density of electrons. In [19], the self-consistent PL model was introduced and allows the authors of [19] to bypass solving the Schrödinger equation. According to the real modeling exercises in [34], the landscape model considerably reduced the computation time, compared to a conventional Schrödinger solver.

Up to now, many of the stated advantages of the landscape theory have mostly been proven useful for numerical purposes. The current article is the first rigorous mathematical treatment of the PL model. The goal of the current work is to introduce a rigorous treatment of the PL equation as an effective equation of the REHF equation in the semi-classical limit. Other related rigorous mathematical treatments of the landscape theory for different models can be found in [3,5,16,39,43].

## 1.3 Results

We limit ourselves to the periodic setting in which physical quantities are periodic on $\Omega = \mathbb{R}^3/(L\mathbb{Z})^3 \cong [0, L]^3$, while the quantum states are on $\mathbb{R}^3$. That is, quantities such as $\rho$, $\kappa$, $V$, or $\phi$ are periodic while the associated operators, such as $H = -\varepsilon^2\Delta + V - \phi$, act on $L^2(\mathbb{R}^3)$ (see Appendix A for more details).

Moreover, let $X = \mathbb{R}^3$ or $\Omega$ and $L^p(X; \mathbb{F})$ be the usual $L^p$ space of $\mathbb{F}$ valued functions on $X$, where $\mathbb{F} = \mathbb{R}$ or $\mathbb{C}$. In the special case when $\mathbb{F} = \mathbb{C}$, we denote $L^p(X) = L^p(X; \mathbb{C})$. We endow $L^p(X; \mathbb{F})$ with its standard $p$-norms. Similarly, we equip $L^2(X; \mathbb{F})$ its standard inner product. Due to the periodic nature of $\Omega$, we identify $L^2(\Omega; \mathbb{F})$ with

$$\left\{ f \in L^2_{\text{loc}}(\mathbb{R}^3; \mathbb{F}) : f \text{ is } (L\mathbb{Z})^3 \text{ periodic and } \int_\Omega |f|^2 < \infty \right\}. \tag{17}$$

We let $H^s(\Omega; \mathbb{F}) \subset L^2(\Omega; \mathbb{F})$ denote the associated Sobolev spaces of order $s$ with periodic boundary conditions. The identification of $H^s(\Omega; \mathbb{F})$ with $H^s$ periodic functions on $\mathbb{R}^3$ persists. When $\mathbb{F} = \mathbb{C}$, we will suppress the symbol $\mathbb{C}$. The conversion from $L^2(\mathbb{R}^3; \mathbb{F})$ to $L^2(\Omega; \mathbb{F})$ is done via the density operator den, introduced in (4). That is, the den of a periodic operator on $L^2(\mathbb{R}^3)$ is a periodic function, with fundamental domain $\Omega$.[3] Next, we restrict our study to the following type of piecewise constant potentials, which can be viewed as a (hence any) realization of a random potential of Anderson type.

**Definition 1.1.** Let $0 < L \in \mathbb{Z}$. An $(L\mathbb{Z})^3$ periodic potential $V$ is called landscape admissible if $V$ is a strictly positive and piecewise constant, given by

$$V(x) = \sum_{j \in \mathbb{Z}^3} \omega_j \chi(x - j), \quad \text{for} \quad x \in \Omega, \tag{18}$$

where $0 \le \omega_j \in \mathbb{R}$ is $(L\mathbb{Z})^3$ periodic in $j$ and $\chi(x)$ is the indicator function of $[0, 1)^3$. We note that a landscape admissible function $V$ is real valued by this definition.

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**3** For simplicity, we restrict ourselves to the periodic boundary condition to avoid technical issues. It is slightly easier to carry out the landscape theory on periodic domains, see, e.g., the work in [2,3,16]. For the REHF with an Anderson type random potential, one would expect similar results for different boundary conditions, especially for relatively large domain size. Such intuition comes from the ergodicity of the random potential. For example, one can see the discussion in [7] for the IDS of the Anderson model with different boundary conditions. Unfortunately, we were not able to extend our results for the REHF and PL (PL equations) to the Dirichlet boundary condition.

Our assumption on the external potential $V$ is that $V$ is Landscape admissible with a positive minimum, and the gap between its maximum and minimum is much smaller compared to its minimum. For simplicity, we will assume the external potential is given in the form

$$V(x) = V_{\min} + \delta V_p(x), \tag{19}$$

where $V_{\min} := \inf V(x) > 0$, $0 \le \delta < 1$, and $V_p(x)$ is a piecewise constant function as (18) satisfying $\inf V_p = 0$, $\sup V_p = 1$.

Throughout the article, we will write $A \lesssim B$ or $A = O(B)$ if $A \le CB$ for some constant $C$ independent of $\varepsilon$, $\delta$, $\beta$, and $\kappa$.

Our first result shows that the density on the right-hand side of (6) can be approximated by the right-hand side of (11). This result will be proved in Section 3.

**Theorem 1.1.** *Let $V$ be a* Landscape admissible *potential given in the form* (19). *In addition, assume that*
(1) $\beta > \beta_*$, $0 < \varepsilon < \varepsilon_*$, *and* $0 \le \delta < \delta_*$, *where* $\beta_* > 1$, $\varepsilon_* < 1$, $\delta_* < 1$ *are constants only depending on* $V_{\min}$, *the dimension $d$, and the domain size $L$.*
(2) $\phi \in H^2(\Omega; \mathbb{R})$ *and* $\|\phi\|_{H^2(\Omega)} \lesssim \delta$,
(3) $V_{\min} - \mu \ge C > 0$, *where $C$ is a constant independent of $\delta$ and $\varepsilon$.*

*Then there exists $V_{\mathrm{cut}} \in \mathbb{R}$ with*

$$0 < V_{\min} - V_{\mathrm{cut}} \approx O(\delta^{1/4}), \tag{20}$$

*and two effective potentials $W_1 = 1/u_1$ and $W_2 = 1/u_2$ satisfying*

$$(-\varepsilon^2 \Delta + (V - V_{\mathrm{cut}} - \phi))u_1 = 1, \tag{21}$$

$$(-\varepsilon^2 \Delta + (V - V_{\mathrm{cut}}))u_2 = 1. \tag{22}$$

*Moreover, the density has the asymptotic expansion*

$$\mathrm{den} f_{\mathrm{FD}}(\beta(-\varepsilon^2\Delta + V - \phi - \mu)) = \frac{1}{(2\pi\varepsilon)^3} \int_{\mathbb{R}^3} \mathrm{d}p\, f_{\mathrm{FD}}(\beta(p^2 + W_1 + V_{\mathrm{cut}} - \mu)) + R_1 \tag{23}$$

$$= \frac{1}{(2\pi\varepsilon)^3} \int_{\mathbb{R}^3} \mathrm{d}p\, f_{\mathrm{FD}}(\beta(p^2 + W_2 - \phi + V_{\mathrm{cut}} - \mu)) + R_2, \tag{24}$$

*where*

$$\|R_1\|_{L^2(\Omega)}, \|R_2\|_{L^2(\Omega)} \lesssim \varepsilon^{-3+1/2}\beta^{-1}e^{-\beta(V_{\mathrm{cut}}-\mu-\delta^{1/4})}. \tag{25}$$

Theorem 1.1 provides the foundation for a rigorous justification of the PL equation. In addition, (22) suggests that a simpler effective equation is also possible. More precisely, let

$$F_{\mathrm{REHF}}(\phi, \mu) := \mathrm{den} f_{\mathrm{FD}}(\beta(-\varepsilon^2\Delta + V - \phi - \mu)), \tag{26}$$

$$F_{\mathrm{PL}}(\phi, \mu) := \frac{1}{(2\pi\varepsilon)^3} \int_{\mathbb{R}^3} \mathrm{d}p\, f_{\mathrm{FD}}(\beta(p^2 + W_1 + V_{\mathrm{cut}} - \mu)), \tag{27}$$

$$F_{\mathrm{LSC}}(\phi, \mu) := \frac{1}{(2\pi\varepsilon)^3} \int_{\mathbb{R}^3} \mathrm{d}p\, f_{\mathrm{FD}}(\beta(p^2 + W_2 - \phi + V_{\mathrm{cut}} - \mu)), \tag{28}$$

where $W_1 = 1/u_1$ and $W_2 = 1/u_2$ and $u_1$ and $u_2$ are given in (21) and (22), respectively. LSC stands for "landscape regularized semi-classical," and we will henceforth call this new $F_{\mathrm{LSC}}$ the landscape regularized semi-classical (LSC) regime. We note that $F_{\mathrm{LSC}}$ is a further simplification of $F_{\mathrm{PL}}$ and more closely resembles the semi-classical approximation (7). Inserting $\rho = F(\phi, \mu)$ for $F = F_{\mathrm{REHF}}, F_{\mathrm{PL}}, F_{\mathrm{LSC}}$ into equation (3), we obtain the REHF, PL, and LSC equation, respectively, for the electric potential $\phi$:

$$-\Delta\phi = \kappa - F(\phi, \mu). \tag{29}$$

One advantage of $F = F_{LCS}$ is that (29) is the Euler-Lagrange equation of a certain (energy) functional (Appendix B). This ensures that the linearization in $\phi$ is self-adjoint, whereas the linearization of $F_{PL}$ is not self-adjoint in general. More importantly, the potential $W_2$ does not depend on $\phi$, and it only depends on the underlying material property due to $V$. One may further incorporate the doping features into $V$ the addition of an ansatz due to doping and electron density. That is, if $\rho_0$ is an a priori estimate for $\rho$, with associated electric potential $\phi_0$, we may look for solutions to (29) of the form $\rho = \rho_0 + \rho'$ and $\phi = \phi_0 + \phi'$. By substituting these expressions into (29) and upon minor modification, we obtain

$$-\Delta\phi' = \frac{1}{(2\pi\varepsilon)^3} \int_{\mathbb{R}^3} dp f_{FD}(\beta(p^2 + \widetilde{W} - \phi' + V_{cut} - \mu)) - \rho_0,$$

where $\widetilde{W} = 1/\tilde{u}$ and $\tilde{u}$ solves

$$(-\varepsilon^2\Delta + V - \phi_0 - V_{cut})\tilde{u} = 1.$$

Hence, all the material and doping properties are stored in $\tilde{W}$, which is independent of $\phi'$.

Finally, to state our main result relating the REHF, PL, LSC equations, and the associated electric fields, we specify additional assumptions.

**Assumption 1.** (Semi-classical regime). The semi-classical parameter

$$\varepsilon < e^{-C\delta^{-1/4}} \tag{30}$$

for some large constant $C > 0$ only depending on $V_{min}$, the dimension $d$, and the domain size $L$.

**Assumption 2.** (Low temperature). There is some $K \in \mathbb{R}$ such that $0 < K < V_{min} - \mu$ and the inverse temperature $\beta$ satisfies

$$K < \frac{\log(\varepsilon^{-3})}{\beta} < V_{min} - \mu, \quad \text{and} \quad \delta \lesssim \left(\frac{\log\beta}{\beta}\right)^4. \tag{31}$$

**Remark 1.2.** The positive temperature assumption $\beta^{-1} > 0$ is crucial for our main results. For technical reasons, the linearization of the density function relies on a large but finite $\beta$, see, e.g., Lemma 6.3. Our approach does not apply to the zero temperature case. At the zero temperature, the REHF equations in disordered media have been studied in [9], when the interaction is short range. Still many questions remain open at the zero temperature, especially for REHF with Anderson background and long interactions. We refer readers to these work and references therein for more related results.

**Assumption 3.** (Conservation of charge). The doping potential $\kappa \in L^2(\Omega; \mathbb{R})$. Moreover,

$$\kappa_0 := \frac{1}{|\Omega|} \int_\Omega \kappa \tag{32}$$

is a fixed constant.

**Theorem 1.3.** (Main result) *Let assumptions in* Theorem 1.1 *and* Assumptions 1–3 *hold. Assume that* $(\phi_0, \mu) \in H^2(\Omega; \mathbb{R}) \times \mathbb{R}$ *solves* (29) *with F being any one of* (26), (27), *or* (28), *and*

$$\|\phi_0\|_{H^2(\Omega)} \lesssim \delta. \tag{33}$$

*Then there exists* $C_1, C_2 > 0$ *and a unique* $\phi \in H^2(\Omega; \mathbb{R})$ *such that* $\|\phi_0 - \phi\|_{H^2(\Omega)} \lesssim \varepsilon^{C_1\delta^{1/4}}$ *and* $(\phi, \mu)$ *solves* (29) *with F being any other one of* (26), (27), *or* (28). *Moreover,*

$$\|\phi_0 - \phi\|_{H^2(\Omega)} \lesssim \varepsilon^{1/2 - C_2\delta^{1/4}}. \tag{34}$$

Theorem 1.3 has an immediate corollary in terms of the density $\rho$. Rearranging (29), the corresponding equations for the density are as follows:

$$\rho = F(\phi, \mu), \tag{35}$$

$$-\Delta\phi = \kappa - \rho. \tag{36}$$

**Corollary 1.4.** *Retain the assumptions in* Theorem 1.3. *Assume that* $(\rho_0, \mu) \in (\kappa + H^{-2}(\Omega; \mathbb{R})) \times \mathbb{R}$ *solves* (35)–(36) *with F being any one of* (26), (27), *or* (28), *and*

$$\|\kappa - \rho_0\|_{H^{-2}(\Omega)} \leq \delta. \tag{37}$$

*Then there exists* $C_1, C_2 > 0$ *and a unique* $\rho \in \kappa + H^{-2}(\Omega; \mathbb{R})$ *such that* $\|\rho_0 - \rho\|_{H^{-2}(\Omega)} \leq \varepsilon^{C_1\delta^{1/4}}$ *and* $(\rho, \mu)$ *solves* (35) *and* (36) *with F being any other one of* (26), (27), *or* (28). *Moreover,*

$$\|\rho_0 - \rho\|_{H^{-2}(\Omega)} \leq \varepsilon^{1/2 - C_2\delta^{1/4}}. \tag{38}$$

**Remark 1.5.** Corollary 1.4 answers the challenge posed in the introduction. It justifies [19, 37] on a mathematically rigorous level in the semi-classical regime at low temperature (or large $\beta$).

**Remark 1.6.** We noted in the paragraph before equation (6) that the dielectric constant is taken to be 1. However, as one will see from the proof of our main result Theorem 1.3, so long as the dielectric constant is strictly positive, the same conclusion can be derived, albeit with more cumbersome proofs.

**Remark 1.7.** Note that in both Theorem 1.3 and Corollary 1.4, a solution to (29) is a pair: either $(\phi, \mu)$ or $(\rho, \mu)$. Because of this particular view of solution, equation (29) has an important dilation symmetry (detailed below). Moreover, since $\kappa$ is real, another important complex conjugation symmetry exists. We now discuss these two symmetries and their consequences in light of Theorem 1.3 and Corollary 1.4.
(1)  (Dilation symmetry)

$$(\phi, \mu) \mapsto (\phi + t, \mu - t) \tag{39}$$

for $t \in \mathbb{R}$.
(2)  (Complex conjugation) If $\kappa$ and $V$ are real valued and $\mu \in \mathbb{R}$, then

$$(\phi, \mu) \mapsto (C\phi, \mu) \tag{40}$$

is a symmetry of (29) where $C\phi = \bar{\phi}$ is the complex conjugation of $\phi$.

Dilation requires one to regard all solutions $(\phi, \mu)$ related by a dilation as a single solution. In this way, the uniqueness of solution is regarded as uniqueness among an equivalence class. Nevertheless, since we fixed $\mu$ in Theorem 1.3 and Corollary 1.4, a particular representative of the equivalence class is chosen, and there is no ambiguity in the word "unique." Perhaps a better way to view this is to consider $\phi + \mu$ as the solution instead of $(\phi, \mu)$. In this way, one avoids the equivalence class description. Nevertheless, since we are interested in the difference of two solutions (34), any choice of either point of view causes no harm. Moreover, the complex conjugation symmetry (and the uniqueness of solution) ensures that any solution to (29) with real $\kappa$, $V$, and $\mu$ is necessarily real. Thus, the conclusions regarding the reality of $\phi$ and $\rho$ in Theorem 1.3 and Corollary 1.4, respectively, are in fact superfluous.

One also note that the PL equation with (27) does not have the dilation symmetry, contrasting the case of (26) and (28). Whether this difference makes numerical approximations using (27) less desirable is out of the scope of this article, since (27) respects the dilation symmetry in leading order $\varepsilon$ if $\varepsilon \ll 1$.

Theorem 1.3 could help us to prove existence of solutions for the three classes of equations REHF, PL, and LSC simultaneously. However, we were unable to prove the smallness assumption (33) in general.

However, we believe this condition should hold in many cases if $\|\kappa\|_{H^2(\Omega)} \leqslant \delta$ (for related results, see [15,25,38]). Nevertheless, we provide an existence result to the simplest case, the LSC equations, via variational principle for completeness sake. Since this type of existence result is well studied in the literature, we will not enumerate all previous works. The interested reader is referred to, for example, [1,11,12,14,36].

**Theorem 1.8.** (LSC existence) *If $\kappa - \kappa_0 \in H^{-2}(\Omega; \mathbb{R})$ (see (32) for definition of $\kappa_0$), there exists a solution $(\phi, \mu) \in H^2(\Omega; \mathbb{R}) \times \mathbb{R}$ to the LSC equation* (28).

**Proof.** This is a direct corollary of Theorem B.1. ☐

## 1.4 Outline of the proof

The proof consists of mainly two parts. The first part is an leading order expansion of electron density, $\rho = \mathrm{den} f_{\mathrm{FD}}(\beta(-\varepsilon^2\Delta + V - \phi - \mu))$ as stated in Theorem 1.1, via the effective potentials $W = 1/u$. We start in Section 2 from several quantitative estimates for the landscape function $u$, solving $(-\varepsilon^2\Delta + v - \phi)u = 1$ (for some abstract $v, \phi$), and the associated effective potential $W = 1/u$ in terms of the parameter $\delta$ and $\varepsilon$. Then we prove the leading order expansion Theorem 1.1 in Section 3 following an analysis of the landscape potential in Section 2. In Section 3, we work in a more general setting for a density $\rho = \mathrm{den} f(-\varepsilon^2\Delta + v)$ for some analytic function $f$ (under mild assumptions). The Schrödinger operator (and the associated density) is conjugated by the landscape function $u^{-1}(-\varepsilon^2\Delta + v)u$, and then estimated by a contour integral $\frac{1}{2\pi i}\int_\Gamma$ (for some $\Gamma$ in the complex plane around the spectrum of the Schrödinger operator). Then we expand the contour integral as a Taylor series of the effective potentials $W$. The leading-order terms in the expansion will contribute to the first terms in equations (23) and (24). The higher order terms in the expansion will contribute to the remainder and will be estimated as the error terms, using the quantitative estimates obtained in Section 2. The remainder/error estimates also rely on some estimates of the Schatten $p$-norm of commutators $[W, R]$ and Kato-Seiler-Simon inequality for a trace.

The second part is to use Theorem 1.1 to prove Theorem 1.3, relating the REHF, PL, LSC equations, and the associated electric fields. To do that, we digress briefly in Section 4 to establish a relationship between the parameters $\varepsilon, \beta, \mu$, etc. as a result of the constraint of the integrability condition

$$\int_\Omega \kappa = \int_\Omega F(\phi, \mu), \tag{41}$$

obtained by integrating (29) over $\Omega$. To prove Theorem 1.3, we rewrite the REHF, PL, and LSC equations in the form $-\Delta\phi = \kappa - F(\phi, \mu)$, where $F$ is one of (26)–(28). We assume that $(\phi_0, \mu)$ is a solution of equation for a choice of $X = $ REHF, PL, or LSC. We look for a solution, $\phi$, of the corresponding equation $Y = $ REHF, PL, and LSC, $Y \neq X$, near $(\phi_0, \mu)$ of the form $\phi = \phi_0 + \varphi$. The first step is to linearize $F$ at $\phi_0$. The linearization leads to an equivalent equation $(-\Delta + M)\varphi = \kappa' + N(\varphi)$, where $L = -\Delta + M$ is a positive operator with $M = d_\phi F(\phi, \mu)|_{\phi=\phi_0}$ the Gâteaux derivative of $F$ at $\phi_0$, and $N$ is a nonlinear operator. The quantitative positive lower bounds of $L$ for all three cases $X$ are obtained in Section 6. The crucial technical Lemma 6.3 to the linear analysis is based on unpublished notes of Chenn and I. M. Sigal, and proved in Lemma 6 of [15], via Fourier transforming the kernel of the density and careful branch-cutting. This lemma is one place/reason that we need to work with a positive temperature $\beta^{-1}$, and are not able to extend our work to the zero temperature case. The nonlinear analysis is presented in Section 7, provided the error estimates given by Theorem 1.1. The results from Section 4 and the assumptions of Theorem 1.3 provide the proper scaling regime to control our estimates in both the linear and nonlinear analysis. Finally, putting together the linear and nonlinear analysis in Sections 6 and 7, the core proof of Theorem 1.3 is finished by a standard fixed point argument in Section 3.

# 2 Landscape function in the semi-classical regime

In this section, we will obtain several estimates for the landscape function $u$ in the semi-classical regime. These estimates will play an important role in the proof of the main result. The landscape function $u$ is the solution to

$$(-\varepsilon^2\Delta + v - \phi)u = 1 \tag{42}$$

on $\Omega = [0, L]^3$ with periodic boundary condition, where $\phi \in H^2(\Omega)$ with $\|\phi\|_{H^2} \leq \delta$ and $v = V - V_{\text{cut}} = v_{\min} + \delta V_P$ is in the form (19) satisfying $0 < v_{\min} := \inf v = \inf V - V_{\text{cut}} \approx \delta^{1/4}$, and $\inf V_p = 0$, $\sup V_p = 1$.

**Theorem 2.1.** *Let $2 \leq p \leq \infty$. Let $v$ be given as earlier. Assume that $0 < \varepsilon, \delta < 1$ are small as in* Theorem 1.1. *Let $W = 1/u$, where $u$ solves the landscape function (42) with periodic boundary condition on $\Omega$, then*

$$\|\nabla W\|_{L^p(\Omega)} \leq C\delta^{1+\frac{1}{4}(\frac{1}{2}-\frac{1}{p})}\varepsilon^{-\frac{p-1}{p}}, \tag{43}$$

$$\|\Delta W\|_{L^p(\Omega)} \leq C\delta^{1+\frac{1}{4}(1-\frac{1}{p})}\varepsilon^{-\frac{2p-1}{p}}, \tag{44}$$

*where $C$ depends on $d$ and $p$ only.*

We start by estimating $\nabla^s u$ in the $L^2$ and $L^\infty$ norms first for $s = 0, 1, 2$. Theorem 2.1 is proved at the end of this section by interpolation. As a remark, we will write the $L^p(\Omega)$ and $H^s(\Omega)$ norms as $\|\cdot\|_p$ and $\|\cdot\|_{H^s}$, respectively, when there is no ambiguity.

**Proposition 2.2.** *Retain the definitions in* Theorem 2.1. *If $u$ solves (42) with periodic boundary condition on $\Omega$, then there is a constant $C$ such that*

$$\|u\|_{L^2(\Omega)} \leq C\delta^{-1/4}, \tag{45}$$

$$\|\nabla u\|_{L^2(\Omega)} \leq C\delta^{1/2}\varepsilon^{-1/2}, \tag{46}$$

$$\|\Delta u\|_{L^2(\Omega)} \leq C\delta^{5/8}\varepsilon^{-3/2}. \tag{47}$$

**Proof of Proposition 2.2.** The first inequality (45) follows from the fact that the Hamiltonian $H = -\varepsilon^2\Delta + v - \phi$ is bounded below by $v_{\min} - C\delta \gtrsim v_{\min}/2 \approx \delta^{1/4}$ for some constant $C$. We prove (46) and (47).

Notice that $V$ is only discontinuous on a subset $\Omega_0 = \{x = (x_1, \ldots, x_d) \in \Omega : x_j \in \mathbb{Z}\} \subset \Omega$ and piecewise constant elsewhere. Let $\Omega_\varepsilon$ be the $\varepsilon$ neighborhood of the discontinuities of $V$:

$$\Omega_\varepsilon = \{x \in \Omega : |x - y| \leq \varepsilon, \quad y \in \Omega_0\}. \tag{48}$$

It is easy to check that $|\Omega_\varepsilon| \lesssim \varepsilon L^d$ (where recall that $\Omega$ is diffeomorphic to $[0, L]^d$). Let $\eta_\varepsilon$ be a standard smooth bump function supported on $B_{\varepsilon/2}(0)$ such that

$$0 \leq \eta_\varepsilon(x) \leq \eta_\varepsilon(0) = \varepsilon^{-d}, \|\eta_\varepsilon\|_{L^1(\mathbb{R}^3)} = 1, \quad |\nabla\eta_\varepsilon| \lesssim \varepsilon^{-d-1}. \tag{49}$$

First, we prove (46) for $u_\varepsilon := \eta_\varepsilon * (1/\tilde{v})$ where $\tilde{v} = v - \phi$. Then we use $u_\varepsilon$ to approximate $u$ for our estimates. Let $v_0$ denote the average of $\tilde{v}$ on $\Omega$ and $v_{\min} \approx \delta^{1/4}$, $v_{\max} = v_{\min} + \delta \approx \delta^{1/4}$. Since $\|\phi\|_{H^2} \leq \delta$ by assumption,

$$\|\tilde{v} - v_0\|_\infty \lesssim \delta. \tag{50}$$

We rewrite

$$u_\varepsilon = \frac{1}{v_0} + u'_\varepsilon, \tag{51}$$

where

$$u'_\varepsilon = \eta_\varepsilon * \left( \frac{1}{\tilde{v}} - \frac{1}{v_0} \right). \tag{52}$$

For any $x \in \Omega$, using (50), we see that

$$|\nabla u'_\varepsilon(x)| \le \int \left| \nabla \eta_\varepsilon(x - y) \left( \frac{1}{\tilde{v}} - \frac{1}{v_0} \right)(y) \right| dy$$

$$\le \max |\nabla \eta_\varepsilon| \frac{1}{v_{\min}^2} \int_{B_{\varepsilon/2}(x)} |(\tilde{v} - v_0)(y)| dy$$

$$\le \max |\nabla \eta_\varepsilon| \delta^{-1/2} \| \tilde{v} - v_0 \|_\infty |B_{\varepsilon/2}(x)|$$

$$\lesssim \delta^{1/2} \varepsilon^d \varepsilon^{-d-1} = \delta^{1/2} \varepsilon^{-1}.$$

Thus, on $\Omega_\varepsilon$, we have

$$\int_{\Omega_\varepsilon} |\nabla u'_\varepsilon|^2 dx \lesssim \frac{\delta^2}{v_{\min}^4} \int_{\Omega_\varepsilon} |\varepsilon^{-1}|^2 dx \le \delta^2 \delta^{-4/4} \varepsilon^{-2} |\Omega_\varepsilon| \le C\delta\varepsilon^{-1}, \tag{53}$$

for some constant $C$. On the other hand, on $\Omega_\varepsilon^C$,

$$|\nabla u'_\varepsilon| = \left| \eta_\varepsilon * \frac{\nabla(\tilde{v})}{\tilde{v}^2} \right| = \left| \eta_\varepsilon * \frac{\nabla \phi}{\tilde{v}^2} \right| \le \frac{1}{v_{\min}^2} |\eta_\varepsilon * \nabla \phi|.$$

It follows that

$$\int_{\Omega_\varepsilon^C} |\nabla u'_\varepsilon|^2 dx \lesssim \frac{1}{v_{\min}^4} \int_{\Omega_\varepsilon^C} |\eta_\varepsilon * \nabla \phi|^2 dx$$

$$\lesssim \delta^{-1} \| \eta_\varepsilon \|_{L^1(\mathbb{R}^3)}^2 \| \nabla \phi \|_2^2 \le \delta^{-1} \cdot 1^2 \cdot \delta^2 = \delta. \tag{54}$$

By combining (53) and (54), we see that

$$\| \nabla u_\varepsilon \|_2 = \| \nabla u'_\varepsilon \|_2 \le C\delta^{1/2}\varepsilon^{-1/2}. \tag{55}$$

Next, we decompose

$$u = u_\varepsilon + u', \tag{56}$$

where $u'$ is defined by this expression. We will control the size of $u'$ using energy estimates. We note that

$$\langle u', Hu' \rangle \ge \varepsilon^2 \| \nabla u' \|_2^2 + \| \sqrt{v - \phi} \, u' \|_2^2 \ge \varepsilon^2 \| \nabla u' \|_2^2 + \frac{1}{2} v_{\min} \| u' \|_2^2. \tag{57}$$

This provides an energy lower bound. On the other hand,

$$Hu' = Hu - Hu_\varepsilon = \varepsilon^2 \Delta u_\varepsilon + 1 - \tilde{v}u_\varepsilon. \tag{58}$$

It follows that

$$|\langle u', Hu' \rangle| \le |\langle \nabla u', \varepsilon^2 \nabla u_\varepsilon \rangle| + |\langle u', 1 - \tilde{v}u_\varepsilon \rangle| \le \varepsilon^2 \| \nabla u' \|_2 \| \nabla u_\varepsilon \|_2 + \| u' \|_2 \| 1 - \tilde{v}u_\varepsilon \|_2. \tag{59}$$

This is an energy upper bound. We now estimate the term $\| 1 - \tilde{v}u_\varepsilon \|_2$. We write $\tilde{v} = v_0 + \delta v'$ where $v_0$ is the mean of $v$ on $\Omega$ and $v'$ is defined by this expression with

$$\| v' \|_\infty \lesssim 1. \tag{60}$$

Together with (51), we note that

$$\tilde{v}u_\varepsilon - 1 = (v_0 + \delta v')(1/v_0 + u'_\varepsilon) - 1 = \delta \frac{v'}{v_0} + v_0 u'_\varepsilon + \delta v' u'_\varepsilon. \tag{61}$$

By using (50) and applying Young's inequality to (52), we see that

$$\|u_\varepsilon'\|_\infty \le \frac{1}{v_{\min}^2}\|\tilde{v} - v_0\|_\infty \le \delta^{1/2}. \tag{62}$$

By applying (60) and (62) to (61), we see that

$$\|1 - \tilde{v}u_\varepsilon\|_\infty \le \delta/v_{\min} + v_{\max}\delta^{1/2} + \delta\delta^{1/2} \le \delta^{3/4}. \tag{63}$$

Thus, on $\Omega_\varepsilon$,

$$\int_{\Omega_\varepsilon} |1 - \tilde{v}u_\varepsilon|^2 dx \le (\delta^{3/4})^2|\Omega_\varepsilon| \le \delta^{3/2}\varepsilon. \tag{64}$$

For any $x \in \Omega_\varepsilon^C$,

$$\left|\frac{1}{\tilde{v}}(x) - u_\varepsilon(x)\right| \le \int_{\mathbb{R}^3} |\eta_\varepsilon(y)|\left|\frac{1}{\tilde{v}}(x) - \frac{1}{\tilde{v}}(x-y)\right| dy \le \frac{1}{v_{\min}^2}\int_{\mathbb{R}^3} |\eta_\varepsilon(y)||\phi(x) - \phi(x-y)|dy. \tag{65}$$

We remark that the domain of integration is in fact $B_{\varepsilon/2}$ since $\eta_\varepsilon$ is supported on a ball of radius $\varepsilon/2$ at the origin. To estimate the last line, we have

$$|\phi(x) - \phi(x-y)| \le \int_0^1 |\nabla\phi(x-ty)\cdot y|dt \le |y|\int_0^1 |\nabla\phi(x-ty)|dt. \tag{66}$$

Since $\eta_\varepsilon(y)$ has support of radius $O(\varepsilon)$ centered at the origin, it follows from equations (65) and (66) that

$$\begin{aligned}
\int_{\Omega_\varepsilon^C} |1 - \tilde{v}u_\varepsilon|^2 dx &\le v_{\max}^2 \int_{\Omega_\varepsilon^C} \left|\frac{1}{\tilde{v}}(x) - u_\varepsilon(x)\right|^2 dx \\
&\le \varepsilon^2 \int_{\Omega_\varepsilon^C} dx \left(\int_{\mathbb{R}^3} dy \int_0^1 dt|\eta_\varepsilon(y)||\nabla\phi(x-ty)|\right)^2.
\end{aligned} \tag{67}$$

We perform Hölder's inequality (in the $dtdy$-integral) on the integrand $|\eta_\varepsilon(y)||\nabla\phi(x-ty)|$ via the grouping

$$|\eta_\varepsilon(y)||\nabla\phi(x-ty)| = |\eta_\varepsilon(y)|^{1/2}(|\eta_\varepsilon(y)|^{1/2}|\nabla\phi(x-ty)|)$$

to obtain

$$\begin{aligned}
\left(\int_{\mathbb{R}^3} dy \int_0^1 dt|\eta_\varepsilon(y)||\nabla\phi(x-ty)|\right)^2 &\\
&\le \left(\int_{\mathbb{R}^3} dy \int_0^1 dt|\eta_\varepsilon(y)|\right)\left(\int_{\mathbb{R}^3} dy \int_0^1 dt|\eta_\varepsilon(y)||\nabla\phi(x-ty)|^2\right) \\
&= \int_{\mathbb{R}^3} dy \int_0^1 dt|\eta_\varepsilon(y)||\nabla\phi(x-ty)|^2.
\end{aligned}$$

By inserting this into equation (67), we obtain

$$\int_{\Omega_\varepsilon^C} |1 - \tilde{v}u_\varepsilon|^2 dx \le \varepsilon^2 \int_{\Omega_\varepsilon^C} dx \int_{\mathbb{R}^3} dy \int_0^1 dt|\eta_\varepsilon(y)||\nabla\phi(x-ty)|^2 \le C\varepsilon^2\|\nabla\phi\|_2^2 \le C\varepsilon^2\delta^2. \tag{68}$$

Combining the estimates on $\Omega_\varepsilon$ (64) and $\Omega_\varepsilon^C$ (68), we have

$$\|1 - \tilde{v}u_\varepsilon\|_2 \leq C\delta^{3/4}\varepsilon^{1/2}. \tag{69}$$

Together with (57) and (59), and using $2ab \leq a^2 + b^2$ for any real numbers $a$, $b$, we see that

$$\varepsilon^2\|\nabla u'\|_2^2 + \frac{1}{2}\delta^{1/4}\|u'\|_2^2 \tag{70}$$

$$\leq (\varepsilon\|\nabla u'\|_2)(\varepsilon C\delta^{1/2}\varepsilon^{-1/2}) + (C\delta^{3/4}\varepsilon^{1/2}\delta^{-1/8})(\delta^{1/8}\|u'\|_2/2) \tag{71}$$

$$\leq \frac{3}{4}\varepsilon^2\|\nabla u'\|_2^2 + \frac{1}{4}\delta^{1/4}\|u'\|_2^2 + C'\delta\varepsilon. \tag{72}$$

Subtracting the first two terms of (72) from both (72) and (70), we see that

$$\varepsilon^2\|\nabla u'\|_2^2 + \delta^{1/4}\|u'\|_2^2 \leq C\delta\varepsilon.$$

Therefore,

$$\|\nabla u'\|_2 \leq \delta^{1/2}\varepsilon^{-1/2} \quad \text{and} \quad \|u'\|_2 \leq \delta^{3/8}\varepsilon^{1/2}. \tag{73}$$

By combining with (55) and (56), we see that $\|\nabla u\|_2 \leq C\delta^{1/2}\varepsilon^{-1/2}$ for some constant $C$. This proves (46).

Finally, we estimate the $L^2$ norm of $-\Delta u$. Recall that $\tilde{v} = V - \phi$. By using equations (42), (69), and (73), we see that

$$\varepsilon^2\|\Delta u\|_2 = \|1 - \tilde{v}u\|_2 \leq \|1 - \tilde{v}u_\varepsilon\|_2 + \|\tilde{v}u'\|_2 \leq C\delta^{3/4}\varepsilon^{1/2} + v_{\max}C\delta^{3/8}\varepsilon^{1/2}. \tag{74}$$

Therefore, $\varepsilon^2\|\Delta u\|_2 \leq C\delta^{5/8}\varepsilon^{1/2}$. Dividing both sides by $\varepsilon^2$ proves (47). □

**Proposition 2.3.** *Retain the definitions in* Theorem 2.1. *If u solves* (42) *with periodic boundary condition, then*

$$\|\nabla u\|_{L^\infty(\Omega)} \leq C\delta^{5/8}\varepsilon^{-1}, \tag{75}$$

$$\|\Delta u\|_{L^\infty(\Omega)} \leq C\delta^{3/4}\varepsilon^{-2}, \tag{76}$$

*where C depends on d and L only.*

**Proof of Proposition 2.3.** Define $\omega$ via $u(x) = \omega(\varepsilon^{-1}x)$. Since $u$ solves the landscape equation (42), $\omega$ solves $(-\Delta + v_\varepsilon)\omega = 1$, where $v_\varepsilon(x) = v(\varepsilon x) - \phi(\varepsilon x)$. Moreover,

$$\|\nabla^s u\|_{L^\infty(\Omega)} = \varepsilon^{-s}\|\nabla^s\omega\|_{L^\infty(\varepsilon^{-1}\Omega)}. \tag{77}$$

Consequently, we estimate the sup-norm of $\nabla\omega$. As mentioned earlier, let $v_0$ denote the average of $v$ on $\Omega$. We decompose $v_\varepsilon = v_0 + \delta v'_\varepsilon$, where $v'_\varepsilon$ is defined by this expression. We remark that the mean of $v'_\varepsilon$ over $\varepsilon^{-1}\Omega$ is 0 and

$$-1 \leq v'_\varepsilon \leq 1. \tag{78}$$

Let $H_0 = -\Delta + v_0$ and $R = H_0^{-1}$. We see that

$$\omega = (H_0 + \delta v'_\varepsilon)^{-1}1 = \sum_{n\geq 0}(-1)^n\delta^n(Rv'_\varepsilon)^n R1 = \frac{1}{v_0}\sum_{n\geq 0}(-1)^n\delta^n(Rv'_\varepsilon)^n1. \tag{79}$$

It follows that

$$\nabla\omega = \frac{1}{v_0}\sum_{n\geq 1}(-1)^n\delta^n\nabla(Rv'_\varepsilon)^n1. \tag{80}$$

We claim that

$$\|R\|_{L^\infty(\varepsilon^{-1}\Omega)\rightarrow L^\infty(\varepsilon^{-1}\Omega)} \leq \frac{C_1}{v_0}, \tag{81}$$

$$\|\nabla Rv'_\varepsilon\|_{L^\infty} \leq C_2\frac{\delta}{\sqrt{v_0}}, \tag{82}$$

for some constants $C_1$ and $C_2$. For the sake of continuity, we defer the proof of the claims to the end of this section as they are simple corollaries of Young's inequality. Since the integral kernel of $R$ is positive and by using equations (78), (81), and (82), we see that (80) can be estimated as follows:

$$\|\nabla\omega\|_\infty \le \frac{C}{v_0(1 - \delta/v_0)}\frac{\delta}{\sqrt{v_0}} \le C\frac{\delta}{v_{min}^{3/2}} \lesssim \delta^{5/8},$$

since $v_0 \ge v_{min} \gtrsim \delta^{1/4}$. Together with equations (75) and (77) is proved pending claims (81) and (82).

Now we prove the claims (81) and (82). Equation (81) is standard. For the sake of completeness, we carry out the corresponding estimates. Let $g(x) = \frac{e^{-\sqrt{v_0}|x|}}{4\pi|x|}$. Then

$$(Rf)(x) = g * f.$$

It follows from Young's inequality that

$$\|R\|_{L^\infty(\varepsilon^{-1}\Omega) \to L^\infty(\varepsilon^{-1}\Omega)} \le C\int_{\mathbb{R}^3} dx\frac{e^{-\sqrt{v_0}|x|}}{4\pi|x|} = \frac{C}{v_0} \tag{83}$$

for some constant $C$. Similarly, we estimate (82). We note that

$$(\nabla R v_\varepsilon')(x) = (\nabla g) * v_\varepsilon'. \tag{84}$$

Since

$$\int_{\mathbb{R}^3} |\nabla g| = \int_{\mathbb{R}^3} dx\, g(x)(\sqrt{v_0} + |x|^{-1}) = \frac{C}{\sqrt{v_0}} \tag{85}$$

for some universal constant $C$, claim (82) follows by Young's inequality.

Finally, using

$$-\Delta\omega = 1 - v_\varepsilon\omega,$$

we see that

$$\|\Delta\omega\|_\infty = \|1 - v_\varepsilon\omega\|_\infty. \tag{86}$$

By equations (79) and (81), and the fact $\delta = v_{max} - v_{min} \ll \delta^{1/4} \approx v_{min}$,

$$\|1 - v_\varepsilon\omega\|_\infty \le C\sum_{n \ge 1}\delta^n\|R\|_\infty^n \le C_1\frac{\delta/v_{min}}{1 - C_2\delta/v_{min}} \le C\frac{\delta}{v_{min}} \lesssim \delta^{3/4}, \tag{87}$$

for some constant $C$. Together with (77) and (86), this proves (76). The proof of Proposition 2.3 is now complete. $\qquad\square$

**Proof of Theorem 2.1.** Since $W = 1/u$,

$$|\nabla W| = (1/u^2)|\nabla u| \le v_{max}^2|\nabla u|.$$

We now interpolate between equations (46) and (75). Recall $v_{min} \approx \delta^{1/4}$, $v_{max} = v_{min} + \delta \approx \delta^{1/4}$, we see that

$$\|\nabla W\|_p \le v_{max}^2\|\nabla u\|_p \lesssim \delta^{2/4}(\delta^{5/8}\varepsilon^{-1})^{\frac{2-p}{p}}(\delta^{1/2}\varepsilon^{-1/2})^{2/p} \lesssim \delta^{1+\frac{1}{4}(\frac{1}{2}-\frac{1}{p})}\varepsilon^{-\frac{p-1}{p}}.$$

This proves (43). By differentiating $\nabla W$ once more, we see that

$$|\Delta W| \le 2W^3|\nabla u|^2 + W^2|\Delta u| \le 2v_{max}^3|\nabla u|^2 + v_{max}^2|\Delta u|. \tag{88}$$

Since

$$\|\Delta W\|_p \le \|\Delta W\|_\infty^{\frac{p-2}{p}}\|\Delta W\|_2^{2/p}, \tag{89}$$

equations (75), (76), and (88) show that

$$\|\Delta W\|_\infty \lesssim \delta^{3/4}(\delta^{5/8}\varepsilon^{-1})^2 + \delta^{2/4}\delta^{3/4}\varepsilon^{-2} \lesssim \delta^{5/4}\varepsilon^{-2}. \tag{90}$$

Similarly, equations (46), (75), (76), and (88) show that

$$\|\Delta W\|_2 \lesssim \delta^{3/4}\|\nabla u\|_\infty\|\nabla u\|_2 + \delta^{2/4}\|\Delta u\|_2 \tag{91}$$

$$\lesssim \delta^{3/4}(\delta^{5/8}\varepsilon^{-1})(\delta^{1/2}\varepsilon^{-1/2}) + \delta^{2/4}(\delta^{5/8}\varepsilon^{-3/2}) \tag{92}$$

$$\lesssim \delta^{9/8}\varepsilon^{-3/2}. \tag{93}$$

By combining (90) and (93) and using (89), one can compute that

$$\|\Delta W\|_p \le C\delta^{\frac{5p-1}{4p}}\varepsilon^{-\frac{2p-1}{p}}. \tag{94}$$

This proves (44). □

# 3 Leading-order expansion of electron density

We first state a more general theorem from which Theorem 1.1 follows. Then, we prove Theorem 1.1 while delaying the proof of the more general theorem until the end of the section. Let

$$\mathbb{H}_c = \{z \in \mathbb{C} : \Re z + c > 0\}. \tag{95}$$

We have the following general result.

**Theorem 3.1.** *Let* $2 \le p < 3$. *Assume the following hypotheses hold.*
(1) *Suppose that $f$ is analytic on $\mathbb{H}_c$ for some constant $c > 0$ and*

$$\int_{-c}^{\infty} |f(x + iy)|\mathrm{d}x \lesssim O(1) \tag{96}$$

   *uniformly in $y$ for $y$ in on any compact set.*
(2) $v = \tilde{v} - \phi \ge 0$, *where* $\tilde{v} = V - V_{\mathrm{cut}}$ *and* $\phi$ *are as in* Theorem 2.1.
(3) $\varphi \in H^2(\Omega; \mathbb{R})$ *and* $\|\varphi\|_{H^2(\Omega)} \lesssim \delta$.
(4) *The parameters* $0 < \varepsilon < \varepsilon_*$, *and* $0 < \delta < \delta_*$, *where* $\varepsilon_* < 1$, $\delta_* < 1$ *are constants only depending on* $V_{\min}$, *the dimension $d$, and domain size $L$.*
(5) $W = 1/u$ *denotes the landscape potential, where $u$ solves*

$$(-\varepsilon^2\Delta + v)u = 1. \tag{97}$$

*Then,*

$$\mathrm{den}f(-\varepsilon^2\Delta + v - \varphi) = \frac{1}{(2\pi\varepsilon)^3}\int_{\mathbb{R}^3} \mathrm{d}pf(p^2 + W - \varphi) + \varepsilon^{-3+1/p}\mathrm{Rem}, \tag{98}$$

*where*

$$\|\mathrm{Rem}\|_{L^p(\Omega)} \le C_p \int_{-\delta^{1/4}}^{\infty} |f(z)| \tag{99}$$

*for some $p$-dependent constant $C_p > 0$.*

**Proof of Theorem 1.1.** Let $V$ and $\phi$ be as given through the assumptions of Theorem 1.1. We would like to apply Theorem 3.1 to both (23) and (24) simultaneously.

   We note that the Fermi-Dirac function has poles on the imaginary axis in $i\pi\mathbb{Z}$. Thus, we decompose $V = V_{\min} + \delta V_p = V_{\mathrm{cut}} + \tilde{v}$ as in (19), where we choose $V_{\mathrm{cut}} \approx V_{\min} - \delta^{1/4}$ such that

$$\tilde{v}_{\max} = C^{-1}\delta^{1/4}, \tag{100}$$

where $C$ is the constant given in lower bound of the integral in (99). Consequently, we pick $f(z)$ in Theorem 3.1 to be

$$f(z) = f_{\mathrm{FD}}(\beta(z + V_{\mathrm{cut}} - \mu)). \tag{101}$$

Thus, $\mathbb{H}_c$ is chosen with $c = V_{\max} - \mu$.

To prove (23), we apply Theorem 3.1 with the potential $v = \tilde{v} - \phi = V - V_{\mathrm{cut}} - \phi$ and $\varphi = 0$. To prove (24), we apply Theorem 3.1 with $v = \tilde{v} = V - V_{\mathrm{cut}}$ and $\phi = 0$. Finally, we check that the remaining assumptions of Theorem 3.1 are satisfied for the aforementioned choices. Notice in either case, $v_{\min} \approx \delta^{1/4} - \delta \approx \delta^{1/4}$ and $v_{\max} \approx v_{\min} + \delta \approx \delta^{1/4}$.

By the second item of Theorem 1.1 and the Sobolev inequality, $\|\varphi\|_{\infty} \lesssim \delta$. Since $\delta \ll 1$ and $V - \mu \geq C > 0$ (Assumptions 1 and 3 of Theorem 1.1), we see that $V_{\mathrm{cut}} - \mu \geq O(1) > 0$. Hence, the function $f(z) = f_{\mathrm{FD}}(\beta(z + V_{\mathrm{cut}} - \mu))$ is analytic on $\mathbb{H}_{V_{\mathrm{cut}}-\mu}$ (definition (95)), and Assumption 1 of Theorem 3.1 is satisfied. Clearly, items 2–4 of Theorem 3.1 are satisfied by $v$ and $\varphi$.

Item 5 of Theorem 3.1 can also be satisfied since $\tilde{v} > 0$.

It follows by Theorem 3.1 that the $L^2$ norm of the remainder Rem (98) is bounded above by

$$\varepsilon^{-3+1/2} \int_{-\delta^{1/4}}^{\infty} \mathrm{d}x f_{\mathrm{FD}}(\beta(x + V_{\mathrm{cut}} - \mu)) \lesssim \varepsilon^{-3+1/2}\beta^{-1}e^{-\beta(V_{\mathrm{cut}}-\mu-\delta^{1/4})}. \tag{102}$$

This proves the errors in (23) and (24). □

The remainder of this section is devoted to the proof of Theorem 3.1.

**Proof of Theorem 3.1.** First, we remark that the potential functions $v$ and $\phi$ are real and bounded. It follows that their associated Hamiltonian $-\Delta + v - \phi$ is self-adjoint (on $L^2(\mathbb{R}^3)$), so that the spectral theory of self-adjoint operator and its associated analytic tools apply. Moreover, the landscape function $u$ solving (97), and the landscape potential $W = 1/u$ are also real.

Let $f$ be a meromorphic function as given in the hypotheses of Theorem 3.1. We note that

$$u^{-1}(-\varepsilon^2\Delta + v)u = -\varepsilon^2\Delta - 2\varepsilon^2\nabla u \cdot \nabla + u^{-1}. \tag{103}$$

Let us denote

$$U = -2u^{-1}\varepsilon^2\nabla u \cdot \nabla + u^{-1} - \varphi. \tag{104}$$

Consequently,

$$\mathrm{den}f(-\varepsilon^2\Delta + v - \varphi) = \mathrm{den}f(-\varepsilon^2\Delta + U). \tag{105}$$

Since $-\varepsilon^2\Delta + U$ has the same spectrum as $-\varepsilon^2\Delta + v - \varphi$, we see that the spectrum of $-\varepsilon^2\Delta + U$ is contained in $[v_{\min} - O(\delta), \infty) \subset [v_{\min}/2, \infty)$, by item (2) of the assumptions in Theorem 3.1. Thus, by using Cauchy's theorem, we can write

$$f(-\varepsilon^2\Delta + U) = \frac{1}{2\pi i}\int_{\Gamma} f(z)(z - (-\varepsilon^2\Delta + U))^{-1}, \tag{106}$$

where the contour $\Gamma$ is given in Figure 1.

For simplicity, we will denote

$$\oint := \frac{1}{2\pi i}\int_{\Gamma} \mathrm{d}z \tag{107}$$

for the rest of the article. Let

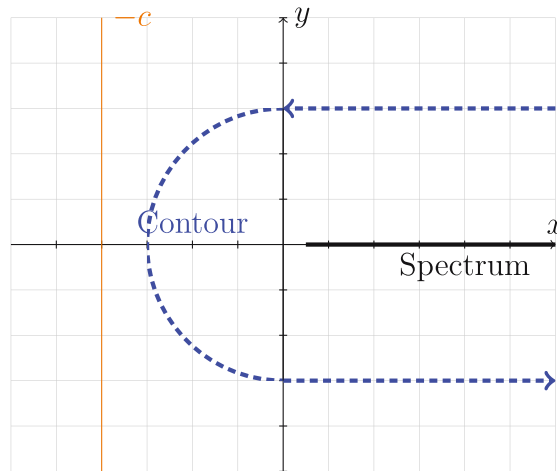$$W = 1/u, \tag{108}$$

**Figure 1:** We identify the complex plane $\mathbb{C}$ with $\mathbb{R}^2$ via $z = x + iy$ for $(x, y) \in \mathbb{R}^2$. The contour $\Gamma$ is denoted by the blue dashed line, extending to positive real infinity. The spectrum of $-\varepsilon^2\Delta + v - \varphi$ is contained in the solid black line. The orange line is where $\Re z = -c$ and $f(z)$ is analytic for $\Re z > -c$.

$$\tilde{W} = 1/u - \varphi. \tag{109}$$

Then,

$$\text{den}f(-\varepsilon^2\Delta + v - \varphi) = \text{den}f(-\varepsilon^2\Delta + U) \tag{110}$$

$$= \text{den}\oint f(z)R(W, \tilde{W}), \tag{111}$$

where

$$R(W, \tilde{W}) = (z - (-\varepsilon^2\Delta + U))^{-1} = (z - (-\varepsilon^2\Delta + 2\varepsilon^2 W^{-1}\nabla W \cdot \nabla + \tilde{W}))^{-1}. \tag{112}$$

To extract leading orders and for $z \in \mathbb{C}$ not in the positive real line, we define

$$R := (z + \varepsilon^2\Delta)^{-1}, \tag{113}$$

$$R_R(\tilde{W}) := \sum_{n \geq 0} R^{n+1}\tilde{W}^n, \tag{114}$$

$$R_L(\tilde{W}) := \sum_{n \geq 0} \tilde{W}^n R^{n+1}. \tag{115}$$

It follows from (111) that

$$\text{den}f(-\varepsilon^2\Delta + v - \varphi) = \text{den}\oint f(z)R_L(\tilde{W}) + \oint f(z)(R(W, \tilde{W}) - R_L(\tilde{W})). \tag{116}$$

Translation invariance of $-\Delta$ shows that for any $n$,

$$\text{den}R^n = \frac{1}{(2\pi\varepsilon)^3}\int_{\mathbb{R}^3}(z - p^2)^{-n}\mathrm{d}p.$$

By using Cauchy's formula and Taylor's theorem, the first term $\text{den}\oint f(z)R_L(\tilde{W})$ can be computed as follows:

$$\text{den}\oint f(z)R_L(\tilde{W}) = \sum_{n \geq 0}\oint f(z)\text{den}\tilde{W}^n R^{n+1} \tag{117}$$

$$= \frac{1}{(2\pi\varepsilon)^3}\sum_{n \geq 0}\int_{\mathbb{R}^3}\mathrm{d}p\oint f(z)\frac{1}{(z - p^2)^{n+1}}\tilde{W}^n \tag{118}$$

$$= \frac{1}{(2\pi\varepsilon)^3} \sum_{n\geq 0} \int_{\mathbb{R}^3} dp \frac{f^{(n)}(p^2)}{n!} \tilde{W}^n \tag{119}$$

$$= \frac{1}{(2\pi\varepsilon)^3} \int_{\mathbb{R}^3} dp f(p^2 + \tilde{W}). \tag{120}$$

Recalling that $\tilde{W} = W - \varphi$, this gives the leading order term in equation (98). It remains to estimate the error term

$$\oint f(z)(R(W, \tilde{W}) - R_L(\tilde{W})). \tag{121}$$

The following Lemma is the main work horse in this estimate, whose proof is delayed until the conclusion of the proof of Theorem 3.1. The Lemma involves the Schatten $p$-norm $\mathfrak{S}^p(\Omega)$ given in Appendix A.    $\square$

**Lemma 3.2.** *Let* $2 \leq p$. *Assume that the assumptions in* Theorem 3.1 *hold and let $W$ and $\tilde{W}$ be given by* (108) *and* (109), *respectively. Then*

$$\|(1 - \varepsilon^2\Delta)(R(W, \tilde{W}) - R_R(\tilde{W}))\|_{\mathfrak{S}^p(\Omega)} \leq \frac{C_1 \varepsilon^{-3/p}}{C_2 - \frac{\delta^{1/4}}{d(z)}} \delta^{\frac{7p-2}{8p}} \varepsilon^{1/p}, \tag{122}$$

$$\|(R(W, \tilde{W}) - R_L(\tilde{W}))(1 - \varepsilon^2\Delta)\|_{\mathfrak{S}^p(\Omega)} \leq \frac{C_1 \varepsilon^{-3/p}}{C_2 - \frac{\delta^{1/4}}{d(z)}} \delta^{\frac{7p-2}{8p}} \varepsilon^{1/p}, \tag{123}$$

*for some $C_1$ and $C_2$ that depend on $p$ and where $d(z)$ is the distance from $z$ to the positive real line.*

Assuming Lemma 3.2, we complete the proof of Theorem 3.1. Let $2 \leq p < 3$ and $q$ be the Hölder conjugate of $p$ such that $\frac{1}{p} + \frac{1}{q} = 1$. Recalling the definition of $R_L(\tilde{W})$ in (115), we may apply Lemma 3.2 and Lemma A.1 (from the Appendix) to obtain

$$\left\| \mathrm{den} \oint f(z)(R(W, \tilde{W}) - R_L(\tilde{W})) \right\|_{L^p(\Omega)} = \left\| \oint f(z)\mathrm{den}[R(W, \tilde{W}) - R_L(\tilde{W})](1 - \varepsilon^2\Delta)(1 - \varepsilon^2\Delta)^{-1} \right\|_{\mathfrak{S}^p(\Omega)} \tag{124}$$

$$\lesssim \frac{\varepsilon^{-3/q}}{\inf\limits_z d(z)} \left\| \oint f(z)[R(W, \tilde{W}) - R_L(\tilde{W})](1 - \varepsilon^2\Delta) \right\|_{\mathfrak{S}^p(\Omega)} \tag{125}$$

$$\lesssim \frac{\varepsilon^{-3}}{\inf\limits_z d(z)} \varepsilon^{1/p} \delta^{1 - \frac{1}{8}(1 + 2/p)} \int_\Gamma |f(z)| \left( 1 - C \frac{\delta^{1/4}}{\inf\limits_z d(z)} \right)^{-1}, \tag{126}$$

provided $v_{\max}$ is much smaller than $\inf\limits_z d(z)$. Since $v_{\max} \approx \delta^{1/4} \ll c$ provided $\delta$ small, we choose our contour to be such that

$$c \gg d(z) = 2C\delta^{1/4}, \tag{127}$$

where $C$ is from (126). This proves (99).

**Proof of Lemma 3.2.** We will prove (123) only. The proof for (122) is similar. For $W$ and $\tilde{W}$ given in (108) and (109), respectively, recall from (104) that

$$U = 2\varepsilon^2 W^{-1}\nabla W \cdot \nabla + \tilde{W}. \tag{128}$$

We expand the resolvent using the resolvent identity

$$
\begin{aligned}
R(W, \tilde{W}) &= (z - (-\varepsilon^2\Delta + U))^{-1} \\
&= (z - (-\varepsilon^2\Delta))^{-1} + (z - (-\varepsilon^2\Delta))^{-1} U (z - (-\varepsilon^2\Delta + U))^{-1} \\
&= \sum_{n\geq 0} (RU)^n R.
\end{aligned} \tag{129}
$$

We will consider each of the $n$th order terms separately. Let us denote

$$\gamma_n = (RU)^n R. \tag{130}$$

Since commutator of $-\varepsilon^2 \Delta$ with $\tilde{W}$ is higher order, to leading order, we have

$$\gamma_n = \tilde{W}^n R^{n+1} + \text{higher order (h.o.)}, \tag{131}$$

where h.o. will be computed after this paragraph. Summing over $n$, to leading order,

$$R(W, \tilde{W}) = \sum_{n \geq 0} \tilde{W}^n R^{n+1} + \text{h.o.} \tag{132}$$

$$= R_L(\tilde{W}) + \text{h.o.} \tag{133}$$

Now we compute the higher order terms coming from $\gamma_n - \tilde{W}^n R^{n+1}$, where $\gamma_n$ is given in (130). Let us introduce the following notations for clarity of exposition.

(1) We denote

$$W_{11} = 2W^{-1} \nabla W. \tag{134}$$

Note that $W_{11}$ is associated with the first order derivative part of

$$U = 2\varepsilon^2 W^{-1} \nabla W \cdot \nabla + \tilde{W}. \tag{135}$$

(2) We denote

$$W_{12} = -2 \nabla \tilde{W}, \tag{136}$$

$$W_{21} = -\Delta \tilde{W}. \tag{137}$$

These terms came from the commutator

$$[R, \tilde{W}] = R(-2\varepsilon^2 \nabla \tilde{W} \cdot \nabla + (-\varepsilon^2 \Delta \tilde{W}))R = R(\varepsilon^2 W_{11} \cdot \nabla + \varepsilon^2 W_{21})R \tag{138}$$

when we commute $\tilde{W}$ in $\gamma_n$ to the left to obtain $\tilde{W}^n R^{n+1}$.

A simple way to keep track of the $W_{ij}$'s is to note that $W_{ij}$ has $i$ derivatives taken, while $j$ stands for the $j$th such quantity (in order of their introduction).

We write $U = \varepsilon^2 W_{11} \cdot \nabla + \tilde{W}$. Then

$$\gamma_n = R(\varepsilon^2 W_{11} \cdot \nabla + \tilde{W})R \cdots R(\varepsilon^2 W_{11} \cdot \nabla + \tilde{W})R. \tag{139}$$

If we write $\gamma_n$ by expanding all the aforementioned brackets, we obtain

$$\gamma_n = (R\tilde{W})^n R + \varepsilon \sum_{i=0}^{n-1} (R\tilde{W})^i (RW_{11} \cdot \varepsilon \nabla)(R\tilde{W})^{n-i-1} R + \gamma_n', \tag{140}$$

where $\gamma_n'$ is defined by this expression and contains terms with at least two factors of $\varepsilon^2 W_{11} \cdot \nabla$. By commuting $\tilde{W}$ to the left, we see that

$$(R\tilde{W})^n R = \tilde{W}^n R^{n+1} + \sum_{0 \leq i < j \leq n} \tilde{W}^{j-1} R^i [R, \tilde{W}] R^{j-i-1} (R\tilde{W})^{n-j} R. \tag{141}$$

It follows that

$$\gamma_n = \tilde{W}^n R^{n+1} \tag{142}$$

$$+ \sum_{0 \leq i < j \leq n} \tilde{W}^{j-1} R^i [R, \tilde{W}] R^{j-i-1} (R\tilde{W})^{n-j} R \tag{143}$$

$$+ \varepsilon \sum_{i=0}^{n-1} (R\tilde{W})^i (RW_{11} \cdot \varepsilon \nabla)(R\tilde{W})^{n-i-1} R \tag{144}$$

$$+ \gamma_n', \tag{145}$$

where we note that the leading term $\tilde{W}^n R^{n+1}$ was used in the computation for (120). We now proceed to estimate the terms (143)–(145) individually.

First, we estimate the Schatten $p$-norm of commutators (Appendix A) of (143) .

**Lemma 3.3.** *Let $2 \le p$. Let $\tilde{W}$ be given in* (109). *Then*

$$\|[R, \tilde{W}]\|_{\mathbb{S}^p(\Omega)} \le C \frac{\varepsilon^{-3/p}}{d(z)^2} \delta^{1+\frac{1}{4}(1/2-1/p)} \varepsilon^{1/p}. \tag{146}$$

*where $d(z)$ is the distance from $z$ to the positive real line.*

**Proof.** We compute

$$[R, \tilde{W}] = R(\varepsilon^2 W_{11} \cdot \nabla + \varepsilon^2 W_{21})R. \tag{147}$$

Kato-Seiler-Simon inequality shows that

$$\|[R, \tilde{W}]\|_{\mathbb{S}^p(\Omega)} \le \varepsilon \|RW_{12}\|_{\mathbb{S}^p(\Omega)} \|\varepsilon \nabla R\|_{\mathbb{S}^\infty(\Omega)} + \|R\|_{\mathbb{S}^\infty(\Omega)} \varepsilon^2 \|W_{21}R\|_{\mathbb{S}^p(\Omega)} \tag{148}$$

$$\le \frac{C\varepsilon^{-3/p}}{d(z)^2}(\varepsilon \|W_{12}\|_p + \varepsilon^2 \|W_{21}\|_p). \tag{149}$$

Recalling definitions (136) and (137), we see that

$$\|W_{12}\|_p \le C \|\nabla \tilde{W}\|_p, \tag{150}$$

$$\|W_{21}\|_p \le C \|\Delta \tilde{W}\|_p. \tag{151}$$

By definition (109) of $\tilde{W}$, Theorem 2.1 proves (146). $\qquad\square$

By applying Lemma 3.3 to equation (143), we see that

$$\left\| \sum_{0 \le i < j \le n} \tilde{W}^{j-1} R^i [R, \tilde{W}] R^{j-i-1} (R\tilde{W})^{n-j} R(1 - \varepsilon^2 \Delta) \right\|_{\mathbb{S}^p(\Omega)} \le \frac{\varepsilon^{-3/p} n^2 C^n}{d(z)^{n+1}} \|\tilde{W}\|_\infty^{n-1} \delta^{\frac{9p-2}{8p}} \varepsilon^{1/p}. \tag{152}$$

This concludes the estimate for (143).

We can estimate (144) in the spirit of the estimate (143) by using an analog of (152). We obtain

$$\left\| \varepsilon \sum_{i=0}^{n-1} (R\tilde{W})^i (RW_{11} \cdot \varepsilon \nabla)(R\tilde{W})^{n-i-1} R(1 - \varepsilon^2 \Delta) \right\|_{\mathbb{S}^p(\Omega)} \le \frac{\varepsilon^{-3/p} n C^n}{d(z)^{n+1}} \|\tilde{W}\|_\infty^{n-1} \varepsilon \|W_{11}\|_p \tag{153}$$

$$\le \frac{\varepsilon^{-3/p} n C^n}{d(z)^{n+1}} \|\tilde{W}\|_\infty^{n-1} \delta^{\frac{9p-2}{8p}} \varepsilon^{1/p}. \tag{154}$$

Finally, we estimate (145). The term $\gamma_n'$ consists of all possible terms of the form

$$RX_1 RX_2 \cdots RX_n R, \tag{155}$$

where $X_i$ is one of $\tilde{W}$ or $\varepsilon W_{11} \cdot (\varepsilon \nabla)$ with at least two of the latter factor. Without loss of generality, we assume that $X_1 = \varepsilon W_{11} \cdot (\varepsilon \nabla)$. By Lemma A.1, Theorem 2.1 and Proposition 2.3, we see that

$$\|RX_1 RX_2 \cdots RX_n R(1 - \varepsilon^2 \Delta)\|_{\mathbb{S}^p(\Omega)} \le \frac{\varepsilon^{-3/p} C}{d(z)} \|R\varepsilon W_{11}\|_{\mathbb{S}^p(\Omega)} \|\varepsilon \nabla RX_2\|_{\mathbb{S}^\infty(\Omega)} \prod_{i \ge 3} \|RX_i\|_{\mathbb{S}^\infty(\Omega)} \tag{156}$$

$$\le \frac{\varepsilon^{-3/p} C^n}{d(z)^{n+1}} (\|\tilde{W}\|_\infty + \varepsilon \|u\|_\infty \|\nabla W\|_\infty)^{n-1} \|\varepsilon \nabla W\|_p \|u\|_\infty \tag{157}$$

$$\leq \frac{\varepsilon^{-3/p}C^n}{d(z)^{n+1}}(\|\tilde{W}\|_\infty + \varepsilon\delta^{-1/4}\|\nabla W\|_\infty)^{n-1}\|\varepsilon\nabla W\|_p\delta^{-1/4}. \tag{158}$$

Combining (152) (for (143)), (154) (for (144)), (158) (for (145)), and using the binomial theorem (or a modification thereof), the fact $\delta \ll v_{\min} \approx \delta^{1/4}$ and Theorem 2.1, we see that

$$\|(\gamma_n - \tilde{W}^n R^{n+1})(1 - \varepsilon^2\Delta)\|_{\mathfrak{S}^p(\Omega)} \leq \frac{\varepsilon^{-3/p}C^n}{d(z)^{n+1}}(\delta^{1/4} + \varepsilon\delta^{-1/4}(\delta^{9/8}\varepsilon^{-1}))^{n-1}\delta^{\frac{7p-2}{8p}}\varepsilon^{1/p} \tag{159}$$

$$\leq \frac{\varepsilon^{-3/p}C^n}{d(z)^{n+1}}(\delta^{1/4} + \varepsilon\delta^{-1/4}(\delta^{9/8}\varepsilon^{-1}))^{n-1}\delta^{\frac{7p-2}{8p}}\varepsilon^{1/p}. \tag{160}$$

Together with (129), (123), and Lemma 3.2 are now proved. □

# 4 Consequence of the integrability condition

Before we move on to the proof of the main result Theorem 1.3, we dedicate this short section to elucidate the implied relationships between different parameters $\varepsilon$, $\delta$, $\beta$, and $\mu$. We achieve this through the integrability of the Poisson equation (41), which we now recall and elaborate.

Let $F = F_{\mathrm{REHF}}$, $F_{\mathrm{PL}}$ or $F_{\mathrm{LSC}}$ (26)–(28). By integrating the left- and right-hand sides of (29), we obtain an equation of the form

$$\kappa_0 := \frac{1}{|\Omega|}\int_\Omega \kappa = \frac{1}{|\Omega|}\int_\Omega F. \tag{161}$$

The goal of this section is to prove bounds on $\mu$ given that (161) holds.

**Lemma 4.1.** *Let $V$ be a bounded potential as in* (19) *and $\kappa_0 \in \mathbb{R} > 0$ and $\|\phi\|_{H^2(\Omega)} \lesssim \delta$. Let Assumptions 1–3 and* (161) *hold. Assume also that* (161) *holds for any $F$ given in* (26)–(28). *Then,*

$$0 < \mu \quad and \quad V - \mu > K. \tag{162}$$

**Proof.** We consider the special case where $F = F_{\mathrm{LSC}}$, and all other cases follow from Theorem 1.1. In this case, Assumption 3 implies

$$\kappa_0 = \frac{1}{(2\pi\varepsilon)^3|\Omega|}\int_\Omega \mathrm{d}x\int_{\mathbb{R}^3} \mathrm{d}p f_{\mathrm{FD}}(\beta(p^2 + W - \phi + V_{\mathrm{cut}} - \mu)), \tag{163}$$

where $u = 1/W$ solves

$$(-\varepsilon^2\Delta + V - V_{\mathrm{cut}})u = 1. \tag{164}$$

Let $\theta(\mu)$ denote the right-hand side of (163). We first note that $\theta(\mu)$ is increasing in $\mu$ since $f_{\mathrm{FD}}$ is a decreasing function. So it suffices for us to check that $\theta(0) < \kappa_0 < \theta(V_{\min} - K)$. For a generic $\eta \in \mathbb{R}$,

$$\int_{\mathbb{R}^3} \mathrm{d}p f_{\mathrm{FD}}(\beta p^2 + \beta(W - \phi + V_{\mathrm{cut}} - \eta)) \tag{165}$$

$$= \frac{4\pi}{\beta^{3/2}}\int_0^\infty \mathrm{d}q q^2 f_{\mathrm{FD}}(q^2 + \beta(W - \phi + V_{\mathrm{cut}} - \eta)). \tag{166}$$

Since $\|\phi\|_{H^2} \lesssim \delta$, we can find a constant $C$ such that

$$W - \phi + V_{\mathrm{cut}} \geq V_{\min} - O(\delta^{1/4}) - O(\delta) \geq V_{\min} - C\delta^{1/4}, \tag{167}$$

$$(W - \phi + V_{\text{cut}}) - (V_{\min} - K) < K + O(\delta^{1/4}) + O(\delta) < K + C\delta^{1/4}. \tag{168}$$

Thus, we see that

$$f_{\text{FD}}(q^2 + \beta(W - \phi + V_{\text{cut}} - 0)) \approx e^{-q^2}e^{-\beta(W-\phi+V_{\text{cut}})}, \tag{169}$$

$$f_{\text{FD}}(q^2 + \beta((W - \phi + V_{\text{cut}}) - (V_{\min} - K))) \approx e^{-q^2}e^{-\beta(W-\phi+V_{\text{cut}}-V_{\min}+K)}, \tag{170}$$

where we recall that $A \approx B$ means $A \lesssim B \lesssim A$. It follows that

$$\theta(0) \lesssim \varepsilon^{-3}\beta^{-3/2}e^{-\beta(V_{\min}-C\delta^{1/4})}, \tag{171}$$

$$\theta(V_{\min} - K) \gtrsim \varepsilon^{-3}\beta^{-3/2}e^{-\beta(K+C\delta^{1/4})} \tag{172}$$

for some constant $C > 0$. Thus, Assumption 2 shows that a solution $0 < \mu_0 < V_{\min} - K$ of $\theta(\mu_0) = \kappa_0$ exists. $\qquad\square$

**Corollary 4.2.** *Let* Assumptions 1–3 *hold. Assume also that* (161) *holds and* $\|\phi\|_{H^2(\Omega)} \lesssim \delta$. *Then*

$$\varepsilon^{-3}\beta^{-3/2}e^{-\beta(V_{\min}-\mu+C\delta^{1/4})} \lesssim 1 \lesssim \varepsilon^{-3}\beta^{-3/2}e^{-\beta(V_{\min}-\mu-C\delta^{1/4})} \tag{173}$$

*for some constant $C > 0$.*

**Proof.** By Theorem 1.1, it suffices for us to assume that (163) hold. Lemma 4.1 shows that $V - \mu > K > 0$. Since $\beta$ is large, the Fermi-Dirac distribution $f_{\text{FD}}(\beta(p^2 + V - \mu))$ is well approximated by $e^{-\beta p^2}e^{-\beta(V-\mu)}$. By integrating $dp$, we have that

$$\int_{\mathbb{R}^3} dp\, e^{-\beta p^2} \approx \beta^{-3/2}, \tag{174}$$

where we recall that $A \approx B$ means $A \lesssim B \lesssim A$. Moreover,

$$e^{-\beta(V_{\min}-\mu+C\delta^{1/4})} \leq e^{-\beta(W-\phi+V_{\text{cut}}-\mu)} \leq e^{-\beta(V_{\min}-\mu-C\delta^{1/4})}. \tag{175}$$

It follows by (163) that (173) is proved. $\qquad\square$

# 5 Proof of the main result: Theorem 1.3

**Proof of Theorem 1.3.** Recall that we can write the REHF, PL, and LSC equations (29) in the form

$$-\Delta\phi = \kappa - F(\phi, \mu), \tag{176}$$

where $F$ is one of (26)–(28).

For a fixed choice of $X$ = REHF, PL, or LSC, let $(\phi_0, \mu)$ denote a solution of equation $X$ satisfying the assumptions of Theorem 1.3. We look for a solution, $\phi$, of the corresponding equation $Y$ = REHF, PL, and LSC, $Y \neq X$, near $(\phi_0, \mu)$ of the form $\phi = \phi_0 + \varphi$. By substituting this ansatz into (29) of the $Y$ equation, we obtain

$$-\Delta\phi_0 - \Delta\varphi = \kappa - F_Y(\phi_0 + \varphi, \mu) \tag{177}$$

$$= \kappa - F_Y(\phi_0, \mu) + F_Y(\phi_0, \mu) - F_Y(\phi_0 + \varphi, \mu). \tag{178}$$

Rearranging, we obtain

$$-\Delta\varphi = \kappa' + F_Y(\phi_0, \mu) - F_Y(\phi_0 + \varphi, \mu), \tag{179}$$

where

$$\kappa' = \kappa - F_Y(\phi_0, \mu) + \Delta\phi_0 \tag{180}$$

$$= F_X(\phi_0, \mu) - F_Y(\phi_0, \mu). \tag{181}$$

Theorem 1.1, and the scaling in Assumption 1 and 2 show that

$$\|\kappa'\|_{L^2(\Omega)} \lesssim \varepsilon^{-3+1/2}\beta^{-1}e^{-\beta(V_{\text{cut}}-\mu-\delta^{1/4})} \lesssim \varepsilon^{1/2}e^{C_1\beta\delta^{1/4}} \lesssim \varepsilon^{1/2}e^{C_2\log(\varepsilon^{-1})\delta^{1/4}} \lesssim \varepsilon^{1/2-C_3\delta^{1/4}} \tag{182}$$

for some constant $C_i$, independent of $\varepsilon$ and $\delta$. Let $M$ denote the Gâteaux derivative of $F$ at $\phi_0$:

$$M = d_\phi F(\phi, \mu)|_{\phi=\phi_0}. \tag{183}$$

We see that (179) can be written as follows:

$$(-\Delta + M)\varphi = \kappa' + N(\varphi), \tag{184}$$

where $N$ is defined by this expression. Let us denote

$$L = -\Delta + M. \tag{185}$$

The rest of the analysis rests upon the following abstract lemma and subsequent theorems.

**Lemma 5.1.** (Main lemma) *Let $\mathcal{H}_1$ and $\mathcal{H}_2$ be two Hilbert spaces such that $\mathcal{H}_1 \subset \mathcal{H}_2$ is dense (in the $\mathcal{H}_2$ topology). Let $L$ be an operator on $\mathcal{H}_2$ with domain $\mathcal{H}_1$ and $N$ be a function on $\mathcal{H}_1$ with range in $\mathcal{H}_2$. Assume that $L$ is invertible on $\mathcal{H}_2$ and there is a $0 < m \in \mathbb{R}$ such that*

$$\|L^{-1}\|_{\mathcal{H}_2 \to \mathcal{H}_1} \le m^{-1}, \tag{186}$$

*and*

$$\|N(\phi_1) - N(\phi_2)\|_{\mathcal{H}_2} < C_N\big(\|\phi_1\|_{\mathcal{H}_1} + \|\phi_2\|_{\mathcal{H}_1}\big)\|\phi_1 - \phi_2\|_{\mathcal{H}_1} \tag{187}$$

*for some constant $C_N$ on a ball of radius at least $Cm^{-1}\|\kappa'\|_{\mathcal{H}_2}$ centered the origin for some constant $C > 0$. Let $\kappa' \in \mathcal{H}_2$. If*

$$\|\kappa'\|_{\mathcal{H}_2} \ll m \text{ and} \tag{188}$$

$$C_N\|\kappa'\|_{\mathcal{H}_2} \ll m^2, \tag{189}$$

*then there exists a unique solution $\varphi$ on the set*

$$\left\{\varphi \in \mathcal{H}_1 : \|\varphi\|_{\mathcal{H}_1} \le \frac{1}{100}mC_N^{-1}\right\} \tag{190}$$

*to the equation*

$$L\varphi = \kappa' + N(\varphi). \tag{191}$$

*Moreover*,

$$\|\varphi\|_{\mathcal{H}_1} \lesssim m^{-1}\|\kappa'\|_{\mathcal{H}_2}. \tag{192}$$

**Proof.** This is just the implicit function theorem with explicit estimates written out. See, e.g., Chapter XIV of [24].    □

Let $L$ be given by (185) for either one of $F = F_{\text{REHF}}$, $F_{\text{PL}}$, or $F_{\text{LSC}}$ and

$$m_0 = \varepsilon^{\delta^{1/4}}. \tag{193}$$

**Theorem 5.2.** *Let the assumptions of* Theorem 1.3 *hold. Then $L$ is bounded below on $L^2(\Omega)$:*

$$\|Lf\|_{L^2(\Omega)} \ge C_1\|\left(-\Delta + m_0^{C_2}\right)f\|_{L^2(\Omega)} \tag{194}$$

*for some constants C and any $f \in H^2(\Omega)$.*

Let $N$ be defined via (184) for $F$ being any one of $F_{\mathrm{REHF}}$, $F_{\mathrm{PL}}$, or $F_{\mathrm{LSC}}$. Then we have the following result.

**Theorem 5.3.** *Let the assumptions of* Theorem 1.3 *hold. The nonlinear operator N has the following estimate*

$$\|N(\phi_1) - N(\phi_2)\|_{L^2(\Omega)} \leq C_3 m_0^{-C_4}\big(\|\phi_1\|_{H^1(\Omega)} + \|\phi_2\|_{H^1(\Omega)}\big)\|\phi_1 - \phi_2\|_{L^2(\Omega)} \tag{195}$$

*for $\phi_1$ and $\phi_2$ in $H^1(\Omega)$ provided $\|\phi_i\|_{H^1(\Omega)} \lesssim m_0^{C_3}$ for some large constant $C_3$, where $m_0$ is given in (193).*

Theorems 5.2 and 5.3 are proved in Sections 6 and 7, respectively. Section 4 provides some preliminary estimates on parameters $\varepsilon$, $\beta$, $\mu$, etc. due to the integrability condition (41).

Now we apply Lemma 5.1 to (184). We take $\mathcal{H}_1 = H^2(\Omega)$ and $\mathcal{H}_2 = L^2(\Omega)$. By Theorem 5.2, the linear estimate (186) of Lemma 5.1 is satisfied with

$$m = C_1 \varepsilon^{C\delta^{1/4}} \tag{196}$$

for some constant $C_1$ and $C_2$ given in (194). Moreover, Theorem 5.3 shows that $C_N$ of Lemma 5.1 can be taken to be

$$C_N = C_3 \varepsilon^{-C_4 \delta^{1/4}}, \tag{197}$$

where $C_3$ and $C_4$ are constants given in (195). Together with equation (182), we see that

$$\|\kappa'\| \leq C_N \|\kappa'\|_{L^2(\Omega)} \lesssim C_1 \varepsilon^{1/2 - C_3 \delta^{1/4}} \ll \min(m, m^2) \tag{198}$$

by Assumption 1. This proves (189) of Lemma 5.1. Consequently, Theorem 1.3 is proved by Lemma 5.1. We remark that the reality of $\phi$ is established by the complex conjugation symmetry (40) of (29) and the uniqueness of solution from the aforementioned fixed point argument. □

# 6 Linear analysis

In this section, we prove Theorem 5.2 in three parts: in each of the following subsections, we prove a version of Theorem 5.2 for the case of REHF, PL, and LSC in Theorems 6.1, 6.8, and 6.9, respectively.

## 6.1 Proof of Theorem 5.2: REHF case

Let

$$M_{\mathrm{REHF}} = d_\phi F_{\mathrm{REHF}} \mid_{\phi = \phi_0} \tag{199}$$

be the Gâteaux derivative of $F_{\mathrm{REHF}}(\cdot, \mu)$ at $(\phi_0, \mu)$ (cf. (183)). Recall that $L_{\mathrm{REHF}} = -\Delta + M_{\mathrm{REHF}}$ and that $m_0$ is defined by (193).

**Theorem 6.1.** *Let the assumptions of* Theorem 1.3 *hold. Then $L_{\mathrm{REHF}}$ is a positive self-adjoint operator on $L^2(\Omega)$ and*

$$L_{\mathrm{REHF}} \gtrsim -\Delta + m_0^C \tag{200}$$

*for some constant C.*

We begin by recording a few auxiliary lemmas first.

**Lemma 6.2.** *Let the assumptions of* Theorem 1.3 *hold. For any* $\varphi \in L^2(\Omega)$, *we have*

$$M_{\text{REHF}}\varphi = -\text{den}\oint f_{\text{FD}}(\beta(z + V_{\text{cut}} - \mu))(z - h)^{-1}\varphi(z - h)^{-1}, \tag{201}$$

*where*

$$h = -\varepsilon^2\Delta + V - V_{\text{cut}} - \phi_0. \tag{202}$$

*Moreover,* $M_{\text{REHF}}$ *is a bounded positive self-adjoint operator on* $L^2(\Omega)$ *with*

$$\|M_{\text{REHF}}\|_{\mathfrak{S}^\infty(\Omega)} \lesssim m_0^{-C}. \tag{203}$$

*for some constant C.*

**Proof of Lemma 6.2.** We will only prove (203). The rest of the properties are proved in [13]. We remark that $h$ is self-adjoint on $L^2(\mathbb{R}^3)$ since each of the potential functions $V$ and $\phi_0$ is real. Let $f, g \in L^2(\Omega)$. Let $\text{Tr}_\Omega$ denote the trace per volume $\Omega$ operator (Appendix A):

$$\text{Tr}_\Omega A = \frac{1}{|\Omega|}\text{Tr}\chi_\Omega A, \tag{204}$$

where $A$ is an operator on $L^2(\mathbb{R}^3)$ and $\chi_\Omega$ is the indicator function of $\Omega$. Since $V - V_{\text{cut}} - \phi_0$ is bounded, we see that $h$ is self-adjoint. Moreover,

$$\|(1 - \varepsilon^2\Delta)(z - h)^{-1}\|_{\mathfrak{S}^\infty(\Omega)} \lesssim \left(1 + \frac{1}{d(z)}\right), \tag{205}$$

where $d(z)$ is the distance from $z$ to the contour, $\Gamma$ (see Figure 1 for definition of $\Gamma$), of integration in

$$\oint = \frac{1}{2\pi i}\int_\Gamma \mathrm{d}z. \tag{206}$$

Let $\mathfrak{S}^p(\Omega)$ denote the standard Schatten norm associated to $\text{Tr}_\Omega$ (Appendix A). By (205), the definition of den (rigorously defined via (A6)), and the Kato-Seiler-Simon inequality, we see that

$$\frac{1}{|\Omega|}\langle g, M_{\text{REHF}}f\rangle_{L^2(\Omega)} = \oint f_{\text{FD}}(\beta(z - \mu))\,\text{Tr}_\Omega \bar{g}(z - h)^{-1}f(z - h)^{-1} \tag{207}$$

$$\leq \oint |f_{\text{FD}}(\beta(z - \mu))|\|g(z - h)^{-1}\|_{\mathfrak{S}^2(\Omega)}\|f(z - h)^{-1}\|_{\mathfrak{S}^2(\Omega)}$$

$$\leq \oint \left|1 + \frac{1}{d(z)}\right|^2 |f_{\text{FD}}(\beta(z - \mu))|\|g\|_{L^2(\Omega)}\|f\|_{L^2(\Omega)}\|(1 - \varepsilon^2\Delta)^{-1}\|_{\mathfrak{S}^2(\Omega)}^2 \tag{208}$$

$$\leq \varepsilon^{-3}\oint \frac{|f_{\text{FD}}(\beta(z - \mu))|}{d(z)^2}\|g\|_{L^2(\Omega)}\|f\|_{L^2(\Omega)}.$$

Since $f_{\text{FD}}(\beta(z - V_{\text{cut}} - \mu))$ is holomorphic on $\{z : \Re z > \mu - V_{\text{cut}}\}$, we may choose the contour such that $|d(z)| = O(\|V_1\|_\infty) = O(\delta^{1/4})$ (20) and

$$\langle g, M_{\text{REHF}}f\rangle_{L^2(\Omega)} \lesssim \beta^{-1}\delta^{-1/2}\varepsilon^{-3}e^{-\beta(V_{\text{cut}}-\mu-\delta^{1/4})}\|g\|_{L^2(\Omega)}\|f\|_{L^2(\Omega)}, \tag{209}$$

where we note that the additional factor of $\beta^{-1}$ came from integration in $z$. By Corollary 4.2, we see that (203) follows. This proves the $\mathfrak{S}^\infty(\Omega)$ bound for $M_{\text{REHF}}$. One can see that $M_{\text{REHF}}$ is self-adjoint by using the tracial characterization (207) and the cyclicity of trace. □

Let

$$|\nabla| = \sqrt{-\Delta}, \tag{210}$$

where the square root is taken via the Borel functional calculus under periodic boundary condition on $\Omega$. The following lemma is crucial to our linear analysis and is based on unpublished notes of Chenn and I. M. Sigal, and proved in Lemma 6 of [15] with $\varepsilon = 1$.

**Lemma 6.3.** *Assume that $v > 0$.*

$$-\text{den}\oint dz f_{\text{FD}}(\beta(z+v))(z+\varepsilon^2\Delta)^{-1}\varphi(z+\varepsilon^2\Delta)^{-1} = \frac{1}{8\pi^2\varepsilon^3}\int\limits_0^\infty dt f_{\text{FD}}(\beta(t+v))\frac{1}{|\varepsilon\nabla|}\log\left(\left|\frac{\sqrt{4t}+|\varepsilon\nabla|}{\sqrt{4t}-|\varepsilon\nabla|}\right|\right)\varphi. \tag{211}$$

In view of Lemma 6.3, define

$$M_{\text{sc}} = \frac{1}{8\pi^2\varepsilon^3}\int\limits_0^\infty dt f_{\text{FD}}(\beta(t+W+V_{\text{cut}}-\phi_0-\mu))\frac{1}{|\varepsilon\nabla|}\log\left(\left|\frac{\sqrt{4t}+|\varepsilon\nabla|}{\sqrt{4t}-|\varepsilon\nabla|}\right|\right), \tag{212}$$

where $W = 1/u$ and

$$(-\varepsilon^2\Delta + V - V_{\text{cut}})u = 1. \tag{213}$$

We remark that when $M_{\text{sc}}$ acts on the zero-(0-) eigenvectors of $|\nabla|$ (i.e., constants), it is assumed that the integrand in (212) is interpreted as follows:

$$\frac{1}{0}\log\left(\left|\frac{\sqrt{4t}+0}{\sqrt{4t}-0}\right|\right) = \frac{1}{\sqrt{t}} \tag{214}$$

for $t > 0$, to ensure continuity of the integrand. Finally, we recall that $m_0 = \varepsilon^{\delta^{1/4}}$ was defined in (193).

**Lemma 6.4.** *Let the assumptions of* Theorem 1.3 *hold. Let* $p, q \geq 2$ *satisfy* $\frac{1}{p} + \frac{1}{q} = \frac{1}{2}$, *then*

$$\|M_{\text{REHF}}f - M_{\text{sc}}f\|_{L^2(\Omega)} \lesssim \varepsilon^{1/p}m_0^{-C}\|f\|_{L^q(\Omega)} \tag{215}$$

*for some constant C. Consequently, picking $p = 2$ and $q = \infty$, and by Sobolev's inequality,*

$$\|M_{\text{REHF}}f - M_{\text{sc}}f\|_{L^2(\Omega)} \lesssim \varepsilon^{1/2}m_0^{-C}\|f\|_{H^2(\Omega)}. \tag{216}$$

**Proof.** We start with equation (201). Let $u$ solve the shifted landscape equation (213). By conjugating inside den by $u$, we obtain

$$M_{\text{REHF}}f = -\text{den}\oint f_{\text{FD}}(\beta(z+V_{\text{cut}}-\mu))R(W,\tilde{W})fR(W,\tilde{W}), \tag{217}$$

where $W = 1/u$, $\tilde{W} = 1/u - \phi_0$ and $R(W,\tilde{W})$ is defined in (112). Similarly, we recall the definition of $R_R(\tilde{W})$ and $R_L(\tilde{W})$ in (114) and (115), respectively. We write

$$R_L' := R(W,\tilde{W}) - R_L(\tilde{W}), \tag{218}$$

and define $R_R'$ similarly. Then, we may rewrite $M_{\text{REHF}}f$ as follows:

$$M_{\text{REHF}}f = -\text{den}\oint f_{\text{FD}}(\beta(z+V_{\text{cut}}-\mu))R_L(\tilde{W})fR_R(\tilde{W}) \tag{219}$$

$$-\text{den}\oint f_{\text{FD}}(\beta(z+V_{\text{cut}}-\mu))[R_L'fR(W,\tilde{W}) \tag{220}$$

$$+R(W,\tilde{W})fR_R' + R_L'fR_R'] \tag{221}$$

We first consider the leading-order term on right-hand side of (219).

$$M_{\text{lead}} := -\text{den}\oint f_{\text{FD}}(\beta(z+V_{\text{cut}}-\mu))R_L(\tilde{W})fR_R(\tilde{W}). \tag{222}$$

On $L^2(\mathbb{R}^3)$, the operators $(z+\varepsilon^2\Delta)^{-n}$ have integral kernels

$$\frac{1}{(2\pi)^3}\int\limits_{\mathbb{R}^3} dp\frac{1}{(z-\varepsilon^2p^2)^n}e^{ip(x-y)}. \tag{223}$$

By inserting (223) into (222), we see that

$$(M_{\text{lead}}f)(x) = \frac{1}{(2\pi)^6}\oint dz \int_{\mathbb{R}^3\times\mathbb{R}^3\times\mathbb{R}^3} dp\,dy\,dq \sum_{n,m\geq 1} f_{\text{FD}}(\beta(z + V_{\text{cut}} - \mu)) \times \frac{\tilde{W}^{n+m}(x)f(y)}{(z - \varepsilon^2 p^2)^n(z - \varepsilon^2 q^2)^m}e^{i(p-q)(x-y)}. \quad (224)$$

For any real numbers $A$ and $B$, we note that

$$\frac{d^k}{dz^k}\frac{1}{(z-A)(z-B)} = (-1)^k k! \sum_{n+m=k;\, 1\leq m,n}\frac{1}{(z-A)^n(z-B)^m}. \quad (225)$$

It follows by Taylor's theorem that

$$(M_{\text{lead}}f)(x) = \frac{1}{(2\pi)^6}\oint dz \int_{\mathbb{R}^3\times\mathbb{R}^3\times\mathbb{R}^3} dp\,dy\,dq \sum_{k\geq 0} f_{\text{FD}}(\beta(z + V_{\text{cut}} - \mu))$$

$$\times \frac{(-1)^k\tilde{W}^k(x)}{k!}\frac{d^k}{dz^k}\frac{f(y)}{(z - \varepsilon^2 p^2)(z - \varepsilon^2 q^2)}e^{i(p-q)(x-y)}$$

$$= \frac{1}{(2\pi)^6}\oint dz \int_{\mathbb{R}^3\times\mathbb{R}^3\times\mathbb{R}^3} dp\,dy\,dq f_{\text{FD}}(\beta(z + V_{\text{cut}} - \mu))$$

$$\times \frac{f(y)}{(z - \varepsilon^2 p^2 - \tilde{W}(x))(z - \varepsilon^2 q^2 - \tilde{W}(x))}e^{i(p-q)(x-y)}.$$

By Fourier transforming back to the position basis, we have that

$$(M_{\text{lead}}f)(x) = \oint dz f_{\text{FD}}(\beta(z + V_{\text{cut}} - \mu))\text{den}[(z - h(x))^{-1}f(z - h(x))^{-1}](x), \quad (226)$$

where

$$h(x) = -\varepsilon^2\Delta + W(x) - \phi_0(x), \quad (227)$$

and $W = 1/u$ is defined by (213). Note that $h(x)$ depends on $x$ and is a family of translation invariant operators indexed by $x$. Consequently, by Lemma 6.3, we see that

$$M_{\text{lead}} = M_{\text{sc}}, \quad (228)$$

where $M_{\text{sc}}$ is given in (212).

We now estimate the error terms in (220) and (221). We only consider the term

$$\text{den}\oint f_{\text{FD}}(\beta(z + V_{\text{cut}} - \mu))R'_L fR(W, \tilde{W}), \quad (229)$$

and the other terms in (220) and (221) are similar. By Lemma A.1, for any $2 \leq p, q$ and $\frac{1}{p} + \frac{1}{q} = \frac{1}{2}$,

$$\left\|\text{den}\oint f_{\text{FD}}(\beta(z + V_{\text{cut}} - \mu))R'_L fR(W, \tilde{W})\right\|_{L^2(\Omega)} \leq \oint |f_{\text{FD}}(\beta(z + V_{\text{cut}} - \mu))|\frac{\varepsilon^{-3/2}}{d(z)} \quad (230)$$

$$\times \|R'_L(1 - \varepsilon^2\Delta)\|_{\mathbb{S}^p(\Omega)}\|(1 - \varepsilon^2\Delta)^{-1}f\|_{\mathbb{S}^q(\Omega)}\|R(W, \tilde{W})(1 - \varepsilon^2\Delta)\|_{\mathbb{S}^\infty(\Omega)}. \quad (231)$$

Since we chose $V - V_{\text{cut}} \gtrsim \delta^{1/4}$ (see (20) of Theorem 1.1), $d(z)$ can be chosen to be of order $\delta^{1/4} \gg \varepsilon$ (see Figure 1 with $v = V - V_{\text{cut}}$ and $\varphi = \phi_0$). By Kato-Seiler-Simon inequality, Lemma 3.2, and our choice of scaling in Assumption 1, it follows that

$$\left\|\text{den}\oint f_{\text{FD}}(\beta(z + V_{\text{cut}} - \mu))R'_L fR(W, \tilde{W})\right\|_{L^2(\Omega)} \lesssim \varepsilon^{-3+1/p}\beta^{-1}e^{-\beta(V_{\text{cut}} - \mu - \delta^{-1/4})}\|f\|_{L^q(\Omega)}, \quad (232)$$

where the extra factor $\beta$ comes from integrating $f_{\text{FD}}(\beta(z - V_{\text{cut}} - \mu))$ in $z$. Corollary 4.2 shows that (215) holds Lemma 6.4 is proved. $\qquad\square$

Since $M_{\text{REHF}}$ is self-adjoint, we have the following unsurprising corollary for the adjoint $M_{\text{sc}}^*$ of $M_{\text{sc}}$.

**Corollary 6.5.** *Let the assumptions of* Theorem 1.3 *hold. If* $f \in H^2(\Omega)$, *then*

$$\|M_{\mathrm{REHF}}f - M_{\mathrm{sc}}^*f\|_{L^2(\Omega)} \lesssim \varepsilon^{1/2} m_0^{-C} \|f\|_{H^2(\Omega)} \tag{233}$$

*for some constant* $C$ *and* $m_0$ *is given in* (193).

**Proof.** We will use the notations $R(W, \tilde{W})$, $R_R(\tilde{W})$, $R_L(\tilde{W})$, and $R'$ given in (112), (114), (115), and (218), respectively. Let $f \in H^1(\Omega)$. Instead of expanding $M_{\mathrm{REHF}}f$ as in (219), we switch the roll of $R_L$ and $R_R$:

$$M_{\mathrm{REHF}}f = -\mathrm{den}\oint f_{\mathrm{FD}}(\beta(z + V_{\mathrm{cut}} - \mu))R_R(\tilde{W})fR_L(\tilde{W}) \tag{234}$$

$$- \mathrm{den}\oint f_{\mathrm{FD}}(\beta(z + V_{\mathrm{cut}} - \mu))[R_R'fL(W, \tilde{W}) \tag{235}$$

$$+ R(W, \tilde{W})fR_L' + R_R'fR_L']. \tag{236}$$

Since $M_{\mathrm{sc}}$ is computed from (219), we note that (234) is nothing but $M_{\mathrm{sc}}^*$. The higher order terms (235) and (236) are dealt with in the same fashion as Lemma 6.4. The proof of the corollary is complete. $\square$

Let us denote

$$G(x) = x \log\left(\left|\frac{x + 1}{x - 1}\right|\right). \tag{237}$$

In this notation,

$$M_{\mathrm{sc}} = \frac{1}{8\pi^2\varepsilon^3} \int_0^\infty f_{\mathrm{FD}}(\beta(t + W - \phi_0 + V_{\mathrm{cut}} - \mu))\frac{1}{\sqrt{4t}}G\left(\frac{\sqrt{4t}}{\varepsilon|\nabla|}\right)\mathrm{d}t. \tag{238}$$

Define

$$M_0 = \frac{1}{8\pi^2\varepsilon^3}e^{-\beta(W - \phi_0 + V_{\mathrm{cut}} - \mu)} \int_0^\infty e^{-\beta t}\frac{1}{\sqrt{4t}}G\left(\frac{\sqrt{4t}}{\varepsilon|\nabla|}\right)\mathrm{d}t. \tag{239}$$

Since $f_{\mathrm{FD}}(x)$ approaches $e^{-x}$ exponentially fast if $x$ is large, we have the following corollary.

**Corollary 6.6.** *Let the assumptions of* Theorem 1.3 *hold. If* $f \in L^2(\Omega)$, *then*

$$\|M_{\mathrm{REHF}}f - M_0 f\|_{L^2(\Omega)}, \|Mf - M_0^*f\|_{L^2(\Omega)} \lesssim \varepsilon^{1/2} m_0^{-C} \|f\|_{H^2(\Omega)} \tag{240}$$

*for some constant* $C$ *and* $m_0$ *is given in* (193).

Now we are ready to prove Theorem 6.1.

**Proof of Theorem 6.1.** Let

$$m = M_{\mathrm{REHF}} - M_0. \tag{241}$$

Lemma 6.4 and Corollary 6.5 show that

$$\|mf\|_{L^2(\Omega)}, \|m^*f\|_{L^2(\Omega)} \lesssim \varepsilon^{1/2} m_0^{-C} \|f\|_{L^2(\Omega)} \tag{242}$$

for $f \in L^2(\Omega)$, where $C$ is a fixed constant. Since $M_{\mathrm{REHF}}$ is self-adjoint, by (241), we see that

$$M_{\mathrm{REHF}}^2 = (M_0^* + m^*)(M_0 + m) \tag{243}$$

$$= M_0^*M_0 + m^*M_0 + M_0^*m + m^*m. \tag{244}$$

It follows that

$$M_{\text{REHF}}^2 = \frac{1}{64\pi^4\varepsilon^6}\left(\int_0^\infty e^{-\beta t}\frac{1}{\sqrt{4t}}G\left(\frac{\sqrt{4t}}{\varepsilon|\nabla|}\right)\right)e^{-2\beta(W-\phi_0+V_{\text{cut}}-\mu)}\left(\int_0^\infty e^{-\beta t}\frac{1}{\sqrt{4t}}G\left(\frac{\sqrt{4t}}{\varepsilon|\nabla|}\right)\right) + m^*M_0 + M_0^*m + m^*m$$

$$\gtrsim \varepsilon^{-6}e^{-2\beta(V_{\max}+\|\phi_0\|_\infty-\mu)}\left(\int_0^\infty e^{-\beta t}\frac{1}{\sqrt{4t}}G\left(\frac{\sqrt{4t}}{\varepsilon|\nabla|}\right)\right)^2 + m^*M_0 + M_0^*m.$$

By Corollary 4.2, Lemma 6.2, and equation (242), we see that

$$M_{\text{REHF}}^2 \gtrsim m_0^C\left(\int_0^\infty e^{-\beta t}\frac{1}{\sqrt{t}}G(\sqrt{t}/\varepsilon\pi|\nabla|)\right)^2 - \varepsilon m_0^{-C}(1-\Delta)^2, \tag{245}$$

where $m_0$ is given in (193) and $C$ is a constant. Since we know that $M_{\text{REHF}} \geq 0$, we apply $\max(\cdot,0)$ to the right-hand side of (245) (so that we can take its square root). Since the right-hand side of (245) is purely a function of $|\nabla|$, the usual commutative algebra rules apply. Moreover, since the square-root operator is operator monotone, we conclude that

$$M_{\text{REHF}} \gtrsim m_0^C\int_0^\infty e^{-\beta t}\frac{1}{\sqrt{4t}}G\left(\frac{\sqrt{4t}}{\varepsilon|\nabla|}\right) - \varepsilon^{1/2}m_0^{-C}(1-\Delta). \tag{246}$$

To complete the proof of Theorem 6.1, we need the following Lemma, whose proof is delayed until after the current proof.

**Lemma 6.7.**

$$\int_0^\infty e^{-t\beta}\frac{1}{\sqrt{4t}}G\left(\frac{\sqrt{4t}}{\varepsilon|\nabla|}\right)dt \geq \frac{1}{2\sqrt{\beta}(1-\beta\varepsilon^2\Delta)}. \tag{247}$$

By combining equation (246) and Lemma 6.7, we see that

$$-\Delta + M_{\text{REHF}} \gtrsim -\Delta + m_0^C\frac{1}{\sqrt{\beta}(1-\beta\varepsilon^2\Delta)} - \varepsilon^{1/2}m_0^{-C}(1-\Delta) \tag{248}$$

$$\gtrsim -\Delta + m_0^C - \varepsilon^{1/2}m_0^{-C}(1-\Delta). \tag{249}$$

By Assumption 1, the proof of Theorem 6.1 is complete, modulo the proof of Lemma 6.7, which we shall provide in the immediate paragraph that follows. □

**Proof of Lemma 6.7.** Let $p = \varepsilon|\nabla|$ and $x = \frac{\sqrt{4t}}{p}$. By our convention, if $p = 0^+$, then $G(\infty) = 2$. In this case, (247) is bounded below by

$$\int_0^\infty e^{-t\beta}\frac{2}{\sqrt{4t}}dt = \sqrt{\frac{\pi}{\beta}}. \tag{250}$$

Otherwise, we assume that $p > 0$.

By elementary calculus, we have the following two estimates

$$\log\left|\frac{x+1}{x-1}\right| > 2x \quad \text{for } x < 1, \tag{251}$$

$$\log\left|\frac{x+1}{x-1}\right| > \frac{2}{x} \quad \text{for } x > 1. \tag{252}$$

Equation (247) becomes

$$\int_0^\infty e^{-t\beta} \frac{1}{\sqrt{4t}} G(x)\mathrm{d}t \geq 2\int_0^{p^2} \frac{\sqrt{t}}{p^2} e^{-\beta t} + \int_{p^2}^\infty \frac{1}{\sqrt{t}} e^{-\beta t} \tag{253}$$

$$= \frac{4}{\beta^{3/2}p^2} \int_0^{\beta p^2} \sqrt{t}\,e^{-t} + \frac{1}{\sqrt{\beta}} \int_{\beta p^2}^\infty \frac{1}{\sqrt{t}} e^{-t} \tag{254}$$

$$= \frac{1}{\sqrt{\beta}} \left( \frac{4}{\beta p^2} \int_0^{\beta p^2} \sqrt{t}\,e^{-t} + \int_{\beta p^2}^\infty \frac{1}{\sqrt{t}} e^{-t} \right). \tag{255}$$

We can compute the bracketted term explicitly as a function of $\beta p^2$. Elementary calculus shows that the terms in the bracket in (255) is bounded below by $\frac{1}{2(1+\beta p^2)}$.

$$\int_0^\infty e^{-t\beta} \frac{1}{\sqrt{t}} G(x)\mathrm{d}t \geq \frac{1}{2\sqrt{\beta}(1+\beta p^2)}. \tag{256}$$

This proves (247). $\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\square$

## 6.2 Proof of Theorem 5.2: PL case

Let $V$ and $\phi = \phi_0$ satisfy the assumption of Theorem 1.1. Let

$$h = -\varepsilon^2 \Delta + V - \phi_0 - V_{\text{cut}}, \tag{257}$$

where $V_{\text{cut}}$ is given under Theorem 1.1. Let also

$$h_0 = u_0^{-1} h u_0. \tag{258}$$

Let $u_0$ denote the landscape function solving $hu_0 = 1$ and $W_0 = 1/u_0$ its landscape potential. Define the function, $m_{\text{PL}}$, on $\Omega$ via

$$m_{\text{PL}} := -\beta(2\pi\varepsilon)^{-3} \int_{\mathbb{R}^3} \mathrm{d}p f'_{\text{FD}}(\beta(p^2 + W_0 + V_{\text{cut}} - \mu)) W_0. \tag{259}$$

**Theorem 6.8.** *Let the assumptions of* Theorem 1.3 *hold. The linear operator L given in* (185) *with $F = F_{\text{PL}}$ (see* (28)) *is*

$$L = L_{\text{PL}} := -\Delta + m_{\text{PL}} h_0^{-1}, \tag{260}$$

*where $m_{\text{PL}}$, $W_0$, and $u_0$ are seen as multiplication operators. Moreover,*

$$\|L_{\text{PL}} f\|_{L^2(\Omega)} \gtrsim \|(-\Delta + m_0^C) f\|_{L^2(\Omega)} \tag{261}$$

*for some constant C, where $m_0$ is given in* (193).

**Proof.** We differentiate $F_{\text{PL}}$ from (27) to obtain

$$d_\phi F_{\text{PL}} \mid_{\phi=\phi_0} \varphi \tag{262}$$

$$= -\beta\varepsilon^{-3}(2\pi)^{-3/2} \int_{\mathbb{R}^3} \mathrm{d}p f'_{\text{FD}}(\beta(p^2 + W_0 + V_{\text{cut}} - \mu)) W_0^2 d_\phi[(h-\phi)^{-1}1]|_{\phi=0} \varphi \tag{263}$$

$$= m_{\mathrm{PL}} u_0^{-1} h^{-1} \varphi h^{-1} 1 \tag{264}$$

$$= m_{\mathrm{PL}} h_0^{-1} \varphi. \tag{265}$$

This proves (260).

Let $M_{\mathrm{PL}} = m_{\mathrm{PL}} h_0^{-1}$. We note that $L = L_{\mathrm{PL}} := -\Delta + M_{\mathrm{PL}}$. Since $M_{\mathrm{PL}}$ is not self-adjoint, $L_{\mathrm{PL}}$ is not self-adjoint. However, $L_{\mathrm{PL}}$ is almost self-adjoint as described below. We rewrite

$$L_{\mathrm{PL}} = \left( -\Delta + \frac{1}{2}(M_{\mathrm{PL}} + M_{\mathrm{PL}}^*) \right) + \frac{1}{2}(M_{\mathrm{PL}} - M_{\mathrm{PL}}^*) \tag{266}$$

$$=: L_1 + M_{\mathrm{PL}}', \tag{267}$$

where $L_1$ is self-adjoint. We show that $M_{\mathrm{PL}}'$ is small. Indeed, we compute

$$2M_{\mathrm{PL}}' = [m_{\mathrm{PL}}, h_0^{-1}] \tag{268}$$

$$= -h_0^{-1}[m_{\mathrm{PL}}, h_0] h_0^{-1} \tag{269}$$

$$= -h_0^{-1} u_0^{-1} [m_{\mathrm{PL}}, -\varepsilon^2 \Delta] u_0 h_0^{-1} \tag{270}$$

$$= -h_0^{-1} u_0^{-1} (-\varepsilon^2 \Delta m_{\mathrm{PL}} - 2(\varepsilon \nabla m_{\mathrm{PL}}) \cdot (\varepsilon \nabla)) u_0 h_0^{-1}. \tag{271}$$

Recalling that $h u_0 = 1$ where $h$ is given in (257), $\|h^{-1}\|_\infty = \|u_0\|_\infty$ is bounded above by

$$\frac{1}{\inf V - \|\phi_0\|_\infty - V_{\mathrm{cut}}} = O(\delta^{-1/4}), \tag{272}$$

and $\|u_0^{-1}\|_\infty$ is bounded above by

$$\sup V + \|\phi_0\|_\infty - V_{\mathrm{cut}} = O(\delta^{1/4}). \tag{273}$$

Thus, we see that $\|h_0^{-1} u_0^{-1}\|_\infty \lesssim 1$ and $\|u_0 h_0^{-1}\|_\infty \lesssim \delta^{-1/2}$. Hence,

$$\|M_{\mathrm{PL}}' f\|_2 \lesssim \|(\varepsilon^2 \Delta m_{\mathrm{PL}} + 2(\varepsilon \nabla m_{\mathrm{PL}}(\varepsilon \nabla)) u_0 h_0^{-1} f\|_2 \lesssim \delta^{-1/2} \|(-\varepsilon^2 \Delta m_{\mathrm{PL}})\|_4 \|f\|_4 + \|(\varepsilon \nabla m_{\mathrm{PL}})\|_4 \|(\varepsilon \nabla) u_0 h_0^{-1} f\|_4. \tag{274}$$

It follows by the Sobolev inequality, Theorem 2.1, Corollary 4.2, and definition (193) that

$$\|M_{\mathrm{PL}}' f\|_2 \lesssim m_0^{-C} \varepsilon^{1/4} \|f\|_{H^1(\Omega)}. \tag{275}$$

Next, we provide a lower bound for $\frac{1}{4}(M_{\mathrm{PL}} + M_{\mathrm{PL}}^*)^2$. We compute

$$\left( \frac{M_{\mathrm{PL}} + M_{\mathrm{PL}}^*}{2} \right)^2 = (M_{\mathrm{PL}}^* + M_{\mathrm{PL}}')(M_{\mathrm{PL}} - M_{\mathrm{PL}}') \tag{276}$$

$$= M_{\mathrm{PL}}^* M_{\mathrm{PL}} + M_{\mathrm{PL}}' M_{\mathrm{PL}} - M_{\mathrm{PL}}^* M_{\mathrm{PL}}' - (M_{\mathrm{PL}}')^2. \tag{277}$$

We denote $v_{\max} = \sup V + \|\phi_0\|_\infty - V_{\mathrm{cut}} = O(\delta^{1/4})$. By using the explicit form of $M_{\mathrm{PL}}$ in (265), we see that

$$M_{\mathrm{PL}}^* M_{\mathrm{PL}} = u_0 h^{-1} u_0^{-1} m_{\mathrm{PL}}^2 u_0^{-1} h^{-1} u_0 \tag{278}$$

$$\geq \beta^2 \varepsilon^{-6} e^{-2\beta(V_{\mathrm{cut}} - \mu + C\delta^{1/4})} u_0 (v_{\max} - \varepsilon^2 \Delta)^{-2} u_0 \tag{279}$$

$$\geq m_0^{2C} u_0 (v_{\max} - \varepsilon^2 \Delta)^{-2} u_0, \tag{280}$$

where $m_0$ is given in (193) and $C$ is a constant. Note that the last line follows from the scaling Assumptions 1 and 2 and Corollary 4.2. To estimate (280), we have that

$$(v_{\max} - \varepsilon^2 \Delta)^{-1} u_0 = u_0 (v_{\max} - \varepsilon^2 \Delta)^{-1} + (v_{\max} - \varepsilon^2 \Delta)^{-1} [u_0, -\varepsilon^2 \Delta] (v_{\max} - \varepsilon^2 \Delta)^{-1}. \tag{281}$$

It follows from (280), Theorem 2.1, and Sobolev's inequality (which depends on $|\Omega|$) that for any $f \in L^2(\Omega)$,

$$\langle f, M^* M f \rangle \geq m_0^{2C} \|(v_{\max} - \varepsilon^2 \Delta)^{-1} u_0 f\|_2 \tag{282}$$

$$\gtrsim m_0^{2C}\|u_0(v_{\max} - \varepsilon^2\Delta)^{-1}f\|_2 - m_0^{-C'}\varepsilon^{1/4}\|f\|_2 \tag{283}$$

$$\gtrsim m_0^{2C}\|(v_{\max} - \varepsilon^2\Delta)^{-1}f\|_2. \tag{284}$$

for suitable and possibly different constants $C$ and $C'$. Together with (261), (275) is proved by (277). □

## 6.3 Proof of Theorem 5.2: LSC case

Similar to the PL case, let $V$ and $\phi = \phi_0$ satisfy the assumption of Theorem 1.1. Let $u_0$ denote the landscape function associated to the Hamiltonian

$$-\varepsilon^2\Delta + V - V_{\text{cut}}, \tag{285}$$

where $V_{\text{cut}}$ is given under Theorem 1.1. Define the function, $m_{\text{LSC}}$, on $\Omega$ via

$$m_{\text{LSC}} := -\beta(2\pi\varepsilon)^{-3/2}\int_{\mathbb{R}^3} \mathrm{d}p f'_{\text{FD}}(\beta(p^2 + W_0 - \phi_0 + V_{\text{cut}} - \mu)), \tag{286}$$

where $W_0 = 1/u_0$ is the landscape potential.

**Theorem 6.9.** *Let the assumptions of* Theorem 1.3 *hold. The linear operator L given in* (185) *with* $F = F_{\text{LSC}}$ (28) *is*

$$L = -\Delta + m_{\text{LSC}}, \tag{287}$$

*where* $m_{\text{LSC}}$ *is seen as a multiplication operator. Moreover, L is self-adjoint on* $L^2(\Omega)$ *and*

$$L \gtrsim -\Delta + m_0^C \tag{288}$$

*for some constant C, where* $m_0$ *is given in* (193).

**Proof.** We differentiate $F_{\text{LSC}}$ from (28) to obtain

$$d_\phi F_{\text{LSC}}|_{\phi=\phi_0}\phi = -\beta\varepsilon^{-3}(2\pi)^{-3/2}\int_{\mathbb{R}^3}\mathrm{d}p f'_{\text{FD}}(\beta(p^2 + W_0 - \phi_0 + V_{\text{cut}} - \mu))\phi \tag{289}$$

$$= m_{\text{LSC}}\phi, \tag{290}$$

where $m_{\text{LSC}}$ is given in (286). By Assumptions 1 and 2, we may replace $f'_{\text{RD}}(x)$ by $e^{-x}$, and we obtain

$$m_{\text{LSC}} \gtrsim \beta\varepsilon^{-3}e^{-\beta(W_0 + \|\phi_0\|_\infty + V_{\text{cut}} - \mu)}\int_{\mathbb{R}^3}\mathrm{d}p e^{-\beta p^2} \gtrsim \beta^{-1/2}\varepsilon^{-3}e^{-\beta(V_{\max} + \|\phi_0\|_\infty - \mu)}. \tag{291}$$

By Corollary 4.2, Assumptions 1 and 2, we see that $m_{\text{LSC}} \gtrsim m_0^C$ for some constant $C$. This proves (288) and completes the proof of Theorem 6.9. □

# 7 Nonlinear analysis

In this section, we prove Theorem 5.3 in three parts: in each of the following subsections, we prove a version of Theorem 5.3 for the case of REHF, PL, and LSC in Theorems 7.1, 7.3, and 7.2, respectively.

## 7.1 Proof of Theorem 5.3: REHF case

**Theorem 7.1.** *Let the assumptions of* Theorem 1.3 *hold. The nonlinear operator N* (*defined in* (184)) *of the REHF equation has the following estimate*:

$$\|N(\phi_1) - N(\phi_2)\|_{L^2(\Omega)} \leq C_1 m_0^{-C_2}\left(\|\phi_1\|_{H^1(\Omega)} + \|\phi_2\|_{H^1(\Omega)}\right)\|\phi_1 - \phi_2\|_{L^2(\Omega)} \tag{292}$$

for $\phi_1$ and $\phi_2$ in $H^1(\Omega)$ provided that $\|\phi_i\|_{H^1(\Omega)} \lesssim m_0^{C_3}$ for some constant $C_3$ large enough, where $m_0$ is given in (193).

**Proof of Theorem 7.1.** By (184), we see that

$$N(\phi) = -\mathrm{den}f_{\mathrm{FD}}(\beta(h - \phi - \mu)) + \mathrm{den}f_{\mathrm{FD}}(\beta(h - \mu)) + M\phi, \tag{293}$$

where

$$h = -\varepsilon^2\Delta + V - \phi_0 - V_{\mathrm{cut}} \tag{294}$$

(recall from Theorem 1.1 and (20) our choice of $V_{\mathrm{cut}}$). We remark that since $\phi$ is not necessarily real, the operator $h$ is not self-adjoint in general. However, its spectrum lies within a tubular neighborhood of the real with width $O(\|\phi\|_\infty) \lesssim O(\|\phi\|_{H^2}) \lesssim m_0^{C_3} = \varepsilon^{C_3\delta^{1/4}}$ for some constant $C_3$, by assumption of Theorem 7.1. In particular, the spectrum of $h - \phi$ does not intersect our contour of integration since the poles of $f_{\mathrm{FD}}(\beta(z + V_{\mathrm{cut}} - \mu))$ are $-(V_{\mathrm{cut}} - \mu) + i\pi\beta^{-1}\mathbb{Z}$ (Figure 1). Thus, recall that the resolvent identity is

$$(z - A)^{-1} - (z - B)^{-1} = (z - A)^{-1}(A - B)(z - B)^{-1}. \tag{295}$$

By using the Cauchy-integral, the resolvent identity, and (201), we arrive at an explicit formula for $N$:

$$N(\phi) := -\mathrm{den}\oint f_{\mathrm{FD}}(\beta(z + V_{\mathrm{cut}} - \mu))(z - (h - \phi))^{-1}(\phi(z - h)^{-1})^2, \tag{296}$$

where $\oint$ is given in (107).

By applying the resolvent identity to (296) iteratively with $A = h - \phi$ and $B = h$ ($h$ is defined in (294)), we arrive at

$$N(\phi) = \sum_{n \geq 2}\oint f_{\mathrm{FD}}(\beta(z + V_{\mathrm{cut}} - \mu))(-1)^n\mathrm{den}(z - h)^{-1}(\phi(z - h)^{-1})^n, \tag{297}$$

whenever the series converges, which we will demonstrate. Let

$$N_n(\phi) = \oint f_{\mathrm{FD}}(\beta(z + V_{\mathrm{cut}} - \mu))(-1)^n\mathrm{den}(z - h)^{-1}(\phi(z - h)^{-1})^n \tag{298}$$

denote the $n$th order nonlinearity. Our goal is to estimate the difference in the individual $n$th order nonlinearities

$$N_n(\phi_1) - N_n(\phi_2) = \oint f_{\mathrm{FD}}(\beta(z + V_{\mathrm{cut}} - \mu))(-1)^n\mathrm{den}(z - h)^{-1}(\phi_1(z - h)^{-1})^n - (z - h)^{-1}(\phi_2(z - h)^{-1})^n. \tag{299}$$

To do so, we use the following expansion of $n$th degree monomials:

$$a^n - b^n = (a - b)a^{n-1} + b(a - b)a^{n-2} + \cdots + b^{n-1}(a - b). \tag{300}$$

By using this pattern, we see that

$$N_n(\phi_1) - N_n(\phi_2) = \oint f_{\mathrm{FD}}(\beta(z + V_{\mathrm{cut}} - \mu))\mathrm{den}(-1)^n(z - h)^{-1}(\phi_1 - \phi_2)(z - h)^{-1}(\phi_\#(z - h)^{-1})^{n-1}$$
$$+ n - 1 \text{ similar terms}, \tag{301}$$

where $\phi_\#$ denotes $\phi_1$ or $\phi_2$. By using the standard Schatten $p$-norm $\mathfrak{S}^p(\Omega)$ and the Kato-Seiler-Simon inequality, (Appendix A) and by Lemma A.1 of the Appendix, we see that

$$\|N_n(\phi_1) - N_n(\phi_2)\|_2$$
$$\leq n\oint \varepsilon^{-3/2}|f_{\mathrm{FD}}(\beta(z + V_{\mathrm{cut}} - \mu))|\|(\phi_1 - \phi_2)(z - h)^{-1}(\phi_\#(z - h)^{-1})^{n-1}\|_{\mathfrak{S}^2(\Omega)} \tag{302}$$
$$\leq n\oint \varepsilon^{-3}|e^{-\beta(z + V_{\mathrm{cut}} - \mu)}|\|(\phi_\#(z - h)^{-1})^{n-1}\|_{\mathfrak{S}^\infty(\Omega)}\|\phi_1 - \phi_2\|_2.$$

It follows that

$$\|N_n(\phi_1) - N_n(\phi_2)\|_{L^2(\Omega)} \lesssim nm_0^{-C}\|(\phi_\#(z-h)^{-1})^{n-1}\|_{\mathfrak{S}^\infty(\Omega)}\|\phi_1 - \phi_2\|_2, \tag{303}$$

by the scaling in Assumptions 1–2 and Corollary (4.2). Denote $d(z)$ to be the distance from $z$ to the contour. Recall that $m_0$ is given in (193) and $\inf d(z) = O(V_{\min} - V_{\mathrm{cut}}) = O(\delta^{1/4})$ by the choice of the contour (Theorem 1.1). We see that by Hölder's and Sŏbolev inequalities,

$$\|(z-h)^{-1}(\phi_\#(z-h)^{-1})^{n-1}\|_{\mathfrak{S}^\infty(\Omega)} \le \|(z-h)^{-1}\|_{\mathfrak{S}^\infty(\Omega)}\|\phi_\#(z-h)^{-1}\|_{\mathfrak{S}^\infty(\Omega)}^{n-1} \tag{304}$$

$$\lesssim nm_0^{-C}\delta^{-n/4}\|\phi_\#\|_4^{n-1} \tag{305}$$

$$\lesssim nm_0^{-C}\delta^{-n/4}\|\phi_\#\|_{H^1(\Omega)}^{n-1}. \tag{306}$$

By combining with (297) and the assumption that $\|\phi_i\|_{H^2(\Omega)} \lesssim m_0^{C_3}$ (for some constant $C_3$ large) is sufficiently small, we conclude that the claim (292) is proved. $\qquad\square$

## 7.2 Proof of Theorem 5.3: LSC case

We will prove the simpler LSC case first before embarking on the tedious yet similar proof of the PL case.

**Theorem 7.2.** *Let the assumptions of* Theorem 1.3 *hold. Let* $\phi_1, \phi_2 \in H^2(\Omega)$ *with* $\|\phi_i\|_{H^2(\Omega)} \lesssim m_0^{C_3}$ *for some large constant* $C_3$ ($m_0$ *is defined in* (193)). *The nonlinear operator $N$ implicitly defined in* (184) *with* $F = F_{\mathrm{LSC}}$ (28) *satisfies the following estimates*:

$$\|N(\phi_1) - N(\phi_2)\|_{L^2(\Omega)} \le C_1 m_0^{-C_2}(\|\phi_1\|_{H^2(\Omega)} + \|\phi_2\|_{H^2(\Omega)})\|\phi_1 - \phi_2\|_{H^2(\Omega)}, \tag{307}$$

*where $C_1$ and $C_2$ are constants.*

**Proof.** Let $h = -\varepsilon^2\Delta + V - V_{\mathrm{cut}}$. Let $u_0$ denote the landscape function solving $hu_0 = 1$ and $W = 1/u_0$ its landscape potential. Similar to the REHF equation, explicitly, by (28) and Theorem 6.9, we see that

$$N(\phi) = \frac{1}{(2\pi\varepsilon)^3}\int_{\mathbb{R}^3} \mathrm{d}p(f_{\mathrm{FD}}(\beta(p^2 + W - \phi_0 + V_{\mathrm{cut}} - \mu)) - f_{\mathrm{FD}}(\beta(p^2 + W - \phi_0 - \phi + V_{\mathrm{cut}} - \mu))$$
$$+ \beta f'_{\mathrm{FD}}(\beta(p^2 + W - \phi_0 + V_{\mathrm{cut}} - \mu))\phi). \tag{308}$$

By Assumptions 1 and 2, we may replace $f'_{\mathrm{FD}}, f_{\mathrm{FD}}(x)$ by $e^{-x}$. It follows that

$$|N(\phi_1) - N(\phi_2)| \lesssim \varepsilon^{-3}e^{-\beta(W - \|\phi_0\|_\infty + V_{\mathrm{cut}} - \mu)}\int_{\mathbb{R}^3} \mathrm{d}p e^{-\beta p^2}|e^{-\beta\phi_1} - e^{-\beta\phi_2} + \beta(\phi_1 - \phi_2)|$$
$$\lesssim \beta^{-3/2}\varepsilon^{-3}e^{-\beta(V_{\min} - \|\phi_0\|_\infty - \mu)}|e^{-\beta\phi_1} - e^{-\beta\phi_2} + \beta(\phi_1 - \phi_2)| \tag{309}$$
$$\lesssim m_0^{-C}|e^{-\beta\phi_1} - e^{-\beta\phi_2} + \beta(\phi_1 - \phi_2)|.$$

Since $\|\phi_i\|_\infty \lesssim \|\phi_i\|_{H^2(\Omega)} \lesssim m_0^{C_3}$ is smaller than $1/\beta$ by Assumption 2, the Taylor expansion of $e^x$ and (309) proves equation (307). $\qquad\square$

## 7.3 Proof of Theorem 5.3: PL case

**Theorem 7.3.** *Let the assumptions of* Theorem 1.3 *hold. Assume that* $\phi_1, \phi_2 \in H^2(\Omega)$, *and* $\|\phi_i\|_{H^2(\Omega)} \lesssim m_0^{C_3}$ *for some large constant* $C_3$ ($m_0$ *is defined in* (193)). *The nonlinear operator $N$ implicitly defined in* (184) *with* $F = F_{\mathrm{PL}}$ (*see* (27)) *satisfies the following estimates*:

$$\|N(\phi_1) - N(\phi_2)\|_{L^2(\Omega)} \leq C_1 m_0^{-C_2}\Big(\|\phi_1\|_{H^2(\Omega)} + \|\phi_2\|_{H^2(\Omega)}\Big)\|\phi_1 - \phi_2\|_{H^2(\Omega)}, \tag{310}$$

where $C_1$ and $C_2$ are constants.

**Proof.** Let

$$h = -\varepsilon^2\Delta + V - \phi_0 - V_{\text{cut}}. \tag{311}$$

Let $u_0$ denote the landscape function solving $hu_0 = 1$ and $W_0 = 1/u_0$ its landscape potential. Let $W(\phi) = [(h - \phi)^{-1}1]^{-1}$ be the landscape potential of $h - \phi$. Similar to the LSC case, by (27) and Theorem 6.8, we see that

$$N(\phi) = \frac{1}{(2\pi\varepsilon)^3}\int_{\mathbb{R}^3} dp(f_{\text{FD}}(\beta(p^2 + W_0 + V_{\text{cut}} - \mu)) - f_{\text{FD}}(\beta(p^2 + W(\phi) + V_{\text{cut}} - \mu))$$
$$+ \beta f'_{\text{FD}}(\beta(p^2 + W_0 + V_{\text{cut}} - \mu))d_\phi W\mid_{\phi=0}\phi). \tag{312}$$

Again we replace $f'_{\text{FD}}, f_{\text{FD}}(x)$ by $e^{-x}$. Denote by $W_1 = W(\phi_1)$ and $W_2 = W(\phi_2)$. Similar to (309), it follows that

$$|N(\phi_1) - N(\phi_2)| \lesssim m_0^{-C}|e^{-\beta(W_1 - W_0)} - e^{-\beta(W_2 - W_0)} - \beta d_\phi W\mid_{\phi=0}(\phi_1 - \phi_2)|. \tag{313}$$

Direct computation shows that

$$W(\phi) = \frac{1}{(h - \phi)^{-1}1} = \frac{1}{u_0(1 + u_0^{-1}\Sigma_{n\geq 1}(-h^{-1}\phi)^n u_0)} \tag{314}$$

and

$$d_\phi W_{\phi=0}\phi' = W_0^2 h^{-1}\phi' h^{-1}1. \tag{315}$$

Hence,

$$W(\phi) - W_0 - d_\phi W\mid_{\phi=0}\phi = W_0^2(h^{-1}\phi)^2 u_0 + \text{ higher order terms of } \quad h^{-1}\phi.$$

As mentioned earlier, let $v_{\min} := V_{\min} - V_{\text{cut}} = O(\delta^{1/4})$ (20). Since $\|h^{-1}\phi\|_\infty \leq v_{\min}^{-1}\delta \ll 1$ and $\delta \ll v_{\min}^C$ and similar to the estimate of the nonlinearity in the LSC equation, one has

$$\|W(\phi) - W_0 - d_\phi W\mid_{\phi=0}\phi\|_2 \lesssim m_0^{-C}\|\phi^2\|_{H^2} \tag{316}$$

for some constant $C > 0$. Since $\|\phi_i\|_\infty \lesssim \|\phi_i\|_{H^2(\Omega)}$. Therefore,

$$\|e^{-\beta(W_1 - W_0)} - e^{-\beta(W_2 - W_0)} - \beta d_\phi W\mid_{\phi=0}(\phi_1 - \phi_2)\|_2 \lesssim \beta^2 m_0^{-C}\Big(\|\phi_1\|_{H^2} + \|\phi_2\|_{H^2}\Big)\|\phi_1 - \phi_2\|_{H^2}. \tag{317}$$

Assumptions 1 and 2 allow the $\beta^2$ to be absorbed into $m_0^{-C}$. This implies equation (310). □

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# Appendix

# A Trace per volume and associated Schatten norm estimates

Let $\mathcal{L}$ denote a Bravais lattice in $\mathbb{R}^3$ and $\Omega$ its fundamental domain (e.g., the Wigner-Seitz cell). For $l \in \mathbb{R}^3$, let $U_l$ denote the translation operator

$$(U_l f)(x) = f(x - l). \tag{A1}$$

An operator on $L^2(\mathbb{R}^3)$ is said to be translation invariant if $A$ commutes with $U_l$ for all $l \in \mathbb{R}^3$. It is said to be $(\mathcal{L})$ periodic if $A$ commutes with $U_l$ for all $l \in \mathcal{L}$.

Let Tr denote the usual trace on $L^2(\mathbb{R}^3)$. It is evident that no periodic or translation invariant operators have a finite trace. Nonetheless, we consider trace per volume $\Omega$ defined via

$$\mathrm{Tr}_\Omega A := \frac{1}{|\Omega|} \mathrm{Tr} \chi_\Omega A, \tag{A2}$$

where $\chi_\Omega$ is the indicator function of $\Omega$. If $A$ is periodic, $\mathrm{Tr}_\Omega$ is independent of translates of $\Omega$. Associated to $\mathrm{Tr}_\Omega$ is a family of periodic Schatten spaces $\mathfrak{S}^p(\Omega)$ given via

$$\mathfrak{S}^p(\Omega) = \left\{ A \in \mathcal{B}(L^2(\mathbb{R}^3)) \text{ and } (\mathcal{L}) \text{ periodic} : \|A\|_{\mathfrak{S}^p(\Omega)} < \infty \right\}, \tag{A3}$$

where

$$\|A\|_{\mathfrak{S}^p(\Omega)}^p = \mathrm{Tr}_\Omega (A^* A)^{p/2}. \tag{A4}$$

The $\mathfrak{S}^p(\Omega)$ norm inherits most inequality estimates from the usual Schatten $p$-norm with the notable exception that

$$\|A\|_{\mathfrak{S}^\infty(\Omega)} \leq C \|A\|_{\mathfrak{S}^p(\Omega)} \tag{A5}$$

*fails* to hold for $1 \leq p < \infty$ and for any $C > 0$.

Given an operator $A$, its density den$A$ is a measurable function on $\Omega$, if it exists, defined via the Riesz representation theorem and the formula

$$\mathrm{Tr} f A = \int_{\mathbb{R}^3} f \, \mathrm{den} A \tag{A6}$$

for any $f \in C_c^\infty(\mathbb{R}^3)$, where $f$ on the left-hand side is regarded as a multiplication operator on $L^2(\mathbb{R}^3)$. When $A$ has an integral kernel $A(x, y)$, that is,

$$(Af)(x) = \int_{\mathbb{R}^3} A(x, y) f(y) \mathrm{d}y, \tag{A7}$$

then,

$$(\mathrm{den} A)(x) = A(x, x), \tag{A8}$$

whenever $A(x, x)$ is defined and unambiguous. We outline a few special cases, where den$A$ is defined and give its estimates below, which will be frequently used in the proof of the main results.

**Lemma A.1.** *Let $d = 3$ and $\frac{3}{2} < p < 3$. Suppose that $A \in \mathfrak{S}^p(\Omega)$ and $R$ be given by* (113), *then* den$AR$ *and* den$RA \in L^2(\Omega)$. *Moreover,*

$$\|\mathrm{den} AR\|_{L^p(\Omega)}, \|\mathrm{den} RA\|_{L^p(\Omega)} \lesssim \frac{\varepsilon^{-3/q}}{d(z)} \|A\|_{\mathfrak{S}^p(\Omega)}, \tag{A9}$$

*where $\frac{1}{q} + \frac{1}{p} = 1$.*

**Proof.** We prove the case for $RA$ only as the case for $AR$ is similar. We use the $L^p(\Omega)$–$L^q(\Omega)$ duality (where $\frac{1}{p} + \frac{1}{q} = 1$ for $\frac{3}{2} < p, q < \infty$). Let $\phi \in L^p(\Omega)$ and apply Hölder's inequality to

$$\mathrm{Tr}_\Omega[(\phi R)A] \lesssim \|\phi R\|_{\mathfrak{S}^q(\Omega)} \|A\|_{\mathfrak{S}^p(\Omega)}, \tag{A10}$$

where $\mathrm{Tr}_\Omega$ is the trace per volumne $\Omega$. Kato-Seiler-Simon inequality shows

$$\mathrm{Tr}_\Omega[(\phi R)A] \leq C \frac{\varepsilon^{-3/q}}{d(z)} \|\phi\|_{L^q(\Omega)} \|A\|_{\mathfrak{S}^p(\Omega)}, \tag{A11}$$

where $\Im z$ is the imaginary part of $z$. The proof is now completed by the $L^q(\Omega)$–$L^p(\Omega)$ duality and the Riesz representation theorem:

$$|\Omega| \mathrm{Tr}_\Omega(\phi RA) = \mathrm{Tr}(\phi RA) = \langle \phi, \mathrm{den}(RA) \rangle_{L^2(\Omega)}. \tag{A12}$$

$\square$

# B Existence of solution to the PL equation

We show that the LSC equation (see (28) and (29)) has a solution by minimizing its associated energy functional. To this end, let $\eta(p, x)$ be periodic in $x$ and $\rho_\eta = \int_{\mathbb{R}^3} \mathrm{d}p \eta(p, x)$. Let $s(x) = -\frac{1}{2}(x \log(x) + (1 - x) \log(1 - x))$. We define the entropy functional

$$S(\eta) = \int_{\mathbb{R}^3 \times \Omega} \mathrm{d}p \mathrm{d}x s(\eta(p, x)), \tag{A13}$$

whenever the integral is convergent. Otherwise we set $S(\eta) = \infty$. Finally, we define

$$\mathcal{F}_{\mathrm{LSC}}(\eta) = \int_{\mathbb{R}^3 \times \Omega} \mathrm{d}p \mathrm{d}x (\varepsilon^2 p^2 + W + V_{\mathrm{cut}}) \eta(p, x) + \frac{1}{2} \langle (\rho_\eta - \kappa), (-\Delta)^{-1}(\rho_\eta - \kappa) \rangle_{L^2(\Omega)} - \beta^{-1} S(\eta). \tag{A14}$$

The associated space on which we perform our minimization is

$$D_\kappa = \left\{ \eta \in L^1(\mathbb{R}_p^3 \times \Omega_x, (1 + p^2) \mathrm{d}p \mathrm{d}x) : 0 \leq \eta \leq 1, \int_{\mathbb{R}^3 \times \Omega} \eta = \int_\Omega \kappa, \quad \text{and} \quad \rho_\eta \in \kappa + \dot{H}^{-1}(\Omega) \right\}, \tag{A15}$$

where, using the notation $\nabla^{-1} := \nabla(-\Delta)^{-1}$,

$$\dot{H}^{-1}(\Omega) = \left\{ f : \int_\Omega f = 0 \quad \text{and} \quad \nabla^{-1} f \in L^2(\Omega) \right\}. \tag{A16}$$

We note that $D_\kappa$ is not an affine space, but it is convex. Let

$$L_1 \eta = \int_{\mathbb{R}^3} \mathrm{d}p \eta(p, x), \tag{A17}$$

$$L_2 \eta = \int_\Omega \mathrm{d}x \eta(p, x), \tag{A18}$$

and define projections

$$P = \frac{1}{|\Omega|} L_2, \tag{A19}$$

$$\bar{P} = 1 - P. \tag{A20}$$

For simplicity, we will denote

$$L^p(\mathbb{R}^3 \times \Omega, (1 + p)^2 \mathrm{d}p\mathrm{d}x) = L^p((1 + p)^2 \mathrm{d}p\mathrm{d}x) \tag{A21}$$

interchangeably.

**Theorem B.1.** (LSC existence and uniqueness) *Assume that $\bar{P}\kappa \in \dot{H}^{-1}$. Then $\mathcal{F}_{\mathrm{LSC}}$ is convex and has a unique minimizer $\eta \in D_\kappa$. If $-\Delta\phi = \kappa - \rho_\eta$, then $\phi$ solves the PL equation (29) with $F = F_{\mathrm{LSC}}$ (cf. (28)) with $\mu$ induced by the Lagrangian multiplier of the constraint.*

**Proof of Theorem B.1.** We equip $D_\kappa$ with the norm

$$\|\eta\|_{D_\kappa} = \|\eta(p, x)\|_{L^1((1+p^2)\mathrm{d}p\mathrm{d}x)} + \|\bar{P}\rho_\eta\|_{\dot{H}^{-1}(\Omega)}. \tag{A22}$$

Note that $D_\kappa$ is closed with respect to this norm.

 **Step 1: Euler-Lagrange equation.** Let $h(p, x) = \varepsilon^2 p^2 + W + V_{\mathrm{cut}}$. The energy functional can be rewritten as follows:

$$\mathcal{F}_{\mathrm{LSC}}(\eta) = L_1 L_2(h\eta) + \frac{1}{2}\|\nabla^{-1}(L_1\eta - \kappa)\|^2_{L^2(\Omega)} - \beta^{-1} L_1 L_2 s(\eta). \tag{A23}$$

From this, the Euler-Lagrange equation subject to $L_1 L_2 \eta = L_2 \kappa$ is

$$h\eta + (-\Delta)^{-1}(\rho_\eta - \kappa) - \beta^{-1} s'(\eta) - \mu\eta = 0 \tag{A24}$$

for a suitable $\mu$ due to the constraint $L_1 L_2 \eta = L^2 \kappa$. By solving for $\eta$, we see that

$$\eta = f_{\mathrm{FD}}(\beta(h - (-\Delta)^{-1}(\rho_\eta - \kappa) - \mu)). \tag{A25}$$

By integrating equation (A25) with respect to $p$, we define

$$\rho_\eta = \int_{\mathbb{R}^3} \mathrm{d}p f_{\mathrm{FD}}(\beta(\varepsilon^2 p^2 + W + V_{\mathrm{cut}} - \phi - \mu)). \tag{A26}$$

Finally, set $\phi = (-\Delta)^{-1}(\rho_\eta - \kappa)$. We see that $(\phi, \mu)$ solves (29) with (28).

 **Step 2: Coercivity.** Note that without the interaction term (Coulomb term), an unconstrained minimizer to

$$\int_{\mathbb{R}^3 \times \Omega} \mathrm{d}p\mathrm{d}x \left(\frac{1}{2}\varepsilon^2 p^2 + W + V_{\mathrm{cut}}\right)\eta(p, x) - \beta^{-1} S(\eta) \tag{A27}$$

is

$$\eta = f_{\mathrm{FD}}(\beta h). \tag{A28}$$

This shows that

$$\mathcal{F}_{\mathrm{LSC}}(\eta) \geq \frac{1}{2}L_1 L_2(h\eta) + \frac{1}{2}\|\nabla^{-1}(L_1\eta - \kappa)\|^2_{L^2(\Omega)} - C, \tag{A29}$$

$$\gtrsim \|\eta\|_{D_\kappa} - C, \tag{A30}$$

for $\|\eta\|_{D_\kappa}$ large.

 **Step 3: Convergent subsequence.** Since $\mathcal{F}_{\mathrm{LSC}}$ is coercive, we can find a minimizing sequence $\eta_n$. Note that since $0 \leq \eta_n \leq 1$, we have that $\eta_n^p \leq \eta_n$ for all $1 \leq p < \infty$. It follows that

$$\|\eta_n\|^p_{L^p((1+p^2)\mathrm{d}p\mathrm{d}x)} \leq \|\eta_n\|_{L^1((1+p^2)\mathrm{d}p\mathrm{d}x)} < \infty. \tag{A31}$$

In particular, $\eta_n$ converges weakly to some $\eta(p)$ for each $1 < p < \infty$ in $L^p(\mathbb{R}^3 \times \Omega, (1 + p^2)\mathrm{d}p\mathrm{d}x)$. By testing against compactly supported smooth functions, i.e.,

$$\langle \varphi, \eta_n \rangle_{L^2((1+p^2)\mathrm{d}p\mathrm{d}x)} \rightarrow \langle \varphi, \eta \rangle_{L^2((1+p^2)\mathrm{d}p\mathrm{d}x)}$$

for $n \rightarrow \infty$, where $\varphi$ is smooth compactly supported on $\mathbb{R}^3 \times \Omega$, which is in $L^p$ for any $1 \leq p \leq \infty$, we see that the $\eta(p) = \eta(q)$ for any $1 < p, q < \infty$.

So we will denote by $\eta$ the common limit. Moreover, note that for any measurable $f$ on $\mathbb{R}^3 \times \Omega$,

$$\int_{\mathbb{R}^3 \times \Omega} \eta_n f = \int_{\mathbb{R}^3 \times \Omega} (1+p^2)\mathrm{d}p\mathrm{d}x \eta_n \cdot \frac{f}{1+p^2}. \tag{A32}$$

Taking $f = 1$ and noting that $(1+p^2)^{-1} \in L^s((1+p^2)\mathrm{d}p\mathrm{d}x)$ for $s > 5/2$, we see that

$$\int_{\mathbb{R}^3 \times \Omega} \eta = \lim_{n \rightarrow \infty} \int_{\mathbb{R}^3 \times \Omega} \eta_n = \int_{\Omega} \kappa. \tag{A33}$$

By the same reasoning with $f \in L^\infty$, it follows that the weak convergence can be achieved on $L^1(\mathbb{R}^3 \times \Omega, \mathrm{d}p\mathrm{d}x)$.

Next, to see that $0 \leq \eta \leq 1$, let $\chi \geq 0$ denote any compactly supported bounded function with $L^1(\mathbb{R}^3 \times \Omega, \mathrm{d}p\mathrm{d}x)$ norm 1. Then

$$\int_{\mathbb{R}^3 \times \Omega} \eta \chi = \lim_{n \rightarrow \infty} \int \eta_n \chi. \tag{A34}$$

Since $0 \leq \eta_n \leq 1$, we see that

$$0 \leq \int_{\mathbb{R}^3 \times \Omega} \eta \chi \leq 1. \tag{A35}$$

It follows that $0 \leq \eta \leq 1$.

It remains to show that

$$\|\bar{P}L_1\eta\|_{\dot{H}^{-1}(\Omega)} < \infty. \tag{A36}$$

Let $f \in \dot{H}^1(\Omega)$ with mean zero. Then

$$\int_{\mathbb{R}^3 \times \Omega} f\eta \leq \|f\|_{L^6(\Omega)} \int_{\mathbb{R}^3} (1+p^2)^{-5/6}(1+p^2)^{5/6}\|\eta^{6/5}\|_{L^1(\Omega,\mathrm{d}x)}^{5/6}. \tag{A37}$$

By Hardy-Littlewood-Sobolev or Sobolev-Poincare and since $0 \leq \eta \leq 1$, we see that

$$\int_{\mathbb{R}^3 \times \Omega} f\eta \leq \|f\|_{\dot{H}^1(\Omega)}\|(1+p^2)^{-5/6}\|_{L^6(\mathbb{R}^3,\mathrm{d}p)}\|(1+p^2)^{5/6}\eta^{6/5}\|_{L^1(\Omega,\mathrm{d}x)}^{5/6}\|_{L^{6/5}(\mathbb{R}^3,\mathrm{d}p)}. \tag{A38}$$

$$\leq C\|f\|_{\dot{H}^1(\Omega)}\|(1+p^2)\eta^{6/5}\|_{L^1(\mathrm{d}p\mathrm{d}x)}^{5/6}. \tag{A39}$$

Since $0 \leq \eta \leq 1$, we see that

$$\int_{\mathbb{R}^3 \times \Omega} f\eta \leq C\|f\|_{\dot{H}^1(\Omega)}\|(1+p^2)\eta\|_{L^1(\mathrm{d}p\mathrm{d}x)}^{5/6}. \tag{A40}$$

It follows by the Riesz representation theorem that

$$\|\bar{P}L_1\eta\|_{\dot{H}^{-1}} \leq C\|(1+p^2)\eta\|_{L^1(\mathrm{d}p\mathrm{d}x)}^{5/6} < \infty. \tag{A41}$$

Finally, Hardy-Littlewood-Sobolev or Sobolev-Poincare shows any $f \in \dot{H}^1(\Omega)$ with mean zero is also in $L^6(\Omega)$. For such an $f$,

$$\frac{f}{(1+p^2)} \in L^6((1+p^2)\mathrm{d}p\mathrm{d}x). \tag{A42}$$

Weak convergence of $\eta_n$ to $\eta$ in $L^{6/5}((1+p^2)\mathrm{d}p\mathrm{d}x)$ shows weak convergence of $\bar{P}L_1\eta_n$ to $\bar{P}L_1\eta$ in $\dot{H}^{-1}(\Omega)$.

In summary, $\eta_n$ converges weakly to $\eta$ in $L^p$ for $1 \le p < \infty$ and $\bar{P}L_1\eta_n$ converges weakly in $\dot{H}^{-1}(\Omega)$ to $\bar{P}L_1\eta$.

**Step 4: lower semi-continuity.** By using (A23), we write

$$\mathcal{F}_{\mathrm{LSC}}(\eta) = L_1L_2(h\eta) - \beta^{-1}L_1L_2s(\eta). \tag{A43}$$

$$+\frac{1}{2}(\|\bar{P}L_1\eta\|^2_{\dot{H}^{-1}(\Omega)} - 2\,\mathrm{Re}\,\langle L_1\eta, (-\Delta)^{-1}\bar{P}\kappa\rangle_{L^2(\Omega)} + \|\bar{P}\kappa\|^2_{\dot{H}^{-1}(\Omega)}). \tag{A44}$$

From this expression, it is evident that $\mathcal{F}_{\mathrm{LSC}}$ is convex in $\eta$. Hence, we may assume that $\eta_n$ converges strongly in $L^p$ for all $1 < p < \infty$. In particular, we may assume point-wise convergence. By Fatou's Lemma, the entropy term and all linear terms are lower semi-continuous. The Coulomb term $\|\bar{P}L_1\eta\|^2_{\dot{H}^{-1}(\Omega)}$ is lower semi-continuous since it is the composition of a norm and integral operators.

**Step 5: conclusion.** By Steps 2 and 3, we see that there is a minimizing sequence $\eta_n$ converging weakly to $\eta \in D_\kappa$. By Step 4, weak lower semi-continuity and convexity of $\mathcal{F}_{\mathrm{LSC}}$ shows that

$$\mathcal{F}_{\mathrm{LSC}}(\eta) \le \liminf_{n\to} \mathcal{F}_{\mathrm{LSC}}(\eta_n). \tag{A45}$$

Since $\eta_n$ is a minimizing sequence, $\eta$ is a the minimizer (uniqueness is due to convexity). Step 1 shows that the associated $(\phi, \mu)$ of this minimizer solves (29) with (28). The proof of Theorem B.1 is now complete. $\quad\square$