On the Reduced Hartree-Fock Equation with Anderson Type Background Charge Distribution

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Abstract

We demonstrate that the reduced Hartree-Fock equation (REHF) with an Anderson type background charge distribution has a unique stationary solution by explicitly computing a screening mass at positive temperature.

1 Introduction

Density functional theory (DFT) has become the stable of modern quantum science thanks to its tractability. One of its notable applications is in describing the electronic structure of disordered crystals in solid state physics and material sciences. Nevertheless, the disordered nature of certain crystal structures and the long range Coulomb interaction have caused considerable difficulties in their theoretical studies. To illustrate this difficulty, we restrict our attention to dimension three (3) for the rest of the paper.

In condensed matter physics, the density of electrons is governed by the Kohn-Sham (KS) equation of DFT, whose mathematical properties have become an area of intense research, for example, [1, 3, 4, 5, 6, 7, 8, 9, 11, 10, 14, 15, 16, 17, 18, 19, 20]. One central focus of these studies is the existence and uniqueness problem. In this context, a prolific approach is through the use of variational arguments. Given a nuclear charge distribution $\kappa$ on a set $S \subset \mathbb{R}^3$, the Kohn-Sham equation are the Euler-Lagrange equation of the Kohn-Sham energy, which is a functional of the electron density matrix $\gamma$ [12]:

$$E_{KS}(\gamma) = \text{Tr}((-\Delta)\gamma) + \frac{1}{2} \int_{S \times S} dxdy \frac{(\kappa(x) - \rho_\gamma(x))(\kappa(y) - \rho_\gamma(y))}{|x - y|} + Ex(\rho_\gamma),$$

(1)

where $\rho_\gamma(x) = \gamma(x, x)$ is the electron density ($\gamma(x, y)$ is the integral kernel of $\gamma$) and $Ex$ is the exchange-correlation energy depending solely on $\rho_\gamma$, instead of $\gamma$. However,
a major impediment to the variational approach is that the Coulomb self-interaction energy in (1) becomes ill defined if \( S \) is unbounded and \( \kappa - \rho \), lacks decay. A notable example is when \( \kappa \) is the Anderson type disorder.

At zero temperature, some mitigation of the long range Coulomb problem involves studying minimizers of \( E_{KS} \) on a finite domain and then passing to their thermal dynamical limits to include periodic \( \kappa \) and \( \rho \), (see for example, [6, 7, 9]), or introducing a screening mass as in the case of Yukawa potential [4]. On the other hand, a natural screening is observed at positive temperature [8, 14].

In this work, we follow the latter school of thoughts. We show that the Kohn-Sham equation have unique solutions despite the presence of long range Coulomb interaction and disordered background distribution \( \kappa \) at positive temperature. To elucidate the main ideas, we drop the exchange correlation term \( E_x \) in \( E_{KS} \). The resulting energy and equation bear the name of reduced Hartree-Fock (REHF) equation and energy, respectively. Let \( \beta \) denote the inverse temperature. At positive temperature \( \beta^{-1} \), the REHF free energy of \( \gamma \) on \( S \subset \mathbb{R}^3 \) is

\[
F_{\text{REHF}}(\gamma) := E_{\text{REHF}}(\gamma) - \beta^{-1}S(\gamma),
\]

\[
E_{\text{REHF}}(\gamma) := \text{Tr}((-\Delta)\gamma) + \frac{1}{2} \int_{S \times S} dx dy \frac{(\kappa(x) - \rho\gamma(x))(\kappa(y) - \rho\gamma(y))}{|x - y|},
\]

\[
S(\gamma) := -\text{Tr}(\gamma \ln(\gamma) + (1 - \gamma) \ln(1 - \gamma)),
\]

whenever \( F_{\text{REHF}} \) is well defined. We remark that we have not specified the space on which \( \gamma \) acts as well as the exact meaning of \( \text{Tr} \). Since we will be working with and describing the Euler-Lagrange equations later, this inconvenience is only formal. The REHF equation is the Euler-Lagrange equation of \( F_{\text{REHF}} \) with a fixed number of particles \( \text{Tr} \gamma \). Despite the fact that \( F_{\text{REHF}} \) is a functional of \( \gamma \), the REHF equation can be solely written in terms of the electron density \( \rho \) (hence the name DFT), the (auxiliary) electric potential \( \varphi \), and the chemical potential \( \mu \) (i.e. the Lagrange-multiplier):

\[
\rho = \text{den} f_{\text{FD}}(\beta(-\Delta - \varphi - \mu)),
\]

\[
-\Delta \varphi = \kappa - \rho,
\]

where \( f_{\text{FD}} \) is the Fermi-Dirac distribution

\[
f_{\text{FD}}(x) = \frac{1}{1 + e^x}.
\]

Moreover, we have introduced the den operator mapping operators \( A \) on \( L^2(\mathbb{R}^3) \) to its density \( A(x, x) \) where \( A(x, y) \) is its integral kernel. A more precise definition of den can be found in Appendix A or [4]. Nevertheless, one can recover \( \gamma \) via

\[
\gamma = f_{\text{FD}}(\beta(-\Delta - \varphi - \mu)).
\]
However, a yet more advantageous view is to substitute $\rho$ from (4) into (5) to obtain

$$- \Delta \varphi = \kappa - \text{den} f_{\text{FD}}(\beta(-\Delta - \varphi - \mu)).$$

It is in this view that one can see a clearer presence of a screening mass at positive temperature. We will henceforth call equation (8) the reduced Hartree-Fock (REHF) equation for the purpose of this paper.

To specify the class of disorders in $\kappa$ and the solution space on which we study (8), let $L$ denote a (non-degenerate) Bravais lattice in $\mathbb{R}^3$ and $Q$ denote any fundamental domain. That is, $L$ translates of $Q$ tile $\mathbb{R}^3$. A typical example of $Q$ is the Wigner-Seitz cell. Moreover, assume that $\tau = \{\tau_\ell\}_{\ell \in L}$ is a group of ergodic measure preserving $L$-actions on the probability space $\Omega$.

**Definition 1.** A measurable function $f$ on $\mathbb{R}^3 \times \Omega$ is said to be ($L$) stationary if

$$f(x - \ell, \tau_\ell \omega) = f(x, \omega)$$

for all $(x, \omega) \in \mathbb{R}^3 \times \Omega$ and $\ell \in L$.

A notable example of this category is the Anderson potential

$$\kappa(x, \omega) = \sum_{\ell \in L} q_\ell(\omega) \chi(x - \ell),$$

where $\chi \in C^\infty_c(\mathbb{R}^d)$ and the $q_\ell(\omega)$ are i.i.d. random variables. The Anderson type potential is of consideration interest to physicists and mathematicians alike [2, 13].

We define the space of stationary $\kappa$'s and record the conventions used before we state our main result. Let $L^q(Q)$ denote the usual $L^q$ space over $Q$ with the standard $L^q$ norm and $L^2$ inner products when $q = 2$. We will use the notation $L^p_w L^q_x$ to denote the norm-completed

$$\{f(w, x) \in L^q_w(\mathbb{R}^3) \times L^p(\Omega) : f \text{ is stationary and } \|f\|_{L^p_w L^q_x} < \infty\},$$

where

$$\|f\|_{L^p_w L^q_x} := \mathbb{E}\|f\|_{L^p(Q)}.$$  

When $p = \infty$ or $q = \infty$, the associated norm is the usual sup norm. We remark that due to ergodicity, the above norms do not depend on the location of the fundamental domain $Q$ (see Lemma 9 in Appendix A). Consequently, we do not display $Q$ in the subscripts of the norms.

With these notations, equation (8) is to be understood as follows. We require $\kappa \in L^\infty_w L^2_x$ while we look for a solution $(\varphi, \mu)$ in $L^\infty_w H^2_x \times \mathbb{R}$. Nevertheless, $-\Delta - \varphi - \mu$ and $f_{\text{FD}}(\beta(-\Delta - \varphi - \mu))$ are operators on $L^2(\mathbb{R}^3)$, where the latter is defined by the holomorphic functional calculus. Consequently, $\text{den} f_{\text{FD}}(\beta(-\Delta - \varphi - \mu))$ is a stationary function since $\varphi$ is stationary.
Finally, we will use
\[
\hat{f}(k) = (2\pi)^{-3/2} \int_{\mathbb{R}^3} f(x) e^{-ix \cdot k} dx
\]
as our unitary Fourier transform. Moreover, we will denote by \(C_{a,b,\cdots}\) finite constants depending only on the parameters \(a, b, \cdots\). By an abuse of notation and by choosing an even large constant if necessary, \(C\) or \(C_{a,b,\cdots}\) may stand for different constants simultaneously. Lastly, we will write \(A \lesssim B, A \gtrsim B\) if \(A \leq CB\) or \(A \geq CB\) for some absolute constant \(C\), respectively.

### 1.1 Main results

We notice that REHF exhibits a symmetry
\[
(\varphi, \mu) \mapsto (\varphi + t, \mu - t)
\]
for any \(t \in \mathbb{R}\). That is, if \((\varphi, \mu)\) is a solution of (8), then so is \((\varphi + t, \mu - t)\). Therefore, a solution of REHF is an equivalence class of \((\varphi, \mu) \in L^\infty_w L^2_x \times \mathbb{R}\) with respect to (13). Consequently, the notion of uniqueness is defined up to this equivalence class. With this definition of uniqueness, we state our main results.

Let \(Q\) denote a fundamental domain of the lattice \(L\). Let \(\kappa \in L^\infty_w L^2_x\) and \(\kappa_0\) denote its expected spacial average:
\[
\kappa_0 = \frac{1}{|Q|} \mathbb{E} \int_Q \kappa.
\]
Let \(\kappa' = \kappa - \kappa_0\). We have the following main results below. Theorem 2 considers the simplest case where \(\kappa \in \mathbb{R}\) is homogeneous. That is, the material is a jellium. Theorem 3 extends Theorem 2 by considering random disordered background \(\kappa\), as a perturbation from the jellium solution with background potential \(\kappa_0\).

**Theorem 2.** Let \(0 < \kappa \in \mathbb{R}\). There exists positive constants \(c_1, c_2\), (independent of \(\beta, \mu, \) and \(\kappa\)) such that if \(\beta \in \mathbb{R}\) is positive and satisfy
\[
\kappa > \frac{c_1}{\beta^{3/2}},
\]
then there exists a solution \((0, \mu) \in \mathbb{R} \times \mathbb{R}\) to the REHF equation (8). Moreover,
\[
0 < \frac{1}{\beta} \log(\kappa \beta^{3/2}/c_1) < \mu < (\kappa/c_2)^{2/3}.
\]

**Theorem 3.** Let \(\beta \in \mathbb{R}\) and \(\kappa \in L^\infty_w L^2_x\) be real valued. Assume that (15) holds with \(\kappa_0\) and the variation \(\|\kappa'\|_{L^\infty_w L^2_x}\) is sufficiently small. Then the REHF equation (8) has a unique solution \((\varphi, \mu) \in L^\infty_w H^2_x \times \mathbb{R}\) in a neighborhood of \((0, \mu)\) with
\[
\|\varphi\|_{L^\infty_w H^2_x} \leq C_{\beta, \mu, \kappa_0} \|\kappa'\|_{L^\infty_w L^2_x},
\]
for some constant \(C_{\beta, \mu, \kappa_0}\) and \(\mu > 0\).
By our remark immediately after Definition 1, we see that Theorem 3 provides existence and uniqueness results for Anderson background charge distributions.

The paper is organized as follows. In section 2, we provide a proof for Theorem 2 in the case \( \kappa = \kappa_0 \) is a constant. Then, we prove Theorem 3 perturbatively by linearizing the REHF equation at the constant solution to the case \( \kappa = \kappa_0 \). The main proof of Theorem 3 is given in Section 3, modulo the core linear and nonlinear analysis. The linearized operator of the REHF equation is studied in Section 4 while the nonlinear analysis is given in Section 5.

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2 Translation invariant solution: proof of Theorem 2

Claim of Theorem 2. If \( \kappa \in \mathbb{R} \) and \( \varphi = 0 \), then equation (8) becomes an equation for \( \mu \):

\[
\kappa = \text{den} f_{\text{FD}}(\beta(-\Delta - \mu)).
\]  
(18)

Translation invariance of \( -\Delta \) on \( L^2(\mathbb{R}^3) \) shows that this equation can be rewritten as

\[
\kappa = \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} dp f_{\text{FD}}(\beta(p^2 - \mu)).
\]  
(19)

Thus, the right hand side of (19) becomes

\[
\frac{1}{(2\pi)^3} 4\pi \int_0^\infty dp \frac{p^2}{1 + e^{-\beta \mu} e^{\beta p^2}}.
\]  
(20)

An upper bound for (20) is

\[
\frac{1}{2\pi^2} \int_0^\infty dp p^2 e^{\beta \mu} e^{-\beta p^2} = \frac{1}{2\pi^2} \beta^{\frac{3}{2}} \int_0^\infty dp \, p^2 e^{-p^2} = \frac{1}{8\pi^{3/2}} \beta^{3/2}.
\]  
(21)
Similarly, a lower bound for (20) is
\[
\frac{1}{2\pi^2} \int_0^{\sqrt{\pi}} dp \frac{p^2}{2} = \frac{1}{12\pi^2} \mu^{3/2}.
\] (23)

As \( \mu \) ranges from 0 to \( \infty \), we note that the lower bound estimate (23) increases from 0 to \( \infty \) while the the upper bound (22) increases from \( c_1 \beta^{-3/2} \) to \( \infty \) for some constant \( c_1 \).

Thus, continuity (in \( \mu \)) of the right hand side of equation (19) implies that a solution \( \mu > 0 \) exists if \( \kappa > c_1 \beta^{-3/2} \). Solving for \( \mu \) in (22) and (23) proves (16). \( \square \)

3 Fixed point argument: proof of Theorem 3

Proof of Theorem 3. By Theorem 2 and assumption (2) of Theorem 3, there exists a solution \((\varphi = 0, \mu)\) with \( \mu > 0 \) to equation (8) with
\[
\kappa = \kappa_0 := \frac{1}{|Q|} \mathbb{E} \int_Q \kappa.
\] (24)

That is, \( \kappa_0 = \text{den} \ f_{FD}(\beta(-\Delta - \mu)) \). For this \( \mu \) fixed, we look for a solution \((\varphi, \mu)\) to the full equation (8) perturbatively. In particular, we linearize (8) at \( \varphi = 0 \). Let
\[
M := d_\varphi \text{den} \ f_{FD}(\beta(-\Delta - \varphi - \mu)) |_{\varphi=0}
\] (25)

and
\[
N(\varphi) := -\left( \text{den} \ f_{FD}(\beta(-\Delta - \varphi - \mu)) - \text{den} \ f_{FD}(\beta(-\Delta - \mu)) - M \varphi \right).
\] (26)

Then we can rewrite equation (8) as
\[
(-\Delta + M)\varphi = \kappa' + N(\varphi).
\] (27)

Let us further denote \( L \) to be the linear operator
\[
L := -\Delta + M.
\] (28)

We have the following estimates for the linear operator \( L \) and the nonlinear operator \( N \), whose proofs are delayed to sections 4 and 5 below for a self-contained treatment.

Theorem 4. Let \( L \) be defined in (25) on \( L^\infty_w L^2 \). Let \( f \in L^\infty_w L^2 \). Then
\[
\|L f\|_{L^\infty_w L^2} \geq \|(m_Q - \Delta) f\|_{L^\infty_w L^2}
\] (29)

where
\[
m_Q = \frac{1}{16} \min(\mu, \sqrt{\mu}) - C_{\beta, \mu} \ell(Q)^{-1}
\] (30)

and \( \ell(Q) \) is the diameter of \( Q \) and \( C_{\beta, \mu} > 0 \) is some constant.
Theorem 5. Let $N$ be defined in (26) and let $\varphi_1, \varphi_2 \in L^\infty_w H^2_x$. There exists a constant $C_{\beta, \mu}$ depending only on $\beta$ and $\mu$ such that if $\|\varphi_i\|_{L^\infty_w H^2_x} \leq \frac{1}{10} C_{\beta, \mu}^{-1}$, then
\[
\|N(\varphi_1) - N(\varphi_2)\|_{L^\infty_w L^2_x} \leq C_{\beta, \mu} (\|\varphi_1\|_{L^\infty_w H^2_x} + \|\varphi_2\|_{L^\infty_w H^2_x}) \|\varphi_1 - \varphi_2\|_{L^\infty_w H^2_x}. \tag{31}
\]

In order to utilize Theorem 4 and ensure a positive lower bound for $L$, we make the following observation. If $\kappa$ is $L$ stationary, it is also $(nL)$ stationary for $0 < n \in \mathbb{Z}$. In particular, by choosing $n$ so large and $\|\kappa'\|_{L^\infty_w L^2_x(Q)}$ so small so that $\|\kappa'\|_{L^\infty_w L^2_x(nQ)}$ is sufficiently small, we may assume that the fundamental domain of $L$ has a sufficiently large diameter. This ensures that (30) is positive. On the other hand, we claim that an $(nL)$ stationary solution associated to a $L$ stationary $\kappa$ is in fact $L$ stationary, provided such solution in unique. Suppose that $(\varphi(x, \omega), \mu) \in L^\infty_w H^2_x \times \mathbb{R}$ is any $(nL)$ stationary unique solution of (8). Since $\kappa$ is $L$ stationary, for $x \in \mathbb{R}^3$ and $\ell \in L$,
\[
-\Delta \varphi(x - \ell, \tau_{\ell}\omega) = \kappa(x, \omega) - \text{den} f_{FD}(\beta(-\Delta - \varphi(x - \ell, \tau_{\ell}\omega) - \mu)). \tag{32}
\]
This shows that $\varphi(x - \ell, \tau_{\ell}\omega)$ is also an $(nL)$ stationary solution of (8). By uniqueness, we see that
\[
\varphi(x - \ell, \tau_{\ell}\omega) = \varphi(x, \omega). \tag{33}
\]
Hence, $\varphi$ is also $L$ stationary. Consequently, it suffices for us to prove Theorem 3 and utilize Theorems 4 under the assumption that $Q$ is sufficiently large. We will make this assumption for the rest of the proof of Theorem 3. At the same time, the uniqueness assumption is established via the fixed point theorem below.

By Theorem 4, if $f \in L^\infty_w L^2_x$, then
\[
\|Lf\|_{L^\infty_w L^2_x} \gtrsim (m_Q - \Delta)f\|_{L^\infty_w L^2_x}, \tag{34}
\]
where $m_Q$ is given in (30) and
\[
m_Q > 0. \tag{35}
\]
Hence, $L$ is invertible and bounded from below by $m_Q$. Thus, we can write (27) as
\[
\varphi = L^{-1} \kappa' + L^{-1} N(\varphi). \tag{36}
\]
To apply the fixed point theorem, we work on the ball
\[
B := \{ \varphi \in L^\infty_w H^2_x : \|\varphi\|_{L^\infty_w H^2_x} < \varepsilon \} \tag{37}
\]
where $\varepsilon \leq \frac{1}{10} C_{\beta, \mu}^{-1}$ is to be determined. If the right hand side of (36) were to map $B$ into $B$, then we require
\[
\|L^{-1}(\kappa' + N(\varphi))\|_{L^\infty_w H^2_x} \leq \varepsilon. \tag{38}
\]
By the choice of \( \varepsilon \leq \frac{1}{10} C_{\beta,\mu}^{-1} \) and by the nonlinear estimates in Theorem 5, we see that condition (38) is satisfied if
\[
m_Q^{-1} \left( \| \kappa' \|_{L_w^\infty L_x^2} + C_{\beta,\mu} \| \varphi \|_{L_w^\infty H_x^2}^2 \right) \leq \varepsilon
\]
where \( C_{\beta,\mu} \) is given in (31). Moreover, in order that \( L^{-1} N \) is a contraction, we require
\[
2m_Q^{-1} C_{\beta,\mu} \varepsilon < 1.
\]
Consequently, we choose
\[
\varepsilon = \min \left( 2m_Q^{-1} \| \kappa' \|_{L_w^\infty L_x^2}, \frac{1}{10} C_{\beta,\mu}^{-1} \right).
\]
We see that this choice of \( \varepsilon \) satisfies (39) and (40) if \( \kappa' \) is sufficiently small:
\[
\| \kappa' \|_{L_w^\infty L_x^2} < \frac{m_Q^2}{4C_{\beta,\mu}}.
\]
Theorem 3 is now proved by the fixed point theorem, where the solution \( \varphi \) of (36) is unique on \( B \) (see (37)) and satisfies
\[
\| \varphi \|_{L_w^\infty H_x^2} \leq \varepsilon \leq 2m_Q^{-1} \| \kappa' \|_{L_w^\infty L_x^2} = C_{\beta,\mu,\kappa_0} \| \kappa' \|_{L_w^\infty L_x^2}
\]
for some constant \( C_{\beta,\mu,\kappa_0} \). We remark that \( C_{\beta,\mu,\kappa_0} \) receives its dependence on \( \kappa_0 \) through \( \mu \) (see Theorem 2).

\[\square\]

4 Linear analysis

The main result of this section is Theorem 4, which concerns the lower bound of the operator \( L \) on \( L_w^\infty L_x^2 \) (see (25)). Since this analysis is the core of the paper, we detail its proofs in pieces. First, we compute an explicit form for \( L \) in Subsection 4.1. Then we prove a lower bound for \( L \) on \( L^2(\mathbb{R}^3) \) in Subsection 4.2. Finally, building on these two results, we will prove Theorem 4 in the last Subsection 4.3.

4.1 Explicit form of the linearization

We first look for an integral representation of \( \text{den} f_{FD}(\beta(-\Delta - \varphi - \mu)) \) (see the right hand side of (8)). Let \( \varphi \in H^2(\Omega) \subset L^\infty(\Omega) \) be such that \( \| \varphi \|_{L^\infty(\Omega)} \leq \| \varphi \|_{H^2(\Omega)} \) is sufficiently small. Thus, the spectrum of \( -\Delta - \varphi \) remains in a small tubular neighborhood of the real axis and bounded from \(-\infty\). Moreover, we note that \( f_{FD}(\beta(z - \mu)) \) is meromorphic on \( \mathbb{C} \) with poles \( \mu + i\pi \beta^{-1} Z \). It follows by Cauchy’s theorem that
\[
\text{den} f_{FD}(\beta(-\Delta - \varphi - \mu)) = \frac{1}{2\pi i} \text{den} \int f_{FD}(\beta(z - \mu))(z - (-\Delta - \varphi))^{-1},
\]

8
Figure 1: We identify the complex plane \( \mathbb{C} \) with \( \mathbb{R}^2 \) via \( z = x + iy \) for \((x,y) \in \mathbb{R}^2\) in the diagram above. The contour \( \Gamma \) is denoted by the blue dashed line, extending to positive real infinity. The spectrum of \( -\Delta - \varphi \) is contained in the solid black line.

where the contour \( \Gamma \) is given in Figure 1. In particular, \( \Gamma \) is chosen to be at most \( \frac{3}{4} \beta^{-1} \) distance away from the real line and contains the spectrum of \( -\Delta - \varphi \). Since we will be using expressions similar to (44) repeatedly, we will denote

\[
\oint := \frac{1}{2\pi i} \int_{\Gamma} dz f_{FD}^\beta(z - \mu) \quad \text{and} \quad \oint \mid f := \frac{1}{2\pi} \int_{\Gamma} dz \mid f_{FD}^\beta(z - \mu) \mid
\]

throughout the paper.

Now, we are ready to compute the linearization of (8). By the resolvent identity

\[
(z - A)^{-1} - (z - B)^{-1} = (z - A)^{-1}(A - B)(z - B)^{-1}
\]

for any operators \( A, B \) on \( L^2(\mathbb{R}^3) \), the linear operator (linearized at \( \varphi = 0 \)) of the REHF equation (8) can be seen to be

\[
L = -\Delta + M \quad \text{where} \quad M \text{ is defined in (25) and}
\]

\[
Mf = - \text{den} \frac{1}{2\pi i} \int_{\Gamma} dz f_{FD}^\beta(z - \mu))(z + \Delta)^{-1} f(z + \Delta)^{-1}.
\]

(47)
The main result of this section is Lemma 6 which yields an explicit formula for $M$.

**Lemma 6.** Assume that $\mu > 0$, then

$$M = \frac{1}{8\pi^2} \frac{1}{|\nabla|} \int_0^\infty \ln \left( \frac{\sqrt{4t} + |\nabla|}{\sqrt{4t} - |\nabla|} \right) f_{FD}(\beta(t - \mu)) dt. \tag{48}$$

Before we start the proof for Lemma 6, we state and prove a preliminary estimate for $M$ below.

**Lemma 7.** $M$ is bounded on $L^\infty_w L^2_x$.

**Proof.** First, we make the important remark that the branch cut of any relevant complex function in the rest of the paper is taken to be the negative real axis. Thus, for $z \in \mathbb{C}$ with $\Re z \geq 0$, the integral kernel of $(z - (-\Delta))^{-1}$ is

$$g_z(x - y) = -\frac{1}{4\pi} \frac{e^{-\sqrt{-z}|x-y|}}{|x-y|}. \tag{49}$$

Then by (47),

$$Mf = -\oint dz g_z^2 * f. \tag{50}$$

We note that $g_z^2(r) = \frac{1}{16\pi^2} \frac{e^{-2\sqrt{-z}|r|}}{|r|^2}$ is $L^1(\mathbb{R}^3)$ and $f_{FD}(\beta(z - \mu))$ decays exponentially in $\beta\Re(z - \mu)$ as $\Re z \to \infty$. It follows by Young's inequality that

$$\|Mf\|_{L^\infty_w L^2_x} \lesssim \|f\|_{L^\infty_w L^2_x}. \tag{51}$$

**Proof of Lemma 6.** The ideas of this proof is based on an unpublished manuscript of I. Chenn and I. M. Sigal. Let $g_z(x - y)$ be the integral kernel of $(z - (-\Delta))^{-1}$ as in (49). It follows that

$$(z + \Delta)^{-1} \varphi(z + \Delta)^{-1}(x, x) = \frac{1}{16\pi^2} \int dy \frac{e^{-2\sqrt{-z}|x-y|}}{|x-y|^2} \varphi(y) \tag{52}$$

for any sufficiently regular $\varphi$. To evaluate (52), we Fourier transform $\frac{e^{-2\sqrt{-z}|x|}}{|x|^2}$:

$$\int e^{-2\sqrt{-z}|x|} e^{-ix \cdot p} dx = \int_0^\infty dr \int_0^\pi d\theta \int_0^{2\pi} d\varphi e^{-2r\sqrt{-z}} e^{-i \cos(\theta) r |p|} r^2 \sin(\theta) \tag{53}$$

$$= 4\pi \int_0^\infty dr \sin(\theta) \frac{\sin(r |p|)}{|p|} e^{-2r\sqrt{-z}} \tag{54}$$

$$= 4\pi \frac{\arctan(|p|/\sqrt{-4z})}{|p|}. \tag{55}$$
By (50), (52), and (55),

\[ M = \frac{1}{8\pi^2} \frac{1}{\sqrt{i}} \int_{\Gamma} f_{\text{FD}}(\beta(z - \mu)) \arctan(|\nabla|/\sqrt{-4z}), \quad (56) \]

where the contour \( \Gamma' \) is homeomorphic to \( \Gamma \) (see Figure 1) and is defined as follows. Let \( 0 < \alpha < \beta^{-1} \) be small and \( L[a, b] \) denote the line segment connecting \( a, b \in \mathbb{C} \). Then, \( \Gamma' = L[\infty + i\alpha, -\alpha + i\alpha] \cup L[-\alpha + i\alpha, -\alpha - i\alpha] \cup L[-\alpha - i\alpha, \infty - i\alpha] \).

Next, we simplify (56) by taking \( \alpha \to 0 \). For ease of notation, we will denote both \( |\nabla| \) and an arbitrary point in its spectrum by \( p \). We note that

\[ \arctan(x) = \frac{i}{2} \left( \log(1 - ix) - \log(1 + ix) \right), \quad (57) \]

where \( \log \) has the branch cut \( (-\infty, 0] \). Moreover, for any \( p > 0 \) fixed, the integrand \( f_{\text{FD}}(\beta(z - \mu)) \arctan(p/\sqrt{-4z}) \) has singularities contained in \( [0, \infty] \cup (\mu + i\beta^{-1}\mathbb{Z}) \), otherwise it is holomorphic near the real axis. Let \( 0 < \alpha \) be small. These observations justify our computation of the integral along another contour which we explicitly parameterize as:

\[ \gamma_1(t) = t + i\alpha, t \in (-\alpha, \infty), \quad (58) \]
\[ \gamma_2(t) = t - i\alpha, t \in (-\alpha, \infty), \quad (59) \]
\[ \gamma_3(t) = -\alpha + it, t \in (-\alpha, \alpha). \quad (60) \]

Note that by holomorphicity outside of the singularity of the integrand, the value of the integral is independent of \( \alpha \). Hence we may take \( \alpha \to 0 \). For notation, let \( f(z) = f_{\text{FD}}(\beta(z - \mu)) \) and for any path \( \gamma : [a, b] \to \mathbb{C} \), let \( \gamma^{-1} \) denote the same path traversed backward. Ignoring pre-factors constants, computing the contour integral (56) along \( \gamma_1^{-1} \) and \( \gamma_2 \), one has

\[ -\frac{1}{8\pi^2} \frac{1}{p_i} \int_{-\alpha}^\infty f(t - i\alpha) \arctan(p/\sqrt{-4(t - i\alpha)}) \]
\[ = -\frac{1}{8\pi^2} \frac{1}{p_i} \int_{-\alpha}^\infty f(t + i\alpha) \arctan(p/\sqrt{-4(t + i\alpha)}) dt \]
\[ = -\frac{1}{8\pi^2} \frac{1}{p_i} \int_{-\alpha}^\infty f(t - i\alpha) \arctan(p/\sqrt{-4t + 4i\alpha}) \]
\[ - f(t + i\alpha) \arctan(p/\sqrt{-4t - 4i\alpha}) dt. \quad (61) \]

Since \( f(x) \) is continuous away from its poles and exponentially decaying for \( \Re z > \mu \), in the limit \( \alpha \to 0 \), it suffices for us to compute

\[ \int_{-\alpha}^\infty f(t) \left( \arctan(p/\sqrt{-4t + 4i\alpha}) - \arctan(p/\sqrt{-4t - 4i\alpha}) \right) dt \quad (62) \]
in place of (61). We split the integral in (62) into
\[
\int_{-\alpha}^{\frac{1}{4}p^2} + \int_{\frac{1}{4}p^2}^{\infty}.
\]
(63)

We compute the first integral in (63) and assume that \( t < \frac{1}{4}p^2 \). We note that
\[
\frac{2}{i} \left( \arctan\left(\frac{p}{\sqrt{-4t + 4i\alpha}}\right) - \arctan\left(\frac{p}{\sqrt{-4t - 4i\alpha}}\right) \right)
= \log\left(1 - i\frac{p}{\sqrt{-4t + 4i\alpha}}\right) - \log\left(1 - i\frac{p}{\sqrt{-4t - 4i\alpha}}\right)
+ \log\left(1 + i\frac{p}{\sqrt{-4t - 4i\alpha}}\right) - \log\left(1 + i\frac{p}{\sqrt{-4t + 4i\alpha}}\right).
\]
(64)

Since \( t, \alpha > 0 \), to keep track of the jump discontinuity in \( \log \), let us write,
\[
\frac{ip}{\sqrt{-4t \pm 4i\alpha}} = \pm \frac{p}{\sqrt{4t \mp i\alpha}} = \pm \frac{p}{\sqrt{4t}} \left(1 \mp \frac{\alpha}{t}\right)^{-1/2}
\]
(65)
for \( t \geq 0 \). Denote \( \delta_\pm = \pm \frac{p}{\sqrt{4t}}((1 \mp i\alpha t)^{-1/2} - 1) \). Hence
\[
1 - \frac{ip}{\sqrt{-4t \pm 4i\alpha}} = 1 \mp \frac{p}{\sqrt{4t}} - \delta_\pm.
\]
(66)

We note that \( \delta_\pm \to 0 \) as \( \alpha \to 0 \) and \( \delta_+ \) and \( \delta_- \) are in the upper half-plane. Since \( t < \frac{1}{4}p^2 \), using \( \lim_{b \to 0^\pm} \log(-a + ib) = \log(a) \pm i\pi \) for \( a > 0 \), we see that
\[
\lim_{\alpha \to 0} \log\left(1 - \frac{ip}{\sqrt{-4t + 4i\alpha}}\right) = \log\left(\frac{p}{\sqrt{4t}} - 1\right) - i\pi
\]
(67)
and similarly
\[
\lim_{\alpha \to 0} \log\left(1 - \frac{ip}{\sqrt{-4t - 4i\alpha}}\right) = \log\left(\frac{p}{\sqrt{4t}} + 1\right).
\]
(68)
So we have that
\[
\lim_{\alpha \to 0} \log\left(1 - \frac{ip}{\sqrt{-4t + 4i\alpha}}\right) - \log\left(1 - \frac{ip}{\sqrt{-4t - 4i\alpha}}\right)
= \log\left(\frac{p}{\sqrt{4t}} - 1\right) - \log\left(\frac{p}{\sqrt{4t}} + 1\right) - i\pi.
\]
(69)

By the same token, and since \( t < \frac{1}{4}p^2 \),
\[
1 + \frac{ip}{\sqrt{-4t \pm 4i\alpha}} = 1 \pm \frac{p}{\sqrt{4t}} + \delta_\pm.
\]
(70)
Using \( \lim_{b \to 0} \log(-a + ib) = \log(a) \pm i\pi \) for \( a > 0 \), we see that
\[
\lim_{\alpha \to 0} \log \left(1 + \frac{ip}{\sqrt{-4t - 4i\alpha}}\right) = \log \left(\frac{p}{\sqrt{4t}} - 1\right) + i\pi, \tag{71}\]
and similarly
\[
\lim_{\alpha \to 0} \log \left(1 + \frac{ip}{\sqrt{-4t + 4i\alpha}}\right) = \log \left(\frac{p}{\sqrt{4t}} + 1\right). \tag{72}\]
So we have that
\[
\lim_{\alpha \to 0} \log \left(1 + \frac{ip}{\sqrt{-4t - 4i\alpha}}\right) - \log \left(1 + \frac{ip}{\sqrt{-4t + 4i\alpha}}\right) = \log \left(\frac{p}{\sqrt{4t}} - 1\right) - \log \left(\frac{p}{\sqrt{4t}} + 1\right) + i\pi. \tag{73}\]
It follows by (64), (69), (73) that
\[
\lim_{\alpha \to 0} \arctan\left(\frac{p}{\sqrt{-4t + 4i\alpha}}\right) - \arctan\left(\frac{p}{\sqrt{-4t - 4i\alpha}}\right) = i \left(\log \left(\frac{p}{\sqrt{4t}} - 1\right) - \log \left(\frac{p}{\sqrt{4t}} + 1\right)\right). \tag{74}\]
Hence, in the limit \( \alpha \to 0 \), the \( \gamma_1^{-1}, \gamma_2 \) portion of the first integral in (63) is
\[
\int_0^{p^2/4} f(t)dt = \int_0^{p^2/4} \left(\log \left(\frac{p}{\sqrt{4t}} - 1\right) - \log \left(\frac{p}{\sqrt{4t}} + 1\right)\right) f(t)dt
= -i \int_0^{p^2/4} \log \left(\frac{p}{\sqrt{4t}}\right) f(t)dt. \tag{75}\]
Now we consider the second integral in (63). In this case, for \( t > p^2/4 \),
\[
\frac{2}{i} \left(\arctan\left(\frac{p}{\sqrt{-4t + 4i\alpha}}\right) - \arctan\left(\frac{p}{\sqrt{-4t - 4i\alpha}}\right)\right) = \log \left(1 - \frac{p}{\sqrt{-4t + 4i\alpha}}\right) - \log \left(1 - \frac{p}{\sqrt{-4t - 4i\alpha}}\right)
+ \log \left(1 + \frac{p}{\sqrt{-4t - 4i\alpha}}\right) - \log \left(1 + \frac{p}{\sqrt{-4t + 4i\alpha}}\right). \tag{76}\]
Via the same argument as (74), we get
\[
\arctan\left(\frac{p}{\sqrt{-4t + 4i\alpha}}\right) - \arctan\left(\frac{p}{\sqrt{-4t - 4i\alpha}}\right) \quad \rightarrow \quad i \left(\log \left(1 - \frac{p}{\sqrt{4t}}\right) - \log \left(1 + \frac{p}{\sqrt{4t}}\right)\right) = i \log \left(\frac{\sqrt{4t} - p}{\sqrt{4t} + p}\right) \tag{77}\]
as $\alpha \to 0$. Putting it as the integrand for the second integral in (63), we get
\[
\int_{\rho^2/4}^{\infty} = i \int_{\rho^2/4}^{\infty} \log \left( \frac{\sqrt{4t} - \rho}{\sqrt{4t} + \rho} \right) f(t) dt = -i \int_{\rho^2/4}^{\infty} \log \left( \frac{\sqrt{4t} + \rho}{\sqrt{4t} - \rho} \right) f(t) dt.
\] (78)

It follows that by (56) and (61)
\[
M = -\frac{1}{8\pi^2} \frac{1}{pt} \left( \int_{0}^{\rho^2/4} + \int_{\rho^2/4}^{\infty} \right) = \frac{1}{8\pi^2} \frac{1}{p} \int_{0}^{\infty} \log \left( \frac{\sqrt{4t} + \rho}{\sqrt{4t} - \rho} \right) f(t) dt,
\] (79)
which is (48). The proof of Lemma 6 is now complete. \qed

4.2 Lower bound of $L$ on $L^2(\mathbb{R}^3)$

**Theorem 8.** The operator $L$ given in (47) is bounded below on $L^2(\mathbb{R}^3)$ by
\[
L \gtrsim -\Delta + m_*
\] (80)
where
\[
m_* = \min(\mu, \sqrt{\mu}).
\] (81)

**Proof.** Let $p = |\nabla|$. By elementary calculus, we have the following two estimates
\[
\ln \left| \frac{x + 1}{x - 1} \right| > 2x \text{ for } x < 1
\] (82)
\[
\ln \left| \frac{x + 1}{x - 1} \right| > \frac{2}{x} \text{ for } x > 1.
\] (83)

In the eigenspace with $p^2/4 < \mu$, we use $f_{FD}(\beta(t - \mu)) \geq \frac{1}{2} \chi_{[0,\mu]}$, where $\chi_S$ is the indicator function on $S \subset \mathbb{R}$. For a particular $p^2/4 < \mu$ fixed, equation (48) shows
\[
M \gtrsim \int_{0}^{p^2/4} \frac{\sqrt{t}}{p^2} + \int_{p^2/4}^{\mu} \frac{1}{\sqrt{t}}
\] (84)
\[
= \frac{1}{p^2} \frac{2}{3} \left[ \int_{0}^{p^2/4} \sqrt{t} dt \right]^{1/2} + 2t^{1/2} \bigg|_{p^2/4}^{\mu}
\] (85)
\[
\geq \frac{1}{6} \sqrt{\mu}.
\] (86)
On the other hand, in the eigenspace with $p^2/4 \geq \mu$, we see that $\frac{1}{2} p^2 + M \geq \frac{1}{2} p^2 \geq 2\mu$. Combining with (86), Theorem 8 is proved. \qed
4.3 Lower bound for $L$ on $L^\infty L^2_x$: proof of Theorem 4

Proof of Theorem 4. Let $Q$ be a fundamental domain of $\mathcal{L}$ and $f \in L^\infty L^2_x$ and $C_c^2(Q)$ denote the set of compactly supported $C^2$ function on $Q$. Then

$$\|(-\Delta + M)f\|_{L^\infty L^2_x} := \sup_{\omega \in \Omega} \|(-\Delta + M)f\|_{L^2(Q)}$$

$$= \sup_{\omega \in \Omega} \sup_{\psi \in C_c^2(Q)} \langle \psi, (-\Delta + M)f \rangle_{L^2(Q)} \|\psi\|_{L^2(Q)}.$$  \hfill (87)

The goal is to choose a nice $\psi$ for a lower bound. Intuitively, we should choose $\psi = (-\Delta + M)^{-1}f$. We accomplish this in 4 steps below.

For notation simplicity below, we follow (45) and also use $r(z) := (z + \Delta)^{-1}$.

In this notation, the linear operator is

$$Lf = -\Delta f + Mf = -\Delta f - \oint r(z)fr(z).$$

**Step 1: Move $-\Delta + M$ onto $\psi$.**

We have a solid understanding of $-\Delta + M$ on $L^2(\mathbb{R}^3)$ functions; so we would like to use it. Since $\psi \in C_c^2(Q)$, we see that

$$\langle \psi, (-\Delta)f \rangle_{L^2(Q)} = \langle (-\Delta)\psi, f \rangle_{L^2(Q)}. \hfill (90)$$

Using the definition (47) of $M$, we see that

$$\langle \psi, Mf \rangle_{L^2(Q)} = -\oint \text{Tr} \tilde{\psi}r(z)fr(z) = -\oint \text{Tr} r(z)\overline{\psi}r(z)f = \langle M\psi, f \rangle_{L^2(\mathbb{R}^3)} \hfill (91)$$

by the cyclicity of trace and the fact the contour $\Gamma$ can be chosen to be invariant under complex conjugation. We remark that since $\varphi \in C_c^2(\mathbb{R}^3)$, Tr is taken to be the trace on $L^2(\mathbb{R}^3)$ instead of $L^2(Q)$. By equations (90) and (91), we see that

$$\langle \psi, (-\Delta + M)f \rangle_{L^2(Q)} = \langle (-\Delta + M)\psi, f \rangle_{L^2(\mathbb{R}^3)}. \hfill (92)$$

**Step 2: choosing $\psi$.**

By Theorem 8, $-\Delta + M$ is bounded from below on $L^2(\mathbb{R}^3)$. In particular, it is invertible. Thus, we choose

$$\psi := \chi(-\Delta + M)^{-1}(f \mid_Q) \hfill (93)$$

where $\chi$ is a compactly supported bump function on $Q$ whose exact properties will be determined later and $f \mid_Q$ is the restriction of $f$ to $Q$. We remark that despite the fact that $\psi$ may not be in $C_c^2(Q)$, it can be approximated arbitrarily close in the $H^2$
norm by functions from $C^2_c(Q)$. Thus, it causes no disruption to our proof to consider $\psi$ instead of a proper $C^2_c(Q)$ function. Moreover, this choice of $\psi$ satisfies (90). It follows that

$$(-\Delta + M)\psi = \chi f|_Q + [-\Delta + M,\chi](-\Delta + M)^{-1}(f|_Q).$$ (94)

Combining with (92), we see that

$$\langle \psi, (-\Delta + M)f \rangle_{L^2(Q)} = \|\chi^{1/2} f\|_{L^2(Q)}^2 + \langle [-\Delta + M,\chi](-\Delta + M)^{-1}(f|_Q),f \rangle_{L^2(\mathbb{R}^3)}.$$ (95)

We estimate the second term in (95) below.

**Step 3: Error estimates for $[\Delta,\chi]$ term.**

A simple computation shows that

$$[-\Delta,\chi] = -2\nabla \chi \cdot \nabla - \Delta \chi.$$ (96)

Using Theorem 8 once more and the fact $\chi$ is supported in $Q$, it follows that

$$\langle [-\Delta,\chi](-\Delta + M)^{-1}(f|_Q),f \rangle_{L^2(\mathbb{R}^3)} = \|\chi^{1/2} f\|_{L^2(Q)}^2 + \langle [-\Delta + M,\chi](-\Delta + M)^{-1}(f|_Q),f \rangle_{L^2(Q)} |\langle [-\Delta,\chi](-\Delta + M)^{-1}(f|_Q),f \rangle_{L^2(\mathbb{R}^3)}| \leq 2m_*^{-1} \|\nabla \chi\|_{L^\infty} \|\Delta \chi\|_{L^\infty} \|f\|_{L^2(Q)}^2,$$ (97)

where $m_*$ is given in (81).

**Step 4: Error estimates for $[M,\chi]$ term.**

Let $u \in L^2(\mathbb{R}^3)$ and $v \in L^2_{\text{loc}}(\mathbb{R}^3)$. Then

$$\langle [M,\chi]u,v \rangle_{L^2(\mathbb{R}^3)} = \oint Tr [r(z)\chi ur(z)v - \chi r(z)ur(z)v]$$

$$= \oint Tr[r(z),\chi]ur(z)v$$

$$= \oint Tr r(z)(2\nabla \chi \nabla + \Delta \chi)r(z)ur(z)v.$$ (100)

By the cyclicity of trace, we move $r(z)$ to the right of $v$ to obtain

$$\langle [M,\chi]u,v \rangle_{L^2(\mathbb{R}^3)} = \oint Tr(2\nabla \chi \nabla + \Delta \chi)r(z)ur(z)v.$$ (101)

Since $\chi$ is supported on $Q$, we may write

$$\langle [M,\chi]u,v \rangle_{L^2(\mathbb{R}^3)} = \oint Tr 1_Q(2\nabla \chi \nabla + \Delta \chi)r(z)ur(z)vz 1_Q,$$ (102)

where $1_Q$ is the indicator function of the set $Q$. Let $g_z$ be the integral kernel of $r(z) = (z + \Delta)^{-1}$ on $L^2(\mathbb{R}^3)$ and recall the definition of $\|\mathbf{f}\|$ from (45). Writing (102)
out explicitly in terms of integral kernels, we obtain

\[
|M, \chi|u, v|_{L^2(\mathbb{R}^3)} \leq 2(\|\nabla \chi\|_{L^\infty} + \|\Delta \chi\|_{L^\infty})
\]

\[
\times \left| \int_Q dx \int_{\mathbb{R}^{3+3}} dy_1 dy_2 |(1 + \nabla) g_z(x - y_1) u(y_1) g_z(y_1 - y_2) v(y_2) g_z(y_2 - x)|. \quad (103)
\]

Using a change of variable \( y_1 \mapsto y_1 + x \) and \( y_2 \mapsto y_2 + x \), we see that

\[
\left| \int_Q dx \int_{\mathbb{R}^{3+3}} dy_1 dy_2 |(1 + \nabla) g_z(y_1) u(y_1 + x) g_z(y_1 - y_2) v(y_2 + x) g_z(y_2)|
\]

\[
= \left| \int_Q dx \int_{\mathbb{R}^{3+3}} dy_1 dy_2 |(1 + \nabla) g_z(y_1 - y_2) v(y_2) g_z(y_2 - x)|. \quad (104)
\]

Applying Hölder with \( \frac{1}{2} + \frac{1}{2} = 1 \) to the \( dx \) integral, we see that

\[
\left| \int_Q dx \int_{\mathbb{R}^{3+3}} dy_1 dy_2 |(1 + \nabla) g_z(y_1) u(y_1 + x) g_z(y_1 - y_2) v(y_2 + x) g_z(y_2)|
\]

\[
\leq \left| \int_Q dx \int_{\mathbb{R}^{3+3}} dy_1 dy_2 |(1 + \nabla) g_z(y_1) g_z(y_1 - y_2) g_z(y_2)||u||_{L^2(\mathbb{R}^3)}||v||_{L^2(\mathbb{R}^3)}
\]

\[
\leq \left| \int_Q dx \int_{\mathbb{R}^{3+3}} dy_1 dy_2 |(1 + \nabla) g_z(y_1) g_z(y_1 - y_2) g_z(y_2)||u||_{L^2(\mathbb{R}^3)}||v||_{L^2(\mathbb{R}^3)}. \quad (105)
\]

We specialize to \( u = (-\Delta + M)^{-1}(f|Q) \) and \( v = f \). By Theorem 8, we note that

\[
||u||_{L^2(\mathbb{R}^3)} \leq m_\ast^{-1} ||f||_{L^2(Q)}, \quad (106)
\]

where \( m_\ast \) is given in (81). Combining (103), (104), (105), and (106), we see that

\[
\sup_{\omega \in \Omega} |\langle [M, \chi]u, v \rangle_{L^2(\mathbb{R}^3)}|
\]

\[
\leq 2m_\ast^{-1}(\|\nabla \chi\|_{L^\infty} + \|\Delta \chi\|_{L^\infty})||f||_{L^\infty L^2_x}
\]

\[
\times \left| \int_Q dx \int_{\mathbb{R}^{3+3}} dy_1 dy_2 |(1 + \nabla) g_z(y_1) g_z(y_1 - y_2) g_z(y_2)|\sup_{\omega \in \Omega} ||f||_{L^2(Q+y_1)}.
\quad (107)
\]

Let

\[
A = 2(\|\nabla \chi\|_{L^\infty} + \|\Delta \chi\|_{L^\infty}). \quad (108)
\]

Since the \( L^\infty L^2_x \) norm is independent of the location of the domain of integration, we see that

\[
\sup_{\omega \in \Omega} |\langle [M, \chi]u, v \rangle_{L^2(\mathbb{R}^3)}| \leq m_\ast^{-1} A ||f||_{L^\infty L^2_x} \left| \int_Q \langle (1 + \nabla) g_z, |g_z|^* g_z \rangle_{L^2(\mathbb{R}^3)} \right|
\]

\[
\leq m_\ast^{-1} A ||f||_{L^\infty L^2_x} \left| \int_Q ||g_z||^2_{L_1(\mathbb{R}^3)} ||g_z||_{L^1(\mathbb{R}^3)} \right|
\]

\[
=: m_\ast^{-1} AC_{\beta, \mu} ||f||_{L^\infty L^2_x}, \quad (109)
\]

\[
= m_\ast^{-1} AC_{\beta, \mu} ||f||_{L^\infty L^2_x}, \quad (111)
\]
where
\[ C_{\beta,\mu} = \left| \int g_{x} \|g_{x}\|^{2}_{H^{1}(\mathbb{R}^{3})} \|g_{x}\|_{L^{1}(\mathbb{R}^{3})} < \infty. \] (112)

**Step 4: Conclusion**

By definition (93), we see that
\[ \|\psi\|_{L^{2}(Q)} \leq m^{-1}_{*} \|f\|_{L^{2}(Q)}. \] (113)

Combining with equations (95), (97), and (111) to obtain
\[ \sup_{\omega \in \Omega} \frac{\langle \psi, (-\Delta + M)f \rangle_{L^{2}(Q)}}{\|\psi\|_{L^{2}(Q)}} \geq m_{*} \sup_{\omega \in \Omega} \frac{\|\chi^{1/2}f\|_{L^{2}(Q)}^{2}}{\|f\|_{L^{2}(Q)}} - C_{\beta,\mu} A \|f\|_{L^{\infty}L^{2}}. \] (114)

Choose \( \omega_{0} \in \Omega \) so that
\[ \|f_{\omega_{0}}\|_{L^{2}(Q)}^{2} \geq \frac{1}{2m} \|f_{\omega_{0}}\|_{L^{2}(Q)}. \] (115)

Assuming \( Q \) is a cube centered at the origin (or by a shift and choosing a different fundamental domain if necessary), we can find a subcube \( Q' \subset Q \) with half the diameter, such that
\[ \|f_{\omega_{0}}\|_{L^{2}(Q')}^{2} \geq \frac{1}{2m} \|f_{\omega_{0}}\|_{L^{2}(Q)}. \] (116)

We can translation \( Q' \) to be concentric to \( Q \) by \( h \in \mathbb{R}^{3} \) so that
\[ \|T_{h}f_{\omega_{0}}\|_{L^{2}(Q/2)}^{2} \geq \frac{1}{2m} \|f_{\omega_{0}}\|_{L^{2}(Q)}, \] (117)

where \( T_{h} \) is the translation by \( h \) and \( Q/2 \) is the concentric cube to \( Q \) with half the side length. Thus, we can choose bump functions \( \chi \) by a translation and a dilation from a reference \( O(1) \) bounded \( C_{\infty} \) function so that \( \chi \big|_{Q/2} = 1 \) and
\[ \|\nabla^{m}\chi\| \leq C_{1} \ell(Q)^{-m}, \] (118)

where \( C_{1} \) is independent of the size of \( Q \) and \( \ell(Q) \) is the diameter of \( Q \). Since the operator \(-\Delta + M\) is translation invariant, and the \( L_{w}^{\infty}L_{2}^{2} \) norm is independent of the choice of \( Q \), we may replace \( f \) by any translations of \( f \). In doing so to (114) and using (115), (117), and the fact \( \chi \big|_{Q/2} = 1 \), we obtain
\[
m_{*} \sup_{\omega \in \Omega} \frac{\|\chi^{1/2}T_{h}f\|_{L^{2}(Q)}^{2}}{\|T_{h}f\|_{L^{2}(Q)}} - AC_{\beta,\mu} \|T_{h}f\|_{L^{\infty}L^{2}} \]
\[
\geq m_{*} \sup_{\omega \in \Omega} \frac{\|T_{h}f\|_{L^{2}(Q/2)}^{2}}{\|T_{h}f\|_{L^{2}(Q)}} - AC_{\beta,\mu} \|f\|_{L^{\infty}L^{2}} \]
\[
\geq m_{*} \frac{\|T_{h}f_{\omega_{0}}\|_{L^{2}(Q/2)}^{2}}{\|f\|_{L^{\infty}L^{2}}} - AC_{\beta,\mu} \|f\|_{L^{\infty}L^{2}} \]
\[
\geq \left( \frac{m_{*}}{24} - AC_{\beta,\mu} \right) \|f\|_{L^{\infty}L^{2}}. \] (119)
It follows by translation invariance of $-\Delta + M$ and $Q$-independence of the $L^\infty_\omega L^2_x$ norm, (88), (114), (118), and (119),

$$\|(\Delta + M)f\|_{L^\infty_\omega L^2_x} = \|(\Delta + M)T_h f\|_{L^\infty_\omega L^2_x}$$

$$\geq \sup_{\psi \in \Omega} \langle \psi, (\Delta + M)T_h f \rangle_{L^2(Q)}$$

$$\geq \left( \frac{m_*}{16} - C_{\beta, \mu} (Q)^{-1} \right) \| f \|_{L^\infty_\omega L^2_x}.$$ (120)

This proves Theorem 4.

5 Nonlinear estimate

Proof of Theorem 5. By the resolvent identity in (46) and using the Cauchy-integral, we arrive at an explicit formula for $N$ (see (26)):

$$N(\varphi) := \text{den} \oint (z - (-\Delta - \varphi))^{-1} \varphi (z + \Delta)^{-1} + M \varphi,$$ (121)

where $\oint$ is defined through (45).

Applying the resolvent identity (46) to (121) repeatedly with $A = -\Delta - \varphi$ and $B = -\Delta$, we arrive at

$$N(\varphi) = \sum_{n \geq 2} (-1)^{n-1} \oint \text{den} (z + \Delta)^{-1} (\varphi (z + \Delta)^{-1})^n,$$ (122)

whenever the series converges in $L^\infty_\omega L^2_x$. Our goal is to estimate the difference in the individual $n$-th order nonlinearities. That is, let

$$N_n(\varphi) := (-1)^{n-1} \oint \text{den} (z + \Delta)^{-1} (\varphi (z + \Delta)^{-1})^n.$$ (123)

We would like to estimate $N_n(\varphi_1) - N_n(\varphi_2)$. To do so, we use

$$a^b - b^n = (a - b)b^{n-1} + a(a - b)b^{n-2} + \cdots + a^{n-1}(a - b).$$ (124)

Applying this to the $n$-fold products of resolvents in $N_n(\varphi_1)$ and $N_n(\varphi_2)$, and writing out the first term explicitly, we see that

$$N_n(\varphi_1) - N_n(\varphi_2)$$

$$=(-1)^{n-1} \oint \text{den} (z + \Delta)^{-1} \left( (\varphi_1 (z + \Delta)^{-1})^n - (\varphi_2 (z + \Delta)^{-1})^n \right)$$ (125)

$$=(-1)^{n-1} \oint \text{den} (z + \Delta)^{-1} (\varphi_1 - \varphi_2)(z + \Delta)^{-1}(\varphi_\# (z + \Delta)^{-1})^{n-1}$$ (126)

$$+ n - 1 \text{ similar terms}$$ (127)
in the $L_\infty^\infty L_2^2$-norm, where $\varphi_\#$ denotes $\varphi_1$ or $\varphi_2$. Let $g_z(x - y)$ be the integral kernel of $(z + \Delta)^{-1}$ as in (49). Then the $n$-th order (difference in) nonlinearity (125) becomes

$$(N_n(\varphi_1) - N_n(\varphi_2))(x) = (-1)^{n-1} \oint dy_1 \cdots dy_n g_z(y_1) g_z(y_1 - y_2) \cdots g_z(y_{n-1} - y_n) g_z(y_n)$$

$$\times (\varphi_1 - \varphi_2)(x - y_1) \prod_{i=2}^n \varphi_\#(x - y_i)$$

$$+ n - 1 \text{ similar terms.}$$

We may take the sup-norm on the factor $\prod_{i=2}^{n-1} \varphi_\#(x - y_i)$. Using the notation $\|f\|$ in (45), we see that

$$|N_n(\varphi_1) - N_n(\varphi_2)|$$

$$\leq \|\varphi_\#\|_{L_{\infty}^1(\Omega)}^{n-1} \oint dy_1 \cdots dy_n |g_z(y_1)| \varphi_1 - \varphi_2|(x - y_1) (|g_z| * \cdots * |g_z|)(y_1)$$

$$+ n - 1 \text{ similar terms}$$

$$= \|\varphi_\#\|_{L_{\infty}^1(\Omega)}^{n-1} \oint k_z |\varphi_1 - \varphi_2|,$$  \hspace{1cm} (128)

where $k_z(x) := |g_z|(x) (|g_z| * \cdots * |g_z|)(x)$. It follows by (128) that

$$\|N_n(\varphi_1) - N_n(\varphi_2)\|_{L^2(Q)} \leq \|\varphi_\#\|_{L_{\infty}^1(\Omega)}^{n-1} \oint \|k_z \|_{L^2(Q)} \|\varphi_1 - \varphi_2\|_{L^2(Q)}.$$  \hspace{1cm} (129)

By Hölder’s inequality, we note that

$$\|k_z \|_{L^2(Q)}^2 = \int_Q dx \left( \int_{\mathbb{R}^3} dy k_z(x - y) |\varphi_1 - \varphi_2|(y) \right)^2$$

$$\leq \int_Q dx \|k_z\|_{L^1(\mathbb{R}^3)} \int_{\mathbb{R}^3} dy k_z(x - y) |\varphi_1 - \varphi_2|^2(y)$$

$$= \|\varphi_1 - \varphi_2\|_{L^2(Q)}^2 \|k_z\|_{L^1(\mathbb{R}^3)}.$$  \hspace{1cm} (130)

Combining (129) and (130), we arrive at

$$\|N_n(\varphi_1) - N_n(\varphi_2)\|_{L^2(Q)} \leq \|\varphi_\#\|_{L_{\infty}^1(\Omega)}^{n-1} \|\varphi_1 - \varphi_2\|_{L^2(Q)} \oint \|k_z\|_{L^1(\mathbb{R}^3)}.$$  \hspace{1cm} (131)

Finally, by definition of $k_z$ below equation (128) and repeated applications of Young’s inequality, we note that

$$\|k_z\|_{L^1(\mathbb{R}^3)} \leq \|g_z\|_{L^2(\mathbb{R}^3)}^2 \|g_z\|_{L_{\infty}^1(\mathbb{R}^3)}^{n-1},$$  \hspace{1cm} (132)
Define
\[ C_{\beta,\mu,n} := \left( \left| \oint g \right|_{L^2(\mathbb{R}^3)} \right)^{1/n} < \infty. \tag{133} \]

We note that \( C_{\beta,\mu,n} \) is bounded for given \( \beta \) and \( \mu \) fixed, uniformly in \( n \). Thus, (131) and the Sobolev inequality show
\[ \| N_n(\varphi_1) - N_n(\varphi_2) \|_{L^2(Q)} \leq C_{\beta,\mu,n}^n \left( \| \varphi_1 \|_{H^2(Q)}^{n-1} + \| \varphi_2 \|_{H^2(Q)}^{n-1} \right) \| \varphi_1 - \varphi_2 \|_{H^2(Q)}. \tag{134} \]

By (122), (134), and the assumption that \( \| \varphi_\# \|_{L^\infty(Q)} < \frac{1}{10} \sup_n C_{\beta,\mu,n}^{-1} \) for \( \# = 1 \) and 2, we complete the proof of Equation (31) of Theorem 5. \( \square \)

## A Stationary norms

We briefly outline properties of the norms used in this article and provide a definition to denote for the sake of completeness. A more in depth study can be found in Sections 2 and 3 of [4]. Let \( \mathcal{L} \) denote a Bravais lattice in \( \mathbb{R}^3 \) and \( Q \) its fundamental domain (for example, the Wigner-Seitz cell). We will often suppress the dependence on \( \omega \in \Omega \) for notation clarify (where \( \Omega \) is the probability space). For \( \ell \in \mathbb{R}^3 \) and \( f_\omega(x) = f(\omega,x) \) a measurable function on \( \Omega \times Q \), given an ergodic measure preserving \( \mathcal{L} \)-action \( \tau \) on \( \Omega \), let \( U_\ell \) denote the ergodic translation operator
\[ (U_\ell f_\omega)(x) := f_{\tau_\ell \omega}(x - \ell). \tag{135} \]

Recall from definition 1 that a function \( f \in L^p_\omega L^q_\ell \) is said to be \( (\mathcal{L}) \) stationary if
\[ U_\ell f = f. \tag{136} \]

**Lemma 9.** Let \( f \in L^p_\omega L^q_\ell \) and \( 1 \leq p, q \leq \infty \), the \( L^p_\omega L^q_\ell \) norm is independent of the location of the fundamental domain \( Q \).

**Proof.** Let \( \tau \) denote the ergodic measure preserving map on \( \Omega \). It suffices to note that \( h(\omega) = \| f_\omega \|_{L^q(Q)} \) is stationary:
\[ \| f_{\tau_\ell \omega} \|_{L^q(Q)} = \| f_\omega \|_{L^q(T_\ell Q)}, \tag{137} \]
where \( T_\ell(x) = x + \ell \) is the shift by \( \ell \). Since \( \tau_\ell \) is ergodic, measure preserving, we see that
\[ \mathbb{E} \| f_\omega \|_{L^q(Q)}^p = \mathbb{E} \| f_\omega \|_{L^q(T_\ell Q)}^p \tag{138} \]
for any \( \ell \in \mathbb{R}^3 \). \( \square \)
A random operator, $A$, on $L^2(\mathbb{R}^3)$ is said to be ($\mathcal{L}$) stationary if $A$ commutes with $U_\ell$ for all $\ell \in \mathbb{R}^3$. Let $\text{Tr}$ denote the usual trace on $L^2(\mathbb{R}^3)$. Given a random operator $A$, its density $\text{den} A$ is a measurable function on $\Omega \times Q$, if it exists, defined via the Riesz representation theorem and the formula

$$E \text{Tr} f A = E \int_{\mathbb{R}^3} f \text{den} A,$$

for all simple $C^\infty_c(\mathbb{R}^3)$-valued function $f$. That is, $f$ is of the form

$$f = \sum_{\alpha} I_{S_\alpha} f_\alpha$$

where the sum is a finite sum over $\alpha$, $I_{S_\alpha}$ is the indicator function of some measurable set $S_\alpha \subset \Omega$, and $f_\alpha$ is a $C^\infty_c(\mathbb{R}^3)$ function. Moreover, the $f$ on the left hand side of (139) is regarded as a multiplication operator on $L^2(\mathbb{R}^3)$. When $A$ has an integral kernel $A(x, y)$ a.s., that is

$$(Af)(x) = \int_{\mathbb{R}^3} A(x, y)f(y)dy,$$

then,

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

whenever $A(x, x)$ is defined and unambiguous.

We outline a few special cases used in the paper where $\text{den} A$ is defined. Define trace per volume $Q$ via

$$\text{Tr}_Q A := \frac{1}{|Q|} \text{Tr} 1_Q A 1_Q,$$

where $1_Q$ is the indicator function of $Q$. If $A$ is stationary, $\text{Tr}_Q$ is independent of translates of $Q$. For $1 \leq p, q \leq \infty$, there is a family of stationary Schatten spaces $L^q_\omega \mathcal{S}^p$ associated to $\text{Tr}_Q$, given via the completions of

$$L^q_\omega \mathcal{S}^p = \{A_\omega \in \mathcal{B}(L^2(\mathbb{R}^3)) \text{ and stationary : } \|A_\omega\|_{L^2 \mathcal{S}^p} < \infty\}$$

with the norm

$$\|A\|_{L^q_\omega \mathcal{S}^p}^q = E \left(\text{Tr}_Q (A^* A)^{p/2}\right)^{q/p}.$$  (145)

If $p$ or $q = \infty$, the usual sup norm is assumed. We remark that the usual (nonrandom) Schatten norm for operators on $X \subset \mathbb{R}^3$ is given as

$$\|A\|_{\mathcal{S}^p(X)}^p = \text{Tr} 1_X (A^* A)^{p/2} 1_X,$$  (146)

where $1_X$ is the indicator function on $X$.

Let $R = (1 - \Delta)^{-1}$. We have the following result.
Lemma 10. Suppose that $A \in L^\infty_\omega \mathbb{S}^2$, then $\text{den} AR$ and $\text{den} RA \in L^\infty_\omega L^2_x$. Moreover,

$$\|\text{den} AR\|_{L^\infty_\omega L^2_x} \|\text{den} RA\|_{L^\infty_\omega L^2_x} \lesssim \|A\|_{L^\infty_\omega \mathbb{S}^2}. \quad (147)$$

Proof. We prove the case for $RA$ only. The case for $AR$ is treated similarly. We use the $L^2(Q)$-$L^2(Q)$ duality. Let $\varphi \in L^2(Q)$ and apply Hölder’s inequality to

$$\text{Tr} 1_Q (\varphi R) A 1_Q \leq \|\varphi R\|_{\mathbb{S}^2(\mathbb{R}^3)} \|A 1_Q\|_{\mathbb{S}^2(\mathbb{R}^3)}. \quad (148)$$

Since $\frac{3}{2} < 2$ and we are in dimension 3, the Kato-Seiler-Simon inequality shows

$$\text{Tr}_Q [(\varphi R) A] \lesssim \frac{1}{|Q|} \|\varphi\|_{L^2(Q)} \|A 1_Q\|_{\mathbb{S}^2(\mathbb{R}^3)}. \quad (149)$$

Since

$$\frac{1}{|Q|} \|A 1_Q\|_{\mathbb{S}^2(\mathbb{R}^3)} = \frac{1}{|Q|} \text{Tr} 1_Q A^* A 1_Q = \|A\|_{\mathbb{S}^2(Q)}^2, \quad (150)$$

we see that

$$\text{Tr}_Q [(\varphi R) A] \lesssim \|\varphi\|_{L^2(Q)} \|A\|_{\mathbb{S}^2(Q)}. \quad (151)$$

The $L^2(\Omega)$-$L^2(\Omega)$ duality and the Riesz representation theorem show that there is some $\text{den} RA \in L^2(\Omega)$ such that

$$\frac{1}{|\Omega|} \int_{\Omega} \varphi \text{den}(RA) = \text{Tr}_Q \varphi RA \quad (152)$$

for all $\varphi \in L^2(Q)$ and

$$\|\text{den} RA\|_{L^2(Q)} \lesssim \|A\|_{\mathbb{S}^2(Q)}. \quad (153)$$

Since we have not specified the dependence of $A$ on $\omega$, we see that (152) and (153) hold for all $\omega$ a.s.. In particular, $\text{den} RA_\omega$ is well defined for a.e. $\omega$. Taking sup$_{\omega \in \Omega}$ in (153) in, we see that (147) is proved. \hfill \Box

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