On the excess charge problem in relativistic quantum mechanics

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Zusammenfassung

Wir untersuchen wie viele Elektronen ein Atom der Kernladungszahl Z binden kann. Dieses ist ein klassisches Problem der mathematischen Physik. Experimentell ist die Überschussladung $Q := N-Z$ höchstens Eins. Ziel dieser Arbeit ist es, eine obere Schranke mathematisch für realistische Modelle großer Atome (Z groß) herzuleiten. Für große Z sind relativistische Modelle wesentlich. Wir untersuchen zwei Modelle.

Das erste Modell wurde von Brown und Ravenhall vorgeschlagen. Während nichtrelativistische Modelle detailliert untersucht wurden, ist im Brown-Ravenhall-Modell nicht einmal klar, dass Q beschränkt ist. Um eine solche Schranke zu gewinnen, folgen wir eine Strategie von Benguria. Wir integrieren die Euler-Lagrange-Gleichung gegen das Moment $|x|$, was in der nichtrelativistischen Quantenmechanik erfolgreich angewendet wurde. Der Hauptunterschied liegt im Coulomb-Potential-Term. In der Schrödinger-Theorie ist$|x|\frac{Z}{|x|}$ konstant. Aber in unserem Fall ist der entsprechende Term $\Lambda^+|x|\Lambda^+\frac{Z}{|x|}\Lambda^+$, was keine Konstante mehr ist. Dabei bezeichnet Λ^+ die Projektion auf den positiven Spektralraum von D_0. Unser erstes Hauptergebnis ist, eine obere Schranke an dieses Operators. Im masselosen Fall zeigen wir sowohl eine positive obere als auch eine positive untere Schranke. Im massiven Fall zeigen wir die Existenz der positiven oberen Schranke.

Im zweiten Teil haben wir Schranken an Q sowohl in der zeitabhängigen nichtrelativistischen Thomas-Fermi-Weizsäcker-Theorie, der zeitabhängigen relativistischen Thomas-Fermi-Theorie als auch in der zeitunabhängigen relativistischen Thomas-Fermi-Weizsäcker-Theorie hergeleitet und bewiesen. Das Thomas-Fermi-Funktional ist ein approximatives Energiefunktional, das von der Teilchendichte ρ abhängt. Der Weizsäcker-Term ist die führende Korrektur zur Thomas-Fermi-Theorie. In der nichtrelativistischen TFW-Theorie wurde die Ionisierungsvermutung von Benguria und Lieb bewiesen.

Wir zeigen zunächst, dass auch im relativistischen Fall die Energie nach unten beschränkt ist. Mithilfe diese Resultats zeigen wir die Existenz eines Minimierers und damit die Existenz einer Lösung, wenn N hinreichend klein ist. Um eine Schranke an Q zu gewinnen, verwenden wir dieselbe Idee wie im ersten Teil. Wir integrieren die Euler-Lagrange-Gleichung gegen das Moment $|x|$ multipliziert mit einer Funktion der Dichte. In diesem Fall ist die Anzahl der Elektronen N kleiner als CZ, wo C ungefähr 2,56 ist.

Abstract

We investigate how many electrons an atom of atomic number Z can bind. This is a classic problem of mathematical physics. Experimentally, the excess charge $Q := N - Z$ is at most one. The aim of this work is to derive an upper bound mathematically for realistic models of large atoms (Z large). For large Z, relativistic models are essential. We investigate two models.

The first model was proposed by Brown and Ravenhall. While non-relativistic models have been studied in detail, it is not even clear in the Brown-Ravenhall model whether Q is bounded. To gain such a bound, we follow a strategy by Benguria. We integrate the Euler-Lagrange equation against the moment $|x|$, which has been successfully applied in non-relativistic quantum mechanics. The main difference lies in the Coulomb potential term. In the Schrödinger theory, $|x|\frac{Z}{|x|}$ is a constant. But in our case the corresponding term is $\Lambda^+|x|\Lambda^+\frac{Z}{|x|}\Lambda^+$, which is no longer a constant. Where Λ^+ denotes the projection onto the positive spectral subspace of D_0. Our first major result is an upper bound of this operator. In the massless case, we show that there is both positive lower and upper bounds. In the massive case, we show the existence of the positive upper bound.

In the second part, we have derived and proved the bounds of Q in both the time-dependent non-relativistic Thomas-Fermi-Weizsäcker theory and the time-dependent relativistic Thomas-Fermi theory as well as in the relativistic time-independent Thomas-Fermi-Weizsäcker theory. The Thomas-Fermi functional is an approximate energy functional that depends on particle density. The Weizsäcker term is the leading correction to the Thomas-Fermi theory. In the non-relativistic TFW theory, the ionization conjecture was proved by Benguria and Lieb.

We first show that in the relativistic case the energy is bounded from below. Using this result, we show the existence of a minimizer and thus the existence of a solution when N is sufficiently small. To gain a bound on Q, we use the same idea as in the first part. We integrate the Euler-Lagrange equation against the moment $|x|$ multiplied by a function of density. In this case, the number of electrons N is smaller than CZ, where C is about 2.56.

Chapter 1

Introduction

1.1 The excess charge problem

The question, how many electrons an atom or molecule can bind, has been studied by many scientists. This is a classic problem of mathematical physics. But the question itself is still open (Lieb and Seiringer [21, p. 228]).

In this dissertation, we only investigate the system of one atom. The nucleus has charge Z. N is the number of electrons which the nucleus can bind. Then the excess charge is

$$Q := N - Z. \tag{1.1}$$

Experimentally, it is at most one. In many-body Schrödinger theory, many authors have studied this problem. The many-body Hamiltonian for N electrons is

$$H_N = \sum_{i=1}^{N} T_i - \alpha Z \sum_{i=1}^{N} \frac{1}{|x_i|} + \alpha \sum_{1 \le i < j \le N} \frac{1}{|x_i - x_j|}. \tag{1.2}$$

The first term sum of T_i is the kinetic energy of the electrons. We neglect the magnetic field in this dissertation. In the non-relativistic case, it is

$$T_{nonrel} = \frac{1}{2} p^2, \tag{1.3}$$

where $p := |\mathfrak{p}|$ and $\mathfrak{p} = \frac{1}{i}\nabla$ is the canonical momentum of the electron. In a simple relativistic case given by Chandrasekhar, it is

$$T_{rel} = \sqrt{p^2 + m^2} - m \tag{1.4}$$

for some $m > 0$ which is the mass of an electron. The second term is the electron-nucleus attractive Coulomb interaction. The electrons are located at $x_i \in \mathbb{R}^3$ for $i = 1, \ldots, N$. The nucleus is located at origin. The constant α is the fine-structure constant. The third term is the electron-electron repulsive interaction. The operator acts on wave functions $\psi \in \bigwedge^N L^2(\mathbb{R}^3; \mathbb{C}^q)$, where q is the number of spin states per electron. The energy is

$$\mathcal{E}_N(\psi) := (\psi, H_N \psi). \tag{1.5}$$

If the infimum of it

$$E_0(N) := \inf\left\{\mathcal{E}_N(\psi) : \int\limits_{\mathbb{R}^3} |\psi(x)|^2 \mathrm{d}x = 1\right\} \tag{1.6}$$

is also a minimum, then E_0 is called the ground state energy. The atom can bind N electrons if $E_0(N) < E_0(N-1)$. By the HVZ theorem (Hunziker [16], Winter [36], Zhislin [38]), the essential spectrum of H_N starts at the ground state energy of H_{N-1}, i.e., $\inf \sigma_{ess}(H_N) = \inf H_{N-1} = E_0(N-1)$. So $E_0(N) < E_0(N-1)$ is equivalent to $E_0(N) < \inf \sigma_{ess}(H_N)$. This means $E_0(N)$ is an eigenvalue.

In the non-relativistic case, the following results are known. Sigal [33, 32] proved the nonexistence of very negative ions, then showed that negative ions of charge $\leq -18Z$ do not exist. Ruskai [29, 30] had showed that $Q \leq cZ^{\frac{6}{5}}$ for some constant c. Lieb [19] showed that $Q < Z + 1$. Later, Lieb, Sigal, Simon, and Thirring [22] proved that $\lim\limits_{Z\to\infty} \frac{N}{Z} = 1$, i.e., $\lim\limits_{Z\to\infty} \frac{Q}{Z} = 0$. Fefferman and Seco [13] proved that $Q = O(Z^\alpha)$ for $\alpha = \frac{47}{56}$. Using the key estimate of their work, Seco, Solovej, and Sigal [31] also gave a bound of the ionization energy. Several years ago, Nam [25] gave a new bound $Q < 0.22Z + 3Z^{1/3}$.

In the relativistic case, the best bound is still $Q < Z+1$ (Lieb and Seiringer [21, p. 229]). It is much more difficult than the non-relativistic problem. The bound $Q < c$ from numerical estimates and experiment observations is still not proved.

The works we introduced above are all time-independent. In the time-dependent setting the definition of the maximal number of electrons is defined by the evolution of the density. We say the atom can bind at least N electrons, if there exists a measurable and bounded subset B of $\mathbb{R}^3$, such that for all positive times t

$$\int\limits_B \mathrm{d}x \rho_t(x) \geq N. \tag{1.7}$$

The maximal number of electrons which the atom can bind is the supremum over all such N. Lenzmann and Lewin [18], inspired by the Rage Theorem (see, e.g., Perry [27, Theorem 2.1]), considered the time average of the number of electrons in any finite ball for long times in the Hartree approximation. They proved

$$\limsup_{T\to\infty} \frac{1}{T} \int\limits_0^T \mathrm{d}t \int\limits_B \mathrm{d}x \rho_t(x) \leq 4Z \tag{1.8}$$

for all balls B of finite radius, where ρ_t is the ground state density, i.e., according to the above definition, $N \leq 4Z$. L. Chen and Siedentop [5] proved the same bounds in the Thomas-Fermi and the Vlasov model.

1.2 Brown-Ravenhall Operators

We focus on the relativistic problems in the dissertation. We estimate the excess charge in two different models. The first one is the Brown-Ravenhall model.

The Dirac operator [6, 7] is a relativistic generalization of Schrödinger's kinetic energy operator. It is a differential operator that is a formal square root of $-\Delta$. The Dirac operator without any magnetic field is given by

$$D_0 = \boldsymbol{\alpha} \cdot \mathfrak{p} + \beta m, \tag{1.9}$$

where $\boldsymbol{\alpha} = (\alpha^1, \alpha^2, \alpha^3)$ and β are 4×4 matrices. A particular representation is

$$\alpha^i = \begin{pmatrix} 0 & \sigma^i \\ \sigma^i & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} \mathbb{I}_{\mathbb{C}^2} & 0 \\ 0 & \mathbb{I}_{\mathbb{C}^2} \end{pmatrix}, \tag{1.10}$$

where σ^i are Pauli matrices. Different from $p = |\mathfrak{p}|$, the Dirac operator is a local operator. The Hamiltonian for relativistic electrons

$$H_N = \sum_{i=1}^{N} D_{0,i} - \alpha Z \sum_{i=1}^{N} \frac{1}{|x_i|} + \alpha \sum_{1 \le i < j \le N} \frac{1}{|x_i - x_j|} \tag{1.11}$$

is not bounded from below. So there is not ground state energy. Brown and Ravenhall [4] showed that, for $N \ge 2$, the spectrum of H_N is the whole real line, and there would be no eigenvalue. They offered a solution of this unphysical behavior using the projection Λ^+ onto the positive spectral subspace of D_0. Then the electron wave function can only live in this positive energy subspace. The projection is given by

$$\Lambda_+ = \frac{1}{2}\left(1 + \frac{\alpha \cdot \mathfrak{p} + m\beta}{\sqrt{p^2 + m^2}}\right). \tag{1.12}$$

Since the many-body model is too complicated for our investigation. We use the reduced Hartree-Fock theory. The energy is

$$\mathcal{E}_Z^{BR}(\psi) = \sum_{i=1}^{N} \left(\psi_i, \Lambda_+ \left(D_0 - \alpha \frac{Z}{|x|} + \frac{\alpha}{2} \int_{\mathbb{R}^3} \mathrm{d}y \frac{\rho(y)}{|x-y|}\right) \Lambda_+ \psi_i\right), \tag{1.13}$$

where $\psi_i \in H^{1/2}(\mathbb{R}^3; \mathbb{C}^4)$, $\psi_1, ..., \psi_N$ orthonormal, and $\rho(x) = \sum_{i=1}^{N} |\psi_i(x)|^2$. So the ground state energy in Brown-Ravenhall model is

$$E_Z^{BR}(N) := \inf\left\{\mathcal{E}_Z^{BR}(\psi) : \int_{\mathbb{R}^3} |\psi_i(x)|^2 \mathrm{d}x = 1, \psi_i \in H^{1/2}(\mathbb{R}^3; \mathbb{C}^4), \psi_1, ..., \psi_N \text{ orthonormal in } L^2\right\}. \tag{1.14}$$

The ionization conjecture is

Conjecture 1. *There exists a constant $c > 0$ such that for all $Z > 0$, if $E_Z^{BR}(N)$ has a minimizer, then $Q \le c$.*

Whether Q is bounded in Brown-Ravenhall model is still not clear. The method we want to use here is proposed by Benguria [1], which is integrating the Euler-Lagrange equation against $\psi_i|x|$. We will give an upper bound in this direction. We need two important parts to prove that $N < cZ$.

Theorem 1. *For Λ_+ given in (1.12), we have*

$$2\Lambda_+ < \Lambda_+|x|\Lambda_+\frac{1}{|x|}\Lambda_+ + \Lambda_+\frac{1}{|x|}\Lambda_+|x|\Lambda_+ < \frac{8}{3}\Lambda_+, \quad m = 0 \tag{1.15}$$

and

$$\Lambda_+|x|\Lambda_+\frac{1}{|x|}\Lambda_+ + \Lambda_+\frac{1}{|x|}\Lambda_+|x|\Lambda_+ < \frac{8}{3}\Lambda_+, \quad m \neq 0. \tag{1.16}$$

The second part is

Conjecture 2. *This a constant c, such that*

$$c\Lambda_+ < \Lambda_+|x|\Lambda_+\int_{\mathbb{R}^3} \mathrm{d}y\frac{\rho(y)}{|x-y|}\Lambda_+ + \Lambda_+\int_{\mathbb{R}^3} \mathrm{d}y\frac{\rho(y)}{|x-y|}\Lambda_+|x|\Lambda_+. \tag{1.17}$$

Theorem 1 is the first main result we will show in this dissertation. The corresponding inequality in Schrödinger theory is trivial. Because there is no projection in between, $\Lambda_+|x|\Lambda_+\frac{1}{|x|}\Lambda_+$ just becomes $|x|\frac{1}{|x|}$, which is a constant. The Conjecture 2 is still unsolved. We are even not very confident that it is correct. If it is proved, then the bound $N < cZ$ should be also correct.

1.3 Thomas-Fermi-Weizsäcker theory

Thomas-Fermi theory [35, 14] is the earliest density functional theory. Compared to many-body Schrödinger theory, it is a semiclassical approximation and is conjectured a lower bound of the total energy (Lieb and Seiringer [21, p. 127]). But the electron density behaves incorrect when it is very close and very far from nucleus (Benguria, Brézis, and Lieb [2]). Weizsäcker added a gradient term as a leading order correction to the kinetic energy. Benguria and Lieb proved $Q < 0.7335$ in Thomas-Fermi-Weizsäcker theory [3]. A second order correction to Thomas-Fermi theory is given by Dirac [8]. The energy in Thomas-Fermi-Dirac-Weizsäcker theory is

$$\begin{aligned}\mathcal{E}_Z^{TFDW}(\rho) =& \frac{3}{10}\gamma_{TF}\int_{\mathbb{R}^3}\rho^{\frac{5}{3}}(x)\mathrm{d}x - \int_{\mathbb{R}^3}\frac{Z\rho(x)}{|x|}\mathrm{d}x + \frac{1}{2}\iint_{\mathbb{R}^3\times\mathbb{R}^3}\frac{\rho(x)\rho(y)}{|x-y|}\mathrm{d}x\mathrm{d}y \\ &+ c^W\int_{\mathbb{R}^3}|\nabla\sqrt{\rho(x)}|^2\mathrm{d}x - c^D\int_{\mathbb{R}^3}\rho^{\frac{4}{3}}(x)\mathrm{d}x,\end{aligned} \tag{1.18}$$

where $\gamma_{TF} := (\frac{6\pi^2}{q})^{\frac{2}{3}}$, c^W and c^D are positive constants. The ionization conjecture for the non-relativistic TFW theory was proved by Frank, Nam, and van den Bosch [15].

In the non-relativistic time-dependent TF theory, L. Chen and Siedentop proved that an atom of atomic number Z cannot bind more than $4Z$ electrons. We prove the same result in the non-relativistic time-dependent TFW theory. We also consider the problem in the relativistic case. But in that case, we drop the Weizsäcker term.

The relativistic Thomas-Fermi-Dirac-Weizsäcker model was derived by Engel and Dreizler [9, 10]. But we only use the Dirac term in some parts. The energy of the relativistic Thomas-Fermi-Weizsäcker model is

$$\begin{aligned}
&\mathcal{E}_Z^{rTFW}(p) = \\
&\frac{1}{8\pi^2}\int \mathrm{d}x \Bigg(p(x)\sqrt{p^2(x)+m^2}(2p^2(x)+m^2) - m^4 \operatorname{arsinh}\left(\frac{p(x)}{m}\right) - \frac{8}{3}mp^3(x) \\
&+ 3\lambda(\nabla p(x))^2 \frac{p(x)}{\sqrt{p^2(x)+m^2}}\left(1 + 2\frac{p(x)}{\sqrt{p^2(x)+m^2}} \operatorname{arsinh}\left(\frac{p(x)}{m}\right)\right) \\
&- \frac{8\alpha Z p^3(x)}{3|x|} + \frac{4\alpha}{9\pi^2}\int \mathrm{d}y \frac{p^3(x)p^3(y)}{|x-y|}\Bigg),
\end{aligned} \tag{1.19}$$

where $p = (c_{TF}\rho)^{\frac{1}{3}}$ and $c_{TF} := 3\pi^2$ in this theory. The function p is in the following space

$$p \in P := \{p | p \in L^4 \bigcap H^1, D[p^3] < \infty, \|\nabla F(p)\|_2 < \infty\}, \tag{1.20}$$

where $F(p)$ is given in (3.39). The first main result is

Theorem 2. *For any $Z > 0$, the energy $\mathcal{E}_Z^{rTFW}$ has a global minimizer $p_0 \in P := \{p|p \in L^4 \bigcap H^1, D[p^3] < \infty, \|\nabla F(p)\|_2 < \infty\}$, $N := \frac{1}{c_{TF}}\int p_0^3(x)\mathrm{d}x$. The excess charge Q satisfies $Q < 1.56Z$.*

The second main result is

Theorem 3. *For $\kappa := \frac{Z}{c}$ fixed, $N \le 2Z + CZ^{\frac{3}{4}}$.*

The method to prove Theorem 2 follows Benguria's idea: We integrate the Euler-Lagrange equation against $\psi_i|x|$. The method to prove Theorem 3 follows Frank, Nam, and van den Bosch [15], which they use in the non-relativistic TFDW theory. In the non-relativistic case, the bound derived by this method is much better than $Z + 1$, which is derived by Benguria's method. But in our relativistic case, there are several disadvantages which we can not handle them very well, so that the constant C may be very large, i.e., $Z + CZ^{\frac{3}{4}}$ could be much larger than $1.56Z$.

1.4 Structure of the Dissertation

In Chapter 2, we discuss the excess charge problem in the reduced Hartree-Fock approximation of the Brown-Ravenhall model. We convert the problem to Fourier space, then decompose the operator using spherical spinors. Then we give a proof of Theorem 1 and look ahead how to prove Conjecture 1.

In Section 3.1 and 3.2 we present the bounds of the excess charge for the time-dependent non-relativistic TFW theory and the time-dependent relativistic TF theory. In the rest of Chapter 3, we deal with the time-independent relativistic TFW theory. First we prove that the energy can be bounded from below by N and $D[\rho]$. Then we show the existence of a global minimizer. Finally, we show two different bounds of excess charge Q.

In the appendices, we prove the positivity of two functions used in our investigation of the Brown-Ravenhall theory.

Chapter 2

Inequality in Brown-Ravenhall Model

2.1 Ionization Conjecture

Here we give the idea to prove the bound $N < cZ$. Since $E_Z^{BR}(N)$ has a minimizer, there are eigenfunctions $\psi_i \in \Lambda^+ L^2(\mathbb{R}^3;\mathbb{C}^4)$ and $\|\psi_i\|_2 = 1$ such that

$$\Lambda^+ \left(D_0 - \alpha \frac{Z}{|x|} + \alpha \int_{\mathbb{R}^3} \mathrm{d}y \frac{\rho(y)}{|x-y|} \right) \psi_i = \lambda_i \psi_i. \tag{2.1}$$

The eigenvalues λ_i are less than m. The main strategy is mentioned before. We multiply the Euler-Lagrange equation by $\psi_i |x|$ and integrate. So we have

$$\sum_{i=1}^{N} \left(\psi_i, |x| \Lambda_+ \left(D_0 - \alpha \frac{Z}{|x|} + \alpha \int_{\mathbb{R}^3} \mathrm{d}y \frac{\rho(y)}{|x-y|} - \lambda_i \right) \psi_i \right) = 0. \tag{2.2}$$

The bound of the first summand is known (Lieb [19]).

$$\Re \left(\psi_i, |x| \Lambda_+ \left(D_0 - m \right) \psi_i \right) = \Re \left(\psi_i, |x| (\sqrt{p^2 + m^2} - m) \psi_i \right) > 0. \tag{2.3}$$

The control of the second term is from our Theorem 1.

$$- \Re \alpha Z \sum_{i=1}^{N} \left(\psi_i, |x| \Lambda_+ \frac{1}{|x|} \psi_i \right) > -\frac{4}{3} \Re \alpha Z \sum_{i=1}^{N} \left(\psi_i, \psi_i \right) = -\frac{4}{3} \alpha Z N. \tag{2.4}$$

We also need to build a relation between the third term and N^2. That is why we want to solve the Conjecture 2. From Conjecture 2, we have

$$\alpha \Re \sum_{i=1}^{N} \left(\psi_i, |x| \Lambda_+ \int_{\mathbb{R}^3} \mathrm{d}y \frac{\rho(y)}{|x-y|} \psi_i \right) > \frac{c\alpha}{2} N^2. \tag{2.5}$$

Combining the three inequalities (2.3), (2.4), and (2.5), we have $-\frac{4}{3}\alpha ZN + \frac{\alpha c}{2}N^2 < 0$, i.e.,

$$N < \frac{8}{3c}Z. \tag{2.6}$$

The bound $N < cZ$ is implied by (2.6).

There are two main reasons why we guess Conjecture 2 is correct. The first one is that it is true if there is no projection. This is used in the non-relativistic Schrödinger theory. Using triangle inequality $\frac{|x|+|y|}{|x-y|} \geq 1$, the constant c in Conjecture 2 is 1 in this case. The second reason is Theorem 1. In Theorem 1, we show that the operator $\Lambda_+|x|\Lambda_+\frac{1}{|x|}\Lambda_+ + \Lambda_+\frac{1}{|x|}\Lambda_+|x|\Lambda_+$ has both upper and lower bound. [1] It means that the projection Λ^+ does not change the operator a lot in such form. So we hope the Conjecture 2 is also not so different from the non-relativistic case.

2.2 Problem in Fourier Space

We want to solve the problem in Fourier space, i.e., the $\mathfrak{p}$ space. Because the projection Λ^+ given in (1.12) in Fourier space is just a matrix multiplication operator, it is much easier to deal with than in x space. Then the operator acts on $\phi(\mathfrak{p})$ which is $\phi \in \Lambda^+ L^2(\mathbb{R}^3;\mathbb{C}^4)$. The inequalities in Theorem 1 are equivalent to

$$(\phi,\phi) < \Re(\phi, |x|\Lambda_+\frac{1}{|x|}\phi) < \frac{4}{3}(\phi,\phi), \quad m = 0 \tag{2.7}$$

and

$$\Re(\phi, |x|\Lambda_+\frac{1}{|x|}\phi) < \frac{4}{3}(\phi,\phi), \quad m \neq 0. \tag{2.8}$$

Since ϕ is in the positive spectral subspace, it satisfies

$$\Lambda_+\phi(\mathfrak{p}) = \phi(\mathfrak{p}). \tag{2.9}$$

It can be written as

$$\phi(\mathfrak{p}) = \frac{1}{N(\mathfrak{p})}\begin{pmatrix}(E(\mathfrak{p})+m)u(\mathfrak{p})\\ \sigma\cdot\mathfrak{p}u(\mathfrak{p})\end{pmatrix}, \tag{2.10}$$

where $N(\mathfrak{p}) = \sqrt{2E(\mathfrak{p})(E(\mathfrak{p})+m)}$, $E(\mathfrak{p}) = \sqrt{p^2+m^2}$ (Evans, Perry, and Siedentop [12]). The function $u \in L^2(\mathbb{R}^3;\mathbb{C}^2)$ is a Pauli spinor. We will prove later that the operator $\Lambda_+|x|\Lambda_+\frac{1}{|x|}\Lambda_+$ commutes with the total angular momentum. So we decompose the operator on invariant subspace. For any $\phi \in L^2(\mathbb{R}^3;\mathbb{C}^4)$, not necessarily in the positive subspace, it

[1] Although we only proved this in massless case, we believe that it has the same lower bound in massive case. But this part is not necessary for the bound $N < cZ$. So we did not spend much time on it.

can be written as

$$\begin{aligned}\phi(\mathfrak{p}) &= \sum_{l,m,s}\begin{pmatrix}\frac{f_{l,m,s}(p)}{p}\Omega_{l,m,s}(\omega_{\mathfrak{p}})\\ \frac{g_{l,m,s}(p)}{p}\Omega_{l,m,s}(\omega_{\mathfrak{p}})\end{pmatrix}\\ &= \sum_{l,m,s}\begin{pmatrix}\frac{f_{l,m,s}(p)}{p}\Omega_{l,m,s}(\omega_{\mathfrak{p}})\\ \frac{g_{l+2s,m,-s}(p)}{p}\Omega_{l+2s,m,-s}(\omega_{\mathfrak{p}})\end{pmatrix}\\ &=: \sum_{l,m,s}\phi_{l,m,s}(\mathfrak{p})\end{aligned}\tag{2.11}$$

with $l = 0, 1, 2\ldots$, $m = -l - \frac{1}{2}, \ldots, l + \frac{1}{2}$, and $s = -\frac{1}{2}, \frac{1}{2}$, where $p = |\mathfrak{p}|$ and $\omega_p = \frac{\mathfrak{p}}{p}$, $\Omega_{l,m,s}$ are spherical spinors

$$\Omega_{l,m,s}(\omega) := \begin{cases}\begin{pmatrix}\sqrt{\frac{l+s+m}{2(l+s)}}Y_{l,m-\frac{1}{2}}(\omega)\\ \sqrt{\frac{l+s-m}{2(l+s)}}Y_{l,m+\frac{1}{2}}(\omega)\end{pmatrix} & s = \frac{1}{2}\\ \begin{pmatrix}-\sqrt{\frac{l+s-m+1}{2(l+s)+2}}Y_{l,m-\frac{1}{2}}(\omega)\\ \sqrt{\frac{l+s+m+1}{2(l+s)+2}}Y_{l,m+\frac{1}{2}}(\omega)\end{pmatrix} & s = -\frac{1}{2}\end{cases}.\tag{2.12}$$

The $Y_{l,k}$ are normalized spherical harmonics on the unit sphere $\mathbb{S}^2$ (Messiah [24, p. 494]).

2.3 Massless Case

The methods to prove the inequalities in Theorem 1 in the massless and massive case are totally different. As we discussed above, we only need the upper bound to prove the bound $N < cZ$. The proof in massive case also works in massless case. But proving the massless case, we understand the operator $\Lambda_+|x|\Lambda_+\frac{1}{|x|}\Lambda_+ + \Lambda_+\frac{1}{|x|}\Lambda_+|x|\Lambda_+$ better. It describes the exact spectrum of this operator.

In the massless case, the operator is homogeneous in $\mathfrak{p}$. This is a huge advantage comparing to the massive operator. We have $D_0 = \alpha\cdot\mathfrak{p}$ and $\Lambda_+ = \frac{1}{2}\left(1 + \frac{\alpha\cdot\mathfrak{p}}{p}\right)$. The massless inequality (1.15) in Theorem 1 is equivalent to

$$2\Lambda_+ < \Lambda_+|x|\frac{\alpha\cdot\mathfrak{p}}{p}\frac{1}{|x|}\Lambda_+ + \Lambda_+\frac{1}{|x|}\frac{\alpha\cdot\mathfrak{p}}{p}|x|\Lambda_+ < \frac{10}{3}\Lambda_+.\tag{2.13}$$

First we prove the following equation

$$\left(\phi_{l',m',s'}(\mathfrak{p}), |x|\frac{\alpha\cdot\mathfrak{p}}{p}\frac{1}{|x|}\phi_{l,m,s}(\mathfrak{p})\right) = 0, \quad (l',m',s') \neq (l,m,s).\tag{2.14}$$

This implies that the subspace is invariant in the decomposition.

Proof of (2.14). In the massless case, $\phi_{l,m,s}$ in the positive subspace can be written as

$$\phi_{l,m,s}(\mathfrak{p}) = \frac{1}{\sqrt{2}}\begin{pmatrix}u(\mathfrak{p})\\ \frac{\sigma\cdot\mathfrak{p}}{p}u(\mathfrak{p})\end{pmatrix} = \begin{pmatrix}\frac{g(p)}{p}\Omega_{l,m,s}(\omega_p)\\ -\frac{g(p)}{p}\Omega_{l+2s,m,-s}(\omega_p)\end{pmatrix}.\tag{2.15}$$

We start to deal with the operator $|x|\frac{\alpha\cdot\mathfrak{p}}{p}\frac{1}{|x|}$, and only consider $\frac{1}{|x|}$ at the beginning. We have

$$
\begin{aligned}
&\frac{1}{|x|}\frac{g(p)}{p}\Omega_{l,m,s}(\omega_p)\\
=&\frac{1}{(2\pi)^{3/2}}\frac{2\Gamma(1)}{2^{\frac{1}{2}}\Gamma(\frac{1}{2})}\int_{\mathbb{R}^3}\mathrm{d}\mathfrak{q}\frac{1}{|\mathfrak{p}-\mathfrak{q}|^2}\frac{g(q)}{q}\Omega_{l,m,s}(\omega_q)\\
=&\frac{1}{(2\pi)^{3/2}}\frac{2}{2^{\frac{1}{2}}\sqrt{\pi}}\int_{\mathbb{R}^3}\mathrm{d}\mathfrak{q}\sum_{l'=0}^{\infty}\frac{1}{2pq}\frac{2l'+1}{2}\int_{-1}^{1}\mathrm{d}u\frac{P_{l'}(u)}{\frac{1}{2}(\frac{p}{q}+\frac{q}{p})-u}P_{l'}(\cos(\theta))\frac{g(q)}{q}\Omega_{l,m,s}(\omega_q)\\
=&\frac{1}{2\pi^2}\int_{\mathbb{R}^3}\mathrm{d}\mathfrak{q}\sum_{l'=0}^{\infty}\frac{2l'+1}{2pq}Q_{l'}(\frac{1}{2}(\frac{p}{q}+\frac{q}{p}))\sum_{m'=-l'}^{l'}\frac{4\pi}{2l'+1}Y^*_{l',m'}(\omega_q)Y_{l',m'}(\omega_p)\frac{g(q)}{q}\Omega_{l,m,s}(\omega_q)\\
=&\frac{1}{2\pi^2}\int_0^{\infty}\mathrm{d}qq^2\frac{2l+1}{2pq}Q_l(\frac{1}{2}(\frac{p}{q}+\frac{q}{p}))\frac{4\pi}{2l+1}\frac{g(q)}{q}\Omega_{l,m,s}(\omega_p)\\
=&\frac{1}{\pi}I_{g,l}(p)\Omega_{l,m,s}(\omega_p).
\end{aligned}
\tag{2.16}
$$

Q_l is the Legendre function of the second kind. $I_{g,l}$ is defined by

$$
I_{g,l}(p) := \int_0^{\infty}\mathrm{d}q\frac{1}{p}Q_l(\frac{1}{2}(\frac{p}{q}+\frac{q}{p}))g(q). \tag{2.17}
$$

Some formulas about the spherical harmonics we use in (2.16) are in Messiah [23, p. 496]. Then we take $\frac{\alpha\cdot\mathfrak{p}}{p}$ into account. We have

$$
\begin{aligned}
&\frac{\alpha\cdot\mathfrak{p}}{p}\frac{1}{|x|}\begin{pmatrix}\frac{g(p)}{p}\Omega_{l,m,s}(\omega_p)\\ -\frac{g(p)}{p}\Omega_{l+2s,m,-s}(\omega_p)\end{pmatrix}\\
=&\frac{\alpha\cdot\mathfrak{p}}{p}\begin{pmatrix}\frac{1}{\pi}I_{g,l}(p)\Omega_{l,m,s}(\omega_p)\\ -\frac{1}{\pi}I_{g,l+2s}(p)\Omega_{l+2s,m,-s}(\omega_p)\end{pmatrix}=\frac{1}{\pi}\begin{pmatrix}I_{g,l+2s}(p)\Omega_{l,m,s}(\omega_p)\\ -I_{g,l}(p)\Omega_{l+2s,m,-s}(\omega_p)\end{pmatrix}.
\end{aligned}
\tag{2.18}
$$

Then we use the integral formula for (f,pf) (Lieb and Loss [20, p. 184]). So we get

$$\begin{aligned}
&\int_{\mathbb{R}^3} \mathrm{d}\mathfrak{p} \begin{pmatrix} \frac{\overline{g'(p)}}{p}\Omega^*_{l',m',s'}(\omega_p) \\ -\frac{\overline{g'(p)}}{p}\Omega^*_{l'+2s',m',-s'}(\omega_p) \end{pmatrix}^T |x| \frac{\alpha\cdot\mathfrak{p}}{p}\frac{1}{|x|} \begin{pmatrix} \frac{g(p)}{p}\Omega_{l,m,s}(\omega_p) \\ -\frac{g(p)}{p}\Omega_{l+2s,m,-s}(\omega_p) \end{pmatrix} \\
&= \frac{1}{2\pi^3}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \mathrm{d}\mathfrak{p}\mathrm{d}\mathfrak{q} \left(\frac{\overline{g'(p)}}{p}\Omega^*_{l',m',s'}(\omega_p) - \frac{\overline{g'(q)}}{q}\Omega^*_{l',m',s'}(\omega_q) \right) \\
&\qquad \frac{1}{|\mathfrak{p}-\mathfrak{q}|^4}\left(I_{g,l+2s}(p)\Omega_{l,m,s}(\omega_p) - I_{g,l+2s}(q)\Omega_{l,m,s}(\omega_q)\right) \\
&\quad + \frac{1}{2\pi^3}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \mathrm{d}\mathfrak{p}\mathrm{d}\mathfrak{q} \left(\frac{\overline{g'(p)}}{p}\Omega^*_{l'+2s',m',-s'}(\omega_p) - \frac{\overline{g'(q)}}{q}\Omega^*_{l'+2s',m',-s'}(\omega_q) \right) \\
&\qquad \frac{1}{|\mathfrak{p}-\mathfrak{q}|^4}\left(I_{g,l}(p)\Omega_{l+2s,m,-s}(\omega_p) - I_{g,l}(q)\Omega_{l+2s,m,-s}(\omega_q)\right) \\
&=: I_1(\phi_{l',m',s'},\phi_{l,m,s}) + I_2(\phi_{l',m',s'},\phi_{l,m,s}).
\end{aligned} \tag{2.19}$$

Then we decompose $\frac{1}{|\mathfrak{p}-\mathfrak{q}|^4}$,

$$\begin{aligned}
\frac{1}{|\mathfrak{p}-\mathfrak{q}|^4} &= \sum_{l=0}^{\infty}\frac{1}{4p^2q^2}\frac{2l+1}{2}\int_{-1}^{1}\mathrm{d}u\frac{P_l(u)}{(\frac{1}{2}(\frac{p}{q}+\frac{q}{p})-u)^2}P_l(\cos(\theta)) \\
&= \sum_{l=0}^{\infty}\frac{1}{4p^2q^2}\frac{2l+1}{2}\int_{-1}^{1}\mathrm{d}u\frac{P_l(u)}{(\frac{1}{2}(\frac{p}{q}+\frac{q}{p})-u)^2}\sum_{m=-l}^{l}\frac{4\pi}{2l+1}Y^*_{l,m}(\omega_q)Y_{l,m}(\omega_p) \\
&= \sum_{l=0}^{\infty}\frac{\pi}{p^2q^2}O_l(\frac{1}{2}(\frac{p}{q}+\frac{q}{p}))\sum_{m=-l}^{l}Y^*_{l,m}(\omega_q)Y_{l,m}(\omega_p).
\end{aligned} \tag{2.20}$$

The function O_l is defined by

$$O_l(x) := \frac{1}{2}\int_{-1}^{1}\mathrm{d}u\frac{P_l(u)}{(x-u)^2}. \tag{2.21}$$

Then we use the following properties of $Y_{l,m}$,

$$\int_0^{2\pi}\mathrm{d}\varphi\int_0^{\pi}\mathrm{d}\theta\sin\theta Y^*_{l,m}(\theta,\varphi) = \begin{cases}\sqrt{4\pi} & m=l=0 \\ 0 & ohterwise\end{cases} \tag{2.22}$$

and $Y_{0,0} = \frac{1}{\sqrt{4\pi}}$. Then we have

$$\begin{aligned}
I_1(\phi_{l',m',s'}, \phi_{l,m,s}) = \frac{1}{2\pi^2}\int\limits_{\mathbb{R}^3}\int\limits_{\mathbb{R}^3} \mathrm{d}\mathfrak{p}\mathrm{d}\mathfrak{q}\frac{1}{p^2q^2}\\
\Bigg(\frac{\overline{g'(p)}}{p}\Omega^*_{l',m',s'}(\omega_p)\sum_{l'=0}^{\infty} O_{l'}(\frac{1}{2}(\frac{p}{q}+\frac{q}{p}))\sum_{m'=-l'}^{l} Y^*_{l',m'}(\omega_q)Y_{l',m'}(\omega_p)I_{g,l+2s}(p)\Omega_{l,m,s}(\omega_p)\\
+\frac{\overline{g'(q)}}{q}\Omega^*_{l',m',s'}(\omega_q)\sum_{l'=0}^{\infty} O_{l'}(\frac{1}{2}(\frac{p}{q}+\frac{q}{p}))\sum_{m'=-l'}^{l} Y^*_{l',m'}(\omega_p)Y_{l',m'}(\omega_q)I_{g,l+2s}(q)\Omega_{l,m,s}(\omega_q)\\
-\frac{\overline{g'(p)}}{p}\Omega^*_{l',m',s'}(\omega_p)\sum_{l'=0}^{\infty} O_{l'}(\frac{1}{2}(\frac{p}{q}+\frac{q}{p}))\sum_{m'=-l'}^{l} Y^*_{l',m'}(\omega_q)Y_{l',m'}(\omega_p)I_{g,l+2s}(q)\Omega_{l,m,s}(\omega_q)\\
-\frac{\overline{g'(q)}}{q}\Omega^*_{l',m',s'}(\omega_q)\sum_{l'=0}^{\infty} O_{l'}(\frac{1}{2}(\frac{p}{q}+\frac{q}{p}))\sum_{m'=-l'}^{l} Y^*_{l',m'}(\omega_p)Y_{l',m'}(\omega_q)I_{g,l+2s}(p)\Omega_{l,m,s}(\omega_p)\Bigg).
\end{aligned} \tag{2.23}$$

If we look at the integral over ω_p and ω_q, it is obvious that

$$I_1(\phi_{l',m',s'}, \phi_{l,m,s}) = 0, \quad (l', m', s') \neq (l, m, s). \tag{2.24}$$

Similarly, $I_2(\phi_{l',m',s'}, \phi_{l,m,s}) = 0$, when $(l', m', s') \neq (l, m, s)$. □

Formula (2.14) implies that

$$\Big(\phi(\mathfrak{p}), |x|\frac{\alpha\cdot\mathfrak{p}}{p}\frac{1}{|x|}\phi(\mathfrak{p})\Big) = \sum_{l,m,s}\Big(\phi_{l,m,s}(\mathfrak{p}), |x|\frac{\alpha\cdot\mathfrak{p}}{p}\frac{1}{|x|}\phi_{l,m,s}(\mathfrak{p})\Big). \tag{2.25}$$

So we only need to prove (2.13) on subspaces, i.e.,

$$(\phi_{l,m,s}, \phi_{l,m,s}) < \mathfrak{R}(\phi_{l,m,s}, |x|\frac{\alpha\cdot\mathfrak{p}}{p}\frac{1}{|x|}\phi_{l,m,s}) < \frac{5}{3}(\phi_{l,m,s}, \phi_{l,m,s}). \tag{2.26}$$

As a byproduct of the proof of (2.14), we have

$$\begin{aligned}
I_1 :=I_1(\phi_{l,m,s}, \phi_{l,m,s}) = \frac{1}{2\pi^2}\int\limits_{\mathbb{R}^3}\int\limits_{\mathbb{R}^3} \mathrm{d}\mathfrak{p}\mathrm{d}\mathfrak{q}\frac{1}{p^2q^2}\\
\Bigg(\frac{\overline{g(p)}}{p}O_0(\frac{1}{2}(\frac{p}{q}+\frac{q}{p}))\int_0^{\infty}\mathrm{d}k\frac{1}{p}Q_{l+2s}(\frac{1}{2}(\frac{p}{k}+\frac{k}{p}))g(k)\\
+\frac{\overline{g(q)}}{q}O_0(\frac{1}{2}(\frac{p}{q}+\frac{q}{p}))\int_0^{\infty}\mathrm{d}k\frac{1}{q}Q_{l+2s}(\frac{1}{2}(\frac{q}{k}+\frac{k}{q}))g(k)\\
-\frac{\overline{g(p)}}{p}O_l(\frac{1}{2}(\frac{p}{q}+\frac{q}{p}))\int_0^{\infty}\mathrm{d}k\frac{1}{q}Q_{l+2s}(\frac{1}{2}(\frac{q}{k}+\frac{k}{q}))g(k)\\
-\frac{\overline{g(q)}}{q}O_l(\frac{1}{2}(\frac{p}{q}+\frac{q}{p}))\int_0^{\infty}\mathrm{d}k\frac{1}{p}Q_{l+2s}(\frac{1}{2}(\frac{p}{k}+\frac{k}{p}))g(k)\Bigg).
\end{aligned} \tag{2.27}$$

Then we use the Mellin transform [23]

$$g^{\#}(t) := \frac{1}{\sqrt{2\pi}} \int_0^\infty g(p) \frac{1}{p^{\frac{1}{2}}} e^{-it\ln p} \mathrm{d}p,$$
$$g(p) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^\infty g^{\#}(t) \frac{1}{p^{\frac{1}{2}}} e^{it\ln p} \mathrm{d}t. \tag{2.28}$$

The function $g^{\#}(t)$ is in $L^2(-\infty, \infty)$. After changing some variables, we have

$$\begin{aligned} I_1 &= \frac{1}{4\pi^3} \int_0^\infty \mathrm{d}k \int_{-\infty}^\infty \int_{-\infty}^\infty \mathrm{d}t\mathrm{d}r \overline{g^{\#}(t)} Q_{l+2s}(\frac{1}{2}(\frac{1}{k}+k)) g^{\#}(r) \frac{1}{k^{\frac{1}{2}}} e^{ir\ln k} f_l(t,r) \int_0^\infty \mathrm{d}p \frac{1}{p} e^{-i(t-r)\ln p} \\ &= \frac{1}{2\pi^2} \int_0^\infty \mathrm{d}k \int_{-\infty}^\infty \int_{-\infty}^\infty \mathrm{d}t\mathrm{d}r \overline{g^{\#}(t)} Q_{l+2s}(\frac{1}{2}(\frac{1}{k}+k)) g^{\#}(r) \frac{1}{k^{\frac{1}{2}}} e^{ir\ln k} f_l(t,r)\delta(t-r) \\ &= \int_{-\infty}^\infty \mathrm{d}r F_l(r) G_{l+2s}(r) |g^{\#}(r)|^2. \end{aligned} \tag{2.29}$$

The function f_l is defined by

$$f_l(t,r) := \int_0^\infty \mathrm{d}q \left(O_0(\frac{1}{2}(\frac{1}{q}+q)) \left(1 + \frac{1}{q^{\frac{3}{2}}} e^{-it\ln q} \frac{1}{q^{\frac{1}{2}}} e^{ir\ln q} \right) - O_l(\frac{1}{2}(\frac{1}{q}+q)) \left(\frac{1}{q^{\frac{1}{2}}} e^{ir\ln q} + \frac{1}{q^{\frac{3}{2}}} e^{-it\ln q} \right) \right). \tag{2.30}$$

Then $F_l(r) := \frac{1}{\pi} f_l(r,r)$. The function $G_l(r)$ is defined by

$$G_l(r) := \frac{1}{2\pi} \int_0^\infty \mathrm{d}k Q_l(\frac{1}{2}(\frac{1}{k}+k)) \frac{1}{k^{\frac{1}{2}}} e^{ir\ln k}. \tag{2.31}$$

We known that the real parts of F_l and G_l are positive, i.e., $\Re F_l(r) > 0$ and $\Re G_l(r) > 0$. The proofs will be given later in this section. We put some parts in the appendices. Similar to I_1, we have an expression for I_2

$$I_2 = \int_{-\infty}^\infty \mathrm{d}r F_{l+2s}(r) G_l(r) |g^{\#}(r)|^2. \tag{2.32}$$

So we have

$$\left(\phi_{l,m,s}(\mathfrak{p}), |x| \frac{\alpha\cdot\mathfrak{p}}{p} \frac{1}{|x|} \phi_{l,m,s}(\mathfrak{p}) \right) = \int_{-\infty}^\infty \mathrm{d}r (F_l(r) G_{l+2s}(r) + F_{l+2s}(r) G_l(r)) |g^{\#}(r)|^2. \tag{2.33}$$

To prove 2.26, now we only need to prove

Lemma 1. $2 < \Re(F_l(r)G_{l+2s}(r) + F_{l+2s}(r)G_l(r)) \le \frac{10}{3}, \quad r \in \mathbb{R}.$

Before the proof of this lemma, we need another relation between F_l and G_l.

Lemma 2. $F_l(r)G_l(r) = 1, \ r \in \mathbb{R}.$

Proof. We consider

$$\begin{aligned}
&\int_{\mathbb{R}^3} \mathrm{d}\mathfrak{p} \frac{\overline{g(p)}}{p} \Omega^*_{l,m,s}(\omega_p)|x|\frac{1}{|x|}\frac{g(p)}{p}\Omega_{l,m,s}(\omega_p) \\
=&\frac{\Gamma(2)}{\pi^{\frac{3}{2}}|\Gamma(-\frac{1}{2})|}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \mathrm{d}\mathfrak{p}\mathrm{d}\mathfrak{q}\left(\frac{\overline{g(p)}}{p}\Omega^*_{l,m,s}(\omega_p) - \frac{\overline{g(q)}}{q}\Omega^*_{l,m,s}(\omega_q)\right) \\
&\frac{1}{|\mathfrak{p}-\mathfrak{q}|^4}\frac{1}{\pi}(I_{g,l}(p)\Omega_{l,m,s}(\omega_p) - I_{g,l}(q)\Omega_{l,m,s}(\omega_q)) \\
=&\int_{-\infty}^{\infty} \mathrm{d}r F_l(r)G_l(r)|g^{\#}(r)|^2.
\end{aligned} \tag{2.34}$$

But we also know

$$\begin{aligned}
&\int_{\mathbb{R}^3} \mathrm{d}\mathfrak{p} \frac{\overline{g(p)}}{p} \Omega^*_{l,m,s}(\omega_p)|x|\frac{1}{|x|}\frac{g(p)}{p}\Omega_{l,m,s}(\omega_p) \\
=&\int_{\mathbb{R}} \mathrm{d}p p^2 \left|\frac{g(p)}{p}\right|^2 = \int_{\mathbb{R}} \mathrm{d}p|g(p)|^2 = \int_{-\infty}^{\infty} \mathrm{d}r|g^{\#}(r)|^2 > 0.
\end{aligned} \tag{2.35}$$

So we have

$$\int_{-\infty}^{\infty} \mathrm{d}r|g^{\#}(r)|^2 = \int_{-\infty}^{\infty} \mathrm{d}r F_l(r)G_l(r)|g^{\#}(r)|^2. \tag{2.36}$$

Since $g^{\#}(r)$ can be any function in $L^2(-\infty,\infty)$, the lemma is proved. □

By this lemma, we know that $F_l(r)G_{l+2s}(r)F_{l+2s}(r)G_l(r) = 1$. So $F_l(r)G_{l+2s}(r) + F_{l+2s}(r)G_l(r)$ has form $x + \frac{1}{x}$. To prove $2 < \Re\left(x + \frac{1}{x}\right)$, our method is to control the argument of $x - 1$. We have following result

Lemma 3. $|\mathrm{Arg}(F_{l+1}(r)G_l(r) - 1)| = |\mathrm{sgn}(r)\mathrm{Arg}(F_{l+1}(|r|)G_l(|r|) - 1)| < \frac{\pi}{4}.$

Proof. We know

$$G_l(r) = \frac{1}{2\pi}\int_0^{\infty} \mathrm{d}k Q_l(\frac{1}{2}(\frac{1}{k}+k))\frac{1}{k^{\frac{1}{2}}}e^{ir\ln k} = \frac{1}{\sqrt{2\pi}}Q_l^{\#}(\frac{1}{2}(\frac{1}{\cdot}+\cdot))(-r). \tag{2.37}$$

By Le Yaouanc, Oliver, and Raynal [17], the function G_l is a quotient of Gamma functions

$$G_l(r) = \frac{1}{4}\frac{\Gamma\left(\frac{l+\frac{1}{2}-ir}{2}\right)\Gamma\left(\frac{l+\frac{3}{2}+ir}{2}\right)}{\Gamma\left(\frac{l+\frac{3}{2}-ir}{2}\right)\Gamma\left(\frac{l+\frac{5}{2}+ir}{2}\right)}. \tag{2.38}$$

They also give another expression of G_l

$$G_l(r) = \frac{1}{\pi}\sum_{n=0}^{\infty}\frac{\Gamma\left(n+\frac{1}{2}\right)\Gamma\left(n+l+1\right)}{\Gamma\left(n+1\right)\Gamma\left(n+l+\frac{3}{2}\right)}\frac{2n+l+1}{(2n+l+1)^2+(r-\frac{i}{2})^2}. \tag{2.39}$$

Obviously, $\frac{\Gamma(n+\frac{1}{2})\Gamma(n+l+1)}{\Gamma(n+1)\Gamma(n+l+\frac{3}{2})}(2n+l+1)$ is positive. So the argument of G_l is decided by

$$\frac{1}{(2n+l+1)^2+(r-\frac{i}{2})^2} = \frac{(2n+l+1)^2+r^2-\frac{1}{4}+ir}{((2n+l+1)^2+r^2-\frac{1}{4})^2+r^2}. \tag{2.40}$$

Consider the real part, we have

$$\Re\frac{1}{(2n+l+1)^2+(r-\frac{i}{2})^2} = \Re\frac{1}{(2n+l+1)^2+(|r|-\frac{i}{2})^2} > 0. \tag{2.41}$$

For the imaginary part, we have

$$\begin{aligned}\Im\frac{1}{(2n+l+1)^2+(r-\frac{i}{2})^2} &= \frac{r}{((2n+l+1)^2+r^2-\frac{1}{4})^2+r^2}\\ &= \operatorname{sgn}(r)\Im\frac{1}{(2n+l+1)^2+(|r|-\frac{i}{2})^2}\end{aligned} \tag{2.42}$$

and

$$\Im\frac{1}{(2n+l+1)^2+(|r|-\frac{i}{2})^2} > 0. \tag{2.43}$$

From (2.41) and (2.42), we know

$$G_l(r) = \overline{G_l(-r)}. \tag{2.44}$$

Then, using Lemma 2, we have

$$F_l(r) = \overline{F_l(-r)}. \tag{2.45}$$

So we know $\Re G_l(r) = \Re G_l(|r|) > 0$, $\Im G_l(|r|) > 0$, and $\Im G_l(r) = \operatorname{sgn}(r)\Im G_l(|r|)$.

Compare the real part and the imaginary part

$$\begin{aligned}&\Re\frac{1}{(2n+l+1)^2+(|r|-\frac{i}{2})^2} - \Im\frac{1}{(2n+l+1)^2+(|r|-\frac{i}{2})^2}\\ =&\frac{(2n+l)^2+2(2n+l)+\frac{1}{2}+(|r|-\frac{1}{2})^2}{((2n+l+1)^2+r^2-\frac{1}{4})^2+r^2} > 0.\end{aligned} \tag{2.46}$$

So we have

$$\Re G_l(|r|) > \Im G_l(|r|) > 0. \tag{2.47}$$

This implies

$$0 < \mathrm{Arg} G_l(|r|) = \arctan\left(\frac{\Im G_l(|r|)}{\Re G_l(|r|)}\right) < \frac{\pi}{4}. \tag{2.48}$$

By the definition of $G_l(r)$, we have

$$\Re G_l(|r|) - \Im G_l(|r|) = \frac{1}{2\pi}\int\limits_0^\infty \mathrm{d}k \int\limits_{\max\{k,\frac{1}{k}\}}^\infty \mathrm{d}z \frac{z^{-l-1}}{\sqrt{1-(\frac{1}{k}+k)z+z^2}}\frac{1}{k^{\frac{1}{2}}}(\cos(r\ln k) - \sin(|r|\ln k)). \tag{2.49}$$

We compute the derivative with respect to l,

$$\begin{aligned}&\frac{\mathrm{d}}{\mathrm{d}l}(\Re G_l(|r|) - \Im G_l(|r|))\\ =&\frac{1}{2\pi}\int\limits_0^\infty \mathrm{d}k \int\limits_{\max\{k,\frac{1}{k}\}}^\infty \mathrm{d}z \frac{(-l-1)z^{-l-2}}{\sqrt{1-(\frac{1}{k}+k)z+z^2}}\frac{1}{k^{\frac{1}{2}}}(\cos(r\ln k) - \sin(|r|\ln k))\\ =&(-l-1)(\Re G_{l+1}(|r|) - \Im G_{l+1}(|r|)) < 0.\end{aligned} \tag{2.50}$$

This means that, $\Re G_l(|r|) - \Im G_l(|r|)$ is a decreasing function. So we have

$$\Re G_l(|r|) - \Im G_l(|r|) > \Re G_{l+1}(|r|) - \Im G_{l+1}(|r|), \tag{2.51}$$

i.e.,

$$\Re(G_l(|r|) - G_{l+1}(|r|)) > \Im(G_l(|r|) - G_{l+1}(|r|)). \tag{2.52}$$

Similar to (2.50), we have

$$\begin{aligned}&\frac{\mathrm{d}}{\mathrm{d}l}\Im G_l(|r|)\\ =&\frac{1}{2\pi}\int\limits_0^\infty \mathrm{d}k \int\limits_{\max\{k,\frac{1}{k}\}}^\infty \mathrm{d}z \frac{(-l-1)z^{-l-2}}{\sqrt{1-(\frac{1}{k}+k)z+z^2}}\frac{1}{k^{\frac{1}{2}}}\sin(|r|\ln k)\\ =&(-l-1)(\Im G_{l+1}(|r|)) < 0.\end{aligned} \tag{2.53}$$

So we have

$$\Re(G_l(|r|) - G_{l+1}(|r|)) > \Im(G_l(|r|) - G_{l+1}(|r|)) > 0. \tag{2.54}$$

From this, we know

$$0 < \mathrm{Arg}(G_l(|r|) - G_{l+1}(|r|)) = \arctan\left(\frac{\Im(G_l(|r|) - G_{l+1}(|r|))}{\Re(G_l(|r|) - G_{l+1}(|r|))}\right) < \frac{\pi}{4}. \tag{2.55}$$

Using Lemma 2 again, we have

$$F_{l+1}(|r|)G_l(|r|) - 1 = \frac{G_l(|r|)}{G_{l+1}(|r|)} - \frac{G_{l+1}(|r|)}{G_{l+1}(|r|)} = \frac{G_l(|r|) - G_{l+1}(|r|)}{G_{l+1}(|r|)} \tag{2.56}$$

and

$$\arg(F_{l+1}(|r|)G_l(|r|) - 1) = \arg(G_l(|r|) - G_{l+1}(|r|)) - \arg(G_{l+1}(|r|)). \tag{2.57}$$

From (2.48) and (2.55), we proved that

$$-\frac{\pi}{4} < \mathrm{Arg}(G_l(|r|) - G_{l+1}(|r|)) - \mathrm{Arg}(G_{l+1}(|r|)) < \frac{\pi}{4}. \tag{2.58}$$

So we know

$$|\mathrm{Arg}(F_{l+1}(|r|)G_l(|r|) - 1)| < \frac{\pi}{4}. \tag{2.59}$$

For $r < 0$, we know

$$F_{l+1}(r)G_l(r) - 1 = \overline{F_{l+1}(|r|)G_l(|r|)} - 1. \tag{2.60}$$

It means that, for any r,

$$|\mathrm{Arg}(F_{l+1}(r)G_l(r) - 1)| = |\mathrm{sgn}(r)\mathrm{Arg}(F_{l+1}(|r|)G_l(|r|) - 1)| < \frac{\pi}{4}. \tag{2.61}$$

□

Now we can start to prove Lemma 1.

Proof of Lemma 1. We need the value of $G_l(0)$ and $F_l(0)$. Use (B.2), we have

$$G_l(0) = \frac{1}{\pi}\int_0^\infty \mathrm{d}k \cosh(\frac{1}{2}k)Q_l(\cosh k) = \frac{1}{2\sqrt{2}}\int_{-1}^1 \mathrm{d}u\frac{P_l(u)}{\sqrt{1-u}}. \tag{2.62}$$

By Erdélyi et al. [11], we have

$$\frac{1}{\sqrt{1-2hu+h^2}} = \sum_{l=0}^\infty h^l P_l(u). \tag{2.63}$$

Choosing $h = 1$, we have (Whittaker and Watson [37, p. 305])

$$G_l(0) = \frac{1}{2}\int_{-1}^1 \mathrm{d}u P_l^2(u) = \frac{1}{2l+1}. \tag{2.64}$$

Using Lemma 2, we directly get

$$F_l(0) = G_l^{-1}(0) = 2l + 1. \tag{2.65}$$

Using Lemma 2 again, we have

$$\begin{aligned} F_l(r)G_{l+1}(r) &= F_{l+1}(r)G_{l+1}(r) - (F_{l+1}(r) - F_l(r))G_{l+1}(r) \\ &= 1 - (F_{l+1}(r) - F_l(r))G_{l+1}(r). \end{aligned} \tag{2.66}$$

After some computations, we get

$$\begin{aligned}&F_{l+1}(r)-F_l(r)\\=&\frac{1}{\pi}\int_0^\infty\frac{\mathrm{d}q}{q}\left(O_l(\frac{1}{2}(\frac{1}{q}+q))-O_{l+1}(\frac{1}{2}(\frac{1}{q}+q))\right)\left(q^{\frac{1}{2}}e^{ir\ln q}+\frac{1}{q^{\frac{1}{2}}}e^{-ir\ln q}\right).\end{aligned}\tag{2.67}$$

Using (A.1), we get a bound for $F_{l+1}(r)-F_l(r)$

$$\begin{aligned}&|F_{l+1}(r)-F_l(r)|\\\le&\frac{1}{\pi}\int_0^\infty\frac{\mathrm{d}q}{q}\left|\left(O_l(\frac{1}{2}(\frac{1}{q}+q))-O_{l+1}(\frac{1}{2}(\frac{1}{q}+q))\right)\right|\left|q^{\frac{1}{2}}e^{ir\ln q}+\frac{1}{q^{\frac{1}{2}}}e^{-ir\ln q}\right|\\=&\frac{1}{\pi}\int_0^\infty\frac{\mathrm{d}q}{q}\left(O_l(\frac{1}{2}(\frac{1}{q}+q))-O_{l+1}(\frac{1}{2}(\frac{1}{q}+q))\right)\left(q^{\frac{1}{2}}+\frac{1}{q^{\frac{1}{2}}}\right)\\=&F_{l+1}(0)-F_l(0)=2(l+1)+1-(2l+1)=2.\end{aligned}\tag{2.68}$$

We also have

$$\begin{aligned}|G_l(r)|=&\left|\int_0^\infty\mathrm{d}kQ_l(\frac{1}{2}(\frac{1}{k}+k))\frac{1}{k^{\frac{1}{2}}}e^{ir\ln k}\right|\le\int_0^\infty\mathrm{d}k\left|Q_l(\frac{1}{2}(\frac{1}{k}+k))\frac{1}{k^{\frac{1}{2}}}e^{ir\ln k}\right|\\\le&\int_0^\infty\mathrm{d}kQ_l(\frac{1}{2}(\frac{1}{k}+k))\frac{1}{k^{\frac{1}{2}}}=G_l(0)=\frac{1}{2l+1}.\end{aligned}\tag{2.69}$$

So we write

$$(F_{l+1}(r)-F_l(r))G_{l+1}(r)=a+ib\tag{2.70}$$

where $a,b\in\mathbb{R}$. Then we have

$$|(F_{l+1}(r)-F_l(r))G_{l+1}(r)|=\sqrt{a^2+b^2}\le\frac{2}{2l+3}.\tag{2.71}$$

It is easy to see that Inequalities (2.68) and (2.69) become equalities if and only if $r=0$. So the Inequality (2.71) becomes equality if and only if $r=0$. Inequality (2.71) leads to

$$\Re F_l(r)G_{l+1}(r)=1-\Re(F_{l+1}(r)-F_l(r))G_{l+1}(r)=1-a\in\left[\frac{2l+1}{2l+3},\frac{2l+5}{2l+3}\right].\tag{2.72}$$

From this, we get

$$\begin{aligned}&F_l(r)G_{l+1}(r)+F_{l+1}(r)G_l(r)=F_l(r)G_{l+1}(r)+(F_l(r)G_{l+1}(r))^{-1}\\&=1-a-ib+\frac{1}{1-a-ib}=1-a-ib+\frac{1-a+ib}{(1-a)^2+b^2}\\&=(1-a)\left(1+\frac{1}{(1-a)^2+b^2}\right)+ib\left(-1+\frac{1}{(1-a)^2+b^2}\right).\end{aligned}\tag{2.73}$$

By (2.72) and (2.73), we have

$$
\begin{aligned}
&0 < \Re(F_l(r)G_{l+1}(r) + F_{l+1}(r)G_l(r)) = (1-a)\left(1 + \frac{1}{(1-a)^2 + b^2}\right) \\
&\le (1-a)\left(1 + \frac{1}{(1-a)^2}\right) = 1 - a + \frac{1}{1-a} \\
&\le \max\left\{\frac{2l+1}{2l+3} + \frac{2l+3}{2l+1}, \frac{2l+5}{2l+3} + \frac{2l+3}{2l+5}\right\} = \frac{2l+1}{2l+3} + \frac{2l+3}{2l+1} \\
&\le \frac{1}{3} + 3 = \frac{10}{3}.
\end{aligned}
\tag{2.74}
$$

The equality holds only for $b = 0$, $l = 0$, $a = \frac{2}{3}$. It means that the equality in (2.71) holds. So r should be 0. We proved the upper bound in the Lemma.

We write

$$
F_{l+1}(r)G_l(r) - 1 = c + id, \tag{2.75}
$$

where $c, d \in \mathbb{R}$. Using Lemma 3, we know $c > |d|$. Similar to (2.73), we have

$$
\begin{aligned}
&F_{l+1}(r)G_l(r) + F_l(r)G_{l+1}(r) = F_{l+1}(r)G_l(r) + (F_{l+1}(r)G_l(r))^{-1} \\
&= 1 + c + id + \frac{1}{1 + c + id} \\
&= (1+c)\left(1 + \frac{1}{(1+c)^2 + d^2}\right) + id\left(1 - \frac{1}{(1+c)^2 + d^2}\right).
\end{aligned}
\tag{2.76}
$$

We compute the real part

$$
\begin{aligned}
&\Re(F_{l+1}(r)G_l(r) + F_l(r)G_{l+1}(r)) = (1+c)\left(1 + \frac{1}{(1+c)^2 + d^2}\right) \\
&> (1+c)\left(1 + \frac{1}{(1+c)^2 + c^2}\right) = (1+c)\frac{2(1+c+c^2)}{1+2c+2c^2} \\
&= \frac{2(1+2c+2c^2+c^3)}{1+2c+2c^2} > 2.
\end{aligned}
\tag{2.77}
$$

So we have

$$
2 < \Re(F_l(r)G_{l+2s}(r) + F_{l+2s}(r)G_l(r)) \le \frac{10}{3}. \tag{2.78}
$$

$\square$

Now the massless part of Theorem 1 follows immediately.

Proof of Theorem 1 (1.15).

$$
\begin{aligned}
0 <& \left(\phi_{l,m,s}, \left(|x|\frac{\alpha\cdot\mathfrak{p}}{p}\frac{1}{|x|} + \frac{1}{|x|}\frac{\alpha\cdot\mathfrak{p}}{p}|x|\right)\phi_{l,m,s}\right)\\
=& 2\Re\int_{-\infty}^{\infty} \mathrm{d}r (F_l(r)G_{l+2s}(r) + F_{l+2s}(r)G_l(r))|g^{\#}(r)|^2\\
<& \frac{20}{3}\int_{-\infty}^{\infty}\mathrm{d}r|g^{\#}(r)|^2 = \frac{20}{3}\int_{\mathbb{R}}\mathrm{d}p|g(p)|^2\\
=& \frac{10}{3}\left(\phi_{l,m,s},\phi_{l,m,s}\right).
\end{aligned}
\tag{2.79}
$$

The last inequality is strict. Because the Inequality (2.74) becomes equality if and only if $r = 0$. But $g^{\#}(r)$ is a L^2 function. The support can not be only $\{0\}$. So we have

$$
\Lambda^+\left(|x|\frac{\alpha\cdot\mathfrak{p}}{p}\frac{1}{|x|} + \frac{1}{|x|}\frac{\alpha\cdot\mathfrak{p}}{p}|x|\right)\Lambda^+ < \frac{10}{3}\Lambda^+. \tag{2.80}
$$

Similarly, we have

$$
2\Lambda^+ < \Lambda^+\left(|x|\frac{\alpha\cdot\mathfrak{p}}{p}\frac{1}{|x|} + \frac{1}{|x|}\frac{\alpha\cdot\mathfrak{p}}{p}|x|\right)\Lambda^+. \tag{2.81}
$$

It means that

$$
2\Lambda_+ < \Lambda_+|x|\Lambda_+\frac{1}{|x|}\Lambda_+ + \Lambda_+\frac{1}{|x|}\Lambda_+|x|\Lambda_+ < \frac{8}{3}\Lambda_+. \tag{2.82}
$$

□

Next we prove the two bounds are best possible. For the upper bound, from (2.74) and (2.79), it is easy to see the upper bound is critical. Now we deal with the lower bound. For $l = 0$, we compute $G_0(r)$

$$
\begin{aligned}
G_0(r) =& \frac{1}{\pi}\int_0^{\infty}\mathrm{d}x Q_0\left(\frac{1}{2}(e^x + e^{-x})\right)\cos\left(\left(r - \frac{i}{2}\right)x\right)\\
=& \frac{1}{2r^2 + \frac{1}{2}}\left(r\tanh(r\pi) + \frac{1}{2}\operatorname{sech}(r\pi) + i\left(\frac{1}{2}\tanh(r\pi) - r\operatorname{sech}(r\pi)\right)\right).
\end{aligned}
\tag{2.83}
$$

Since $|\tanh(r\pi)| < 1$ and $|\operatorname{sech}(r\pi)| \le 1$, it is easy to prove

$$
\lim_{r\to\infty} G_0(r) = \lim_{r\to\infty}\Re G_0(r) = \lim_{r\to\infty}\Im G_0(r) = 0. \tag{2.84}
$$

Using the same idea in (2.53), we can prove that, $\Re G_l(|r|)$ and $\Im G_l(|r|)$ are both decreasing functions with respect to l. So we know

$$
0 \le \lim_{r\to+\infty}\Re G_l(|r|) \le \lim_{r\to+\infty}\Re G_0(|r|) = 0. \tag{2.85}
$$

It is the same for imaginary part. Using (2.44), we have

$$\lim_{r\to\infty} G_l(r) = 0. \tag{2.86}$$

Because of (2.66) and (2.68), we have

$$\lim_{r\to\infty} F_l(r)G_{l+1}(r) = 1 - \lim_{r\to\infty}(F_{l+1}(r) - F_l(r))G_{l+1}(r) = 1. \tag{2.87}$$

From this, we know

$$\begin{aligned} &\lim_{r\to\infty}(F_l(r)G_{l+1}(r) + F_{l+1}(r)G_l(r)) \\ =&\lim_{r\to\infty} F_l(r)G_{l+1}(r) + \lim_{r\to\infty}(F_l(r)G_{l+1}(r))^{-1} \\ =&\lim_{r\to\infty} F_l(r)G_{l+1}(r) + (\lim_{r\to\infty} F_l(r)G_{l+1}(r))^{-1} = 2. \end{aligned} \tag{2.88}$$

So it is easy to see the constant 2 in the lower bound is also critical.

2.4 Massive Case

In the massive case, we prove the inequality in another way. We compute the norm of the operator and use it to bound the operator.

Proof of Theorem 1 (1.16). We want to prove there is a constant c, such that

$$\frac{1}{|x|}\frac{\alpha\cdot\mathfrak{p}+m\beta}{E(\mathfrak{p})}|x| + |x|\frac{\alpha\cdot\mathfrak{p}+m\beta}{E(\mathfrak{p})}\frac{1}{|x|} < c. \tag{2.89}$$

By definition, the norm of operator is

$$\begin{aligned} &\left\|\frac{1}{|x|}\frac{\alpha\cdot\mathfrak{p}+m\beta}{E(\mathfrak{p})}|x| + |x|\frac{\alpha\cdot\mathfrak{p}+m\beta}{E(\mathfrak{p})}\frac{1}{|x|}\right\| \\ =&\sup_{\|\psi\|=1}\left(\psi, \left(\frac{1}{|x|}\frac{\alpha\cdot\mathfrak{p}+m\beta}{E(\mathfrak{p})}|x| + |x|\frac{\alpha\cdot\mathfrak{p}+m\beta}{E(\mathfrak{p})}\frac{1}{|x|}\right)^2\psi\right)^{\frac{1}{2}}. \end{aligned} \tag{2.90}$$

We compute

$$\begin{aligned} &\left(\frac{1}{|x|}\frac{\alpha\cdot\mathfrak{p}+m\beta}{E(\mathfrak{p})}|x| + |x|\frac{\alpha\cdot\mathfrak{p}+m\beta}{E(\mathfrak{p})}\frac{1}{|x|}\right)^2 \\ =&\frac{1}{|x|}\frac{\alpha\cdot\mathfrak{p}+m\beta}{E(\mathfrak{p})}|x|^2\frac{\alpha\cdot\mathfrak{p}+m\beta}{E(\mathfrak{p})}\frac{1}{|x|} + |x|\frac{\alpha\cdot\mathfrak{p}+m\beta}{E(\mathfrak{p})}\frac{1}{|x|^2}\frac{\alpha\cdot\mathfrak{p}+m\beta}{E(\mathfrak{p})}|x| + 2. \end{aligned} \tag{2.91}$$

We want to prove there is a constant c', such that

$$\frac{1}{|x|}\frac{\alpha\cdot\mathfrak{p}+m\beta}{E(\mathfrak{p})}|x|^2\frac{\alpha\cdot\mathfrak{p}+m\beta}{E(\mathfrak{p})}\frac{1}{|x|} < c'. \tag{2.92}$$

We multiply it by $|x|$ from left and right. Then (2.92) is equivalent to

$$\frac{\alpha\cdot\mathfrak{p}+m\beta}{E(\mathfrak{p})}|x|^2\frac{\alpha\cdot\mathfrak{p}+m\beta}{E(\mathfrak{p})}<c'|x|^2. \tag{2.93}$$

Then it is equivalent to

$$\frac{\alpha\cdot\mathfrak{p}+m\beta}{E(\mathfrak{p})}(-\Delta_{\mathfrak{p}})\frac{\alpha\cdot\mathfrak{p}+m\beta}{E(\mathfrak{p})}<c'(-\Delta_{\mathfrak{p}}). \tag{2.94}$$

For every $\psi\in L^2(\mathbb{R}^3;\mathbb{C}^4)$, we have

$$\begin{aligned}\psi(\mathfrak{p})=&\begin{pmatrix}\sum_{l,m,s}\frac{f_{l,m,s}(p)}{p}\Omega_{l,m,s}(\omega_{\mathfrak{p}})\\ \sum_{l,m,s}\frac{g_{l,m,s}(p)}{p}\Omega_{l,m,s}(\omega_{\mathfrak{p}})\end{pmatrix}\\ =&\sum_{l,m,s}\begin{pmatrix}\frac{f_{l,m,s}(p)}{p}\Omega_{l,m,s}(\omega_{\mathfrak{p}})\\ \frac{g_{l+2s,m,-s}(p)}{p}\Omega_{l+2s,m,-s}(\omega_{\mathfrak{p}})\end{pmatrix}=:\sum_{l,m,s}\psi_{l,m,s}(\mathfrak{p}).\end{aligned} \tag{2.95}$$

with $l=0,1,2...$, $m=-l-\frac{1}{2},...,l+\frac{1}{2}$, and $s=-\frac{1}{2},\frac{1}{2}$. In this proof, ψ is not necessarily in the positive spectral subspace. It is not so hard to prove

$$\begin{aligned}&\left(\psi_{l,m,s}(\mathfrak{p}),\frac{\alpha\cdot\mathfrak{p}+m\beta}{E(\mathfrak{p})}(-\Delta_{\mathfrak{p}})\frac{\alpha\cdot\mathfrak{p}+m\beta}{E(\mathfrak{p})}\psi_{l',m',s'}(\mathfrak{p})\right)\\ =&(\psi_{l,m,s}(\mathfrak{p}),(-\Delta_{\mathfrak{p}})\psi_{l',m',s'}(\mathfrak{p}))=0,\quad (l,m,s)\neq(l',m',s').\end{aligned} \tag{2.96}$$

So to prove (2.94), we only need to prove, for all (l,m,s),

$$\left(\psi_{l,m,s}(\mathfrak{p}),\frac{\alpha\cdot\mathfrak{p}+m\beta}{E(\mathfrak{p})}(-\Delta_{\mathfrak{p}})\frac{\alpha\cdot\mathfrak{p}+m\beta}{E(\mathfrak{p})}\psi_{l,m,s}(\mathfrak{p})\right)<c'(\psi_{l,m,s}(\mathfrak{p}),(-\Delta_{\mathfrak{p}})\psi_{l,m,s}(\mathfrak{p})). \tag{2.97}$$

We compute

$$\begin{aligned}&\frac{\alpha\cdot\mathfrak{p}+m\beta}{E(\mathfrak{p})}\psi_{l,m,s}(\mathfrak{p})\\ =&\frac{\alpha\cdot\mathfrak{p}+m\beta}{E(\mathfrak{p})}\begin{pmatrix}\frac{f(p)}{p}\Omega_{l,m,s}(\omega_{\mathfrak{p}})\\ \frac{g(p)}{p}\Omega_{l+2s,m,-s}(\omega_{\mathfrak{p}})\end{pmatrix}=\frac{1}{E(\mathfrak{p})}\begin{pmatrix}(m\frac{f(p)}{p}-g(p))\Omega_{l,m,s}(\omega_{\mathfrak{p}})\\ -(f(p)+m\frac{g(p)}{p})\Omega_{l+2s,m,-s}(\omega_{\mathfrak{p}})\end{pmatrix}.\end{aligned} \tag{2.98}$$

We ignore the lower subscripts of f and g, because they do not play roles here. By Messiah [23, p. 496], we have

$$-\Delta_{\mathfrak{p}}=-\frac{1}{p}\frac{\mathrm{d}^2}{\mathrm{d}p^2}p+\frac{\mathrm{L}^2}{p^2} \tag{2.99}$$

where $\mathrm{L} := \frac{1}{i}(\mathfrak{p} \times \nabla_{\mathfrak{p}})$ is the angular momentum operator in $\mathfrak{p}$ space. Using (2.99), we compute

$$\begin{aligned}
&-\Delta_{\mathfrak{p}} \frac{\alpha\cdot\mathfrak{p}+m\beta}{E(\mathfrak{p})}\psi_{l,m,s}(\mathfrak{p}) \\
=&\begin{pmatrix} -\frac{1}{p}\frac{\mathrm{d}^2}{\mathrm{d}p^2}\left(p\frac{1}{E(p)}(m\frac{f(p)}{p}-g(p))\right)\Omega_{l,m,s}(\omega_{\mathfrak{p}}) \\ \frac{1}{p}\frac{\mathrm{d}^2}{\mathrm{d}p^2}\left(p\frac{1}{E(p)}(f(p)+m\frac{g(p)}{p})\right)\Omega_{l+2s,m,-s}(\omega_{\mathfrak{p}}) \end{pmatrix} + \begin{pmatrix} \frac{l(l+1)}{p^2}\frac{1}{E(p)}(m\frac{f(p)}{p}-g(p))\Omega_{l,m,s}(\omega_{\mathfrak{p}}) \\ -\frac{(l+2s)(l+2s+1)}{p^2}\frac{1}{E(p)}(f(p)+m\frac{g(p)}{p})\Omega_{l+2s,m,-s}(\omega_{\mathfrak{p}}) \end{pmatrix}.
\end{aligned} \tag{2.100}$$

Then we compute

$$\begin{aligned}
&\int_{\mathbb{R}^3} \mathrm{d}\mathfrak{p}\psi_{l,m,s}(\mathfrak{p})^* \frac{\alpha\cdot\mathfrak{p}+m\beta}{E(\mathfrak{p})}(-\Delta_{\mathfrak{p}})\frac{\alpha\cdot\mathfrak{p}+m\beta}{E(\mathfrak{p})}\psi_{l,m,s}(\mathfrak{p}) \\
=&\int_{\mathbb{R}^3} \mathrm{d}p\Bigg(|f'(p)|^2+|g'(p)|^2+\frac{2m}{E(p)^2}\Re(-\overline{g(p)}f'(p)+\overline{f(p)}g'(p)) \\
&+\left(\frac{m^2}{E(p)^4}+\frac{l(l+1)}{p^2}\right)(|f(p)|^2+|g(p)|^2)+\frac{2s(2l+2s+1)}{p^2}\left|\frac{pf(p)+mg(p)}{E(p)}\right|^2\Bigg).
\end{aligned} \tag{2.101}$$

It is easy to prove

$$\begin{aligned}
&\int_{\mathbb{R}^3} \mathrm{d}\mathfrak{p}\psi_{l,m,s}(\mathfrak{p})^*(-\Delta_{\mathfrak{p}})\psi_{l,m,s}(\mathfrak{p}) \\
=&\int_{\mathbb{R}^3} \mathrm{d}p\left(|f'(p)|^2+|g'(p)|^2+\frac{l(l+1)}{p^2}|f(p)|^2+\frac{(l+2s)(l+2s+1)}{p^2}|g(p)|^2\right).
\end{aligned} \tag{2.102}$$

Suppose $s=\frac{1}{2}$, then we have

$$\begin{aligned}
&\int_{\mathbb{R}^3} \mathrm{d}\mathfrak{p}\psi_{l,m,s}(\mathfrak{p})^*\left(\frac{\alpha\cdot\mathfrak{p}+m\beta}{E(\mathfrak{p})}(-\Delta_{\mathfrak{p}})\frac{\alpha\cdot\mathfrak{p}+m\beta}{E(\mathfrak{p})}+\Delta_{\mathfrak{p}}\right)\psi_{l,m,s}(\mathfrak{p}) \\
=&\int_{\mathbb{R}^3} \mathrm{d}p\left(\frac{2p^2+3m^2}{E(p)^4}|f(p)|^2-\frac{2p^2+m^2}{E(p)^4}|g(p)|^2+\frac{4m^3}{pE(p)^4}\Re(\overline{f(p)}g(p))+\frac{4m}{E(p)^2}\Re(\overline{f(p)}g'(p))\right) \\
&+l\int_{\mathbb{R}^3} \mathrm{d}p\left(\frac{2}{E(p)^2}(|f(p)|^2-|g(p)|^2)+\frac{4m}{pE(p)^2}\Re(\overline{f(p)}g(p))\right) \\
\le&\int_{\mathbb{R}^3} \mathrm{d}p\left(\frac{2}{p^2}|f(p)|^2+\frac{-2p^4-5m^2p^2+6m^4}{(p^2+2m^2)E(p)^4}|g(p)|^2+\frac{8p^2}{p^2+2m^2}|g'(p)|^2\right) \\
&+l\int_{\mathbb{R}^3} \mathrm{d}p\left(\frac{1}{p^2}(3|f(p)|^2+|g(p)|^2)\right) \\
\le& 8\int_{\mathbb{R}^3} \mathrm{d}\mathfrak{p}\psi_{l,m,s}(\mathfrak{p})^*(-\Delta_{\mathfrak{p}})\psi_{l,m,s}(\mathfrak{p}).
\end{aligned} \tag{2.103}$$

The last inequality is from Hardy's inequality [21]. For $s = -\frac{1}{2}$, we set $l = l' + 1$, $f(p) = G(p)$, and $g(p) = -F(p)$, similar to (2.103), we have

$$\begin{aligned}
&\int_{\mathbb{R}^3} \mathrm{d}\mathfrak{p}\psi_{l,m,s}(\mathfrak{p})^* \left(\frac{\alpha\cdot\mathfrak{p}+m\beta}{E(\mathfrak{p})}(-\Delta_{\mathfrak{p}})\frac{\alpha\cdot\mathfrak{p}+m\beta}{E(\mathfrak{p})} + \Delta_{\mathfrak{p}} \right)\psi_{l,m,s}(\mathfrak{p}) \\
=&\int_{\mathbb{R}^3} \mathrm{d}p \Bigg(\frac{2m}{E(p)^2}\Re(\overline{F(p)}G'(p) - \overline{G(p)}F'(p)) + \frac{m^2}{E(p)^4}(|G(p)|^2 + |F(p)|^2) \\
&- \frac{2(l'+1)}{p}\frac{p|G(p)|^2 - p|F(p)|^2 - 2m\Re\overline{G(p)}F(p)}{E(p)^2} \Bigg) \\
\le 8&\int_{\mathbb{R}^3} \mathrm{d}p \left(|F'(p)|^2 + |G'(p)|^2 + \frac{(l'+1)(l'+2)}{p^2}|G(p)|^2 + \frac{l'(l'+1)}{p^2}|F(p)|^2 \right) \\
=8&\int_{\mathbb{R}^3} \mathrm{d}\mathfrak{p}\psi_{l,m,s}(\mathfrak{p})^*(-\Delta_{\mathfrak{p}})\psi_{l,m,s}(\mathfrak{p}).
\end{aligned} \tag{2.104}$$

So we proved

$$\frac{1}{|x|}\frac{\alpha\cdot\mathfrak{p}+m\beta}{E(\mathfrak{p})}|x|^2\frac{\alpha\cdot\mathfrak{p}+m\beta}{E(\mathfrak{p})}\frac{1}{|x|} < 9. \tag{2.105}$$

From this, we know

$$|x|\frac{\alpha\cdot\mathfrak{p}+m\beta}{E(\mathfrak{p})}\frac{1}{|x|^2}\frac{\alpha\cdot\mathfrak{p}+m\beta}{E(\mathfrak{p})}|x| < 9. \tag{2.106}$$

It implies

$$\begin{aligned}
&\frac{1}{|x|}\frac{\alpha\cdot\mathfrak{p}+m\beta}{E(\mathfrak{p})}|x|^2\frac{\alpha\cdot\mathfrak{p}+m\beta}{E(\mathfrak{p})}\frac{1}{|x|} \\
=&\left(|x|\frac{\alpha\cdot\mathfrak{p}+m\beta}{E(\mathfrak{p})}\frac{1}{|x|^2}\frac{\alpha\cdot\mathfrak{p}+m\beta}{E(\mathfrak{p})}|x|\right)^{-1} > \frac{1}{9}.
\end{aligned} \tag{2.107}$$

Using the spectral theorem (Reed and Simon [28, p. 263]), we have

$$\begin{aligned}
&\left(\frac{1}{|x|}\frac{\alpha\cdot\mathfrak{p}+m\beta}{E(\mathfrak{p})}|x| + |x|\frac{\alpha\cdot\mathfrak{p}+m\beta}{E(\mathfrak{p})}\frac{1}{|x|}\right)^2 \\
=&\frac{1}{|x|}\frac{\alpha\cdot\mathfrak{p}+m\beta}{E(\mathfrak{p})}|x|^2\frac{\alpha\cdot\mathfrak{p}+m\beta}{E(\mathfrak{p})}\frac{1}{|x|} + \left(\frac{1}{|x|}\frac{\alpha\cdot\mathfrak{p}+m\beta}{E(\mathfrak{p})}|x|^2\frac{\alpha\cdot\mathfrak{p}+m\beta}{E(\mathfrak{p})}\frac{1}{|x|}\right)^{-1} + 2 \\
\le&\sup_{\frac{1}{9}<\lambda<9}(\lambda + \lambda^{-1}) + 2 = \frac{100}{9}.
\end{aligned} \tag{2.108}$$

By (2.90), we have

$$\frac{1}{|x|}\frac{\alpha\cdot\mathfrak{p}+m\beta}{E(\mathfrak{p})}|x| + |x|\frac{\alpha\cdot\mathfrak{p}+m\beta}{E(\mathfrak{p})}\frac{1}{|x|} < \frac{10}{3}. \tag{2.109}$$

□

2.5 Another Attempt

Since the main difficulty is from the term $\int\limits_{\mathbb{R}^3} \mathrm{d}y \frac{\rho(y)}{|x-y|}$, we try to multiply the Euler equation by $\left(\int\limits_{\mathbb{R}^3} \mathrm{d}y \frac{\rho(y)}{|x-y|}\right)^{-1} \psi_i$ to make this term simpler. Equality (2.2) changes to

$$\sum_{i=1}^{N} \left(\psi_i, \left(\int\limits_{\mathbb{R}^3} \mathrm{d}y \frac{\rho(y)}{|x-y|} \right)^{-1} \Lambda_+ \left(D_0 - \alpha \frac{z}{|x|} + \alpha \int\limits_{\mathbb{R}^3} \mathrm{d}y \frac{\rho(y)}{|x-y|} - \lambda_i \right) \Lambda_+ \psi_i \right) = 0. \tag{2.110}$$

We start from an easier case, that we ignore the projection Λ_+. We need to prove

$$\sum_{i=1}^{N} \left(\psi_i, \left(\int\limits_{\mathbb{R}^3} \mathrm{d}y \frac{\rho(y)}{|x-y|} \right)^{-1} \frac{1}{|x|} \psi_i \right) = \int\limits_{\mathbb{R}^3} \mathrm{d}x \frac{\rho(x)}{|x| \int\limits_{\mathbb{R}^3} \mathrm{d}y \frac{\rho(y)}{|x-y|}} < C. \tag{2.111}$$

But we find a counterexample showing that the integral is not bounded: We assume that ρ is spherical symmetric. Using Newton's theorem [26], we have

$$\begin{aligned} \int\limits_{\mathbb{R}^3} \mathrm{d}x \frac{\rho(x)}{|x| \int\limits_{\mathbb{R}^3} \mathrm{d}y \frac{\rho(y)}{|x-y|}} &= \int\limits_{\mathbb{R}^3} \mathrm{d}x \frac{\rho(x)}{|x| \int\limits_{\mathbb{R}^3} \mathrm{d}y \frac{\rho(y)}{max\{|x|,|y|\}}} \\ = \int_0^\infty \mathrm{d}r \frac{r^2 \rho(r)}{r \int_0^\infty \mathrm{d}s s^2 \frac{\rho(y)}{max\{r,s\}}} &= \int_0^\infty \mathrm{d}r \frac{r^2 \rho(r)}{\int_0^r \mathrm{d}s s^2 \rho(y) + r \int_r^\infty \mathrm{d}s s \rho(y)}. \end{aligned} \tag{2.112}$$

We define ρ as following

$$\rho_b(r) = \begin{cases} 1 & r < 1 \\ \dfrac{1}{r^b} & r \geq 1 \end{cases} \tag{2.113}$$

where $b > 3$. We compute

$$\begin{aligned} &\int_0^1 \mathrm{d}r \frac{r^2 \rho_b(r)}{\int_0^r \mathrm{d}s s^2 \rho_b(y) + r \int_r^\infty \mathrm{d}s s \rho_b(y)} \\ = &\int_0^1 \mathrm{d}r \frac{r^2}{\int_0^r \mathrm{d}s s^2 + r \int_r^1 \mathrm{d}s s + r \int_1^\infty \mathrm{d}s s \frac{1}{s^b}} = 3 \left(-\ln 2 + \ln 3 - \ln \frac{b+1}{b} \right) \end{aligned} \tag{2.114}$$

and

$$\int_1^\infty \mathrm{d}r \frac{r^2\rho_b(r)}{\int_0^r \mathrm{d}s s^2\rho_b(y) + r\int_r^\infty \mathrm{d}s s\rho_b(y)}$$
$$= \int_1^\infty \mathrm{d}r \frac{r^2\frac{1}{s^b}}{\int_0^1 \mathrm{d}s s^2 + \int_1^r \mathrm{d}s s^2\frac{1}{s^b} + r\int_r^\infty \mathrm{d}s s\frac{1}{s^b}} = (b-2)(\ln b - \ln(b-3) + \ln(b-2) - \ln(b+1)). \tag{2.115}$$

So we have

$$\int_{\mathbb{R}^3} \mathrm{d}x \frac{\rho_b(x)}{|x|\int_{\mathbb{R}^3} \mathrm{d}y \frac{\rho_b(y)}{|x-y|}} = 3\left(-\ln 2 + \ln 3 - \ln\frac{b+1}{b}\right) \tag{2.116}$$
$$+ (b-2)(\ln b - \ln(b-3) + \ln(b-2) - \ln(b+1)).$$

It is easy to see that

$$\lim_{b\to 3^+}\int_{\mathbb{R}^3} \mathrm{d}x \frac{\rho_b(x)}{|x|\int_{\mathbb{R}^3} \mathrm{d}y \frac{\rho_b(y)}{|x-y|}} = \infty. \tag{2.117}$$

Since it is unbounded without the projection Λ_+, it is not so hopeful that it is bounded with the projection.

Chapter 3

Thomas-Fermi-Weizsäcker theory

3.1 Bound on Excess Charge in the non-relativistic time-dependent Thomas-Fermi-Weizsäcker theory

Lenzmann and Lewin [18] studied the long-time behavior of the repulsive nonlinear Hartree equation. Following their work, L. Chen and Siedentop [5] studied the time-dependent Thomas-Fermi equation and the Vlasov equation. Our work is related to L. Chen and Siedentop's work on TF equation. They deal with the time-dependent TF equation

$$\partial_t \varphi_t = \frac{1}{2}(\nabla \varphi_t)^2 + \frac{\gamma_{TF}}{2}\rho_t^{\frac{2}{3}} - \frac{Z}{|x|} + \rho_t * |\cdot|^{-1}. \tag{3.1}$$

The function φ is the potential of the velocity field, ρ is the density of electrons. They satisfy continuity equation

$$\partial_t \rho_t = \nabla(\rho_t \nabla \varphi_t). \tag{3.2}$$

L. Chen and Siedentop showed that the number of electrons in a bounded measurable set, in temporal average for large time, does not exceed $4Z$.

We add a Weizsäcker term to the Thomas-Fermi equation and want to get the same result. To get the Weizsäcker term, we solve the variational problem

$$\begin{aligned} &\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\int \mathrm{d}x |\nabla\sqrt{\rho+\varepsilon\eta}|^2\Big|_{\varepsilon=0} = \frac{\mathrm{d}}{\mathrm{d}\varepsilon}\int \mathrm{d}x \left|\nabla\left(\sqrt{\rho}\sqrt{1+\frac{\varepsilon\eta}{\rho}}\right)\right|^2\Bigg|_{\varepsilon=0} \\ =& -\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\int \mathrm{d}x (\Delta\sqrt{\rho})\frac{\varepsilon\eta}{\sqrt{\rho}}\Big|_{\varepsilon=0} = \int \mathrm{d}x(-\frac{\Delta\sqrt{\rho}}{\sqrt{\rho}})\eta. \end{aligned} \tag{3.3}$$

So the time-dependent Thomas-Fermi-Weizsäcker equation is

$$\partial_t \varphi_t = \frac{1}{2}(\nabla \varphi_t)^2 + \frac{\gamma_{TF}}{2}\rho_t^{\frac{2}{3}} - \frac{Z}{|x|} + \rho_t * |\cdot|^{-1} - c^W\frac{\Delta\sqrt{\rho}}{\sqrt{\rho}}. \tag{3.4}$$

Our corresponding result is

Theorem 4. *Assume that φ_t and ρ_t is a weak solution of (3.4) and (3.2) with finite energy, assume $B \subset \mathbb{R}^3$ bounded and measurable, and set*

$$N_{TFW}(t,B) := \int_B \mathrm{d}x \rho_t(x). \tag{3.5}$$

Then

$$\limsup_{T\to\infty} \frac{1}{T}\int_0^T \mathrm{d}t N_{TFW}(t,B) \le 4Z. \tag{3.6}$$

The idea of the proof is the same as in the TF case. We only need to deal with the Weizsäcker term related part. The proof for the other part is the same as before.

Proof. We multiply (3.4) by the operator

$$W_R := \nabla g_R \cdot \nabla, \tag{3.7}$$

multiply by ρ, integrate in the space variable, and average in time, where $g_R(x) := R^3 g(|x|/R)$ with $g(r) := r - \arctan(r)$. We define $\psi := \sqrt{\rho}$ and $\phi := \sqrt{\Delta g_R}$, then compute

$$\begin{aligned}
&\int \mathrm{d}x \rho \nabla g_R \cdot \nabla\Big(-\frac{\Delta\sqrt{\rho}}{\sqrt{\rho}}\Big) \\
=&\int \mathrm{d}x \nabla(\psi^2 \nabla g_R)\frac{\Delta\psi}{\psi} \\
=&-2\int \mathrm{d}x\Big(|\nabla(\phi\psi)|^2 - \frac{-\frac{1}{4}\Delta(\phi^2)+|\nabla\phi|^2}{\phi^2}(\phi\psi)^2\Big).
\end{aligned} \tag{3.8}$$

Using the definition of g_R, we know

$$\phi(x) = \sqrt{\Delta g_R(x)} = \sqrt{R^3 \Delta g(|x|/R)} = \frac{R\sqrt{2|x|(2R^2+|x|^2)}}{R^2+|x|^2}. \tag{3.9}$$

So we have

$$\frac{-\frac{1}{4}\Delta(\phi^2)+|\nabla\phi|^2}{\phi^2} = \frac{|x|^8 + 6R^2|x|^6 + 25R^4|x|^4 + 24R^6|x|^2 - 4R^8}{4(R^2+|x|^2)^2|x|^2(2R^2+|x|^2)^2}. \tag{3.10}$$

We compare this to $\frac{1}{4|x|^2}$. The difference is

$$\frac{-\frac{1}{4}\Delta(\phi^2)+|\nabla\phi|^2}{\phi^2} - \frac{1}{4|x|^2} = \frac{12R^4(|x|^2+\frac{1}{2}R^2)^2 - 11R^8}{4(R^2+|x|^2)^2|x|^2(2R^2+|x|^2)^2}. \tag{3.11}$$

Using Hardy's inequality [21], we have

$$\begin{aligned}
&\int \mathrm{d}x \rho \nabla g_R \cdot \nabla\Big(-\frac{\Delta\sqrt{\rho}}{\sqrt{\rho}}\Big) \\
\le&-2\int \mathrm{d}x\left(-\frac{12R^4(|x|^2+\frac{1}{2}R^2)^2 - 11R^8}{4(R^2+|x|^2)^2|x|^2(2R^2+|x|^2)^2}(\phi\psi)^2\right).
\end{aligned} \tag{3.12}$$

We can prove

$$\begin{aligned}&\frac{12R^4(|x|^2+\frac{1}{2}R^2)^2-11R^8}{4(R^2+|x|^2)^2|x|^2(2R^2+|x|^2)^2}(\phi)^2\\ =&\frac{R^4(12(|x|^2+\frac{1}{2}R^2)^2-11R^4)}{2(R^2+|x|^2)^3|x|(2R^2+|x|^2)}\frac{1}{\langle x/R\rangle^2}\le C_R\frac{1}{\langle x/R\rangle^2}\end{aligned} \tag{3.13}$$

where $C_R\approx 0.3338\frac{1}{R}$ and the notation $\langle x\rangle := \sqrt{1+|x|^2}$. So we have

$$\begin{aligned}&\int \mathrm{d}x\rho\nabla g_R\cdot\nabla(-\frac{\Delta\sqrt{\rho}}{\sqrt{\rho}})\\ \le&2C_R\int \mathrm{d}x\frac{\psi^2}{\langle x/R\rangle^2}=2C_R\int \mathrm{d}x\frac{\rho}{\langle x/R\rangle^2}=2C_RM_R(\rho)\end{aligned} \tag{3.14}$$

where $M_R(\rho) := \int \mathrm{d}x\frac{\rho}{\langle x/R\rangle^2}$. Adding this term to L. Chen and Siedentop's result, we have

$$0\le Z\langle M_R(\rho_t)\rangle_\infty + 2c^W C_R\langle M_R(\rho_t)\rangle_\infty - \frac{1}{4}\langle M_R(\rho_t)\rangle_\infty^2 \tag{3.15}$$

where $\langle f(\rho)\rangle_\infty := \limsup_{T\to\infty}\frac{1}{T}\int_0^T \mathrm{d}t f(\rho)$ is set by L. Chen and Siedentop. Since $\lim_{R\to\infty} C_R = 0$, we prove

$$\limsup_{T\to\infty}\frac{1}{T}\int_0^T \mathrm{d}t\int_B \mathrm{d}x\rho_t(x)\le 4Z. \tag{3.16}$$

□

3.2 Bound on Excess Charge in the relativistic time-dependent Thomas-Fermi theory

In this section, we replace the non-relativistic TF term in (3.4) by the relativistic TF term, and still want to have the same result as L. Chen and Siedentop [5]. Comparing to Theorem 4, we drop the Weizsäcker term. We know

$$\gamma(x,\xi)=q\mathbb{1}_{\{H(x,\xi)<0\}}=q\mathbb{1}_{\{T(\xi)-\varphi(x)<0\}}=q\mathbb{1}_{\{\xi<\sqrt{\varphi^2(x)+2m\varphi(x)}\}}, \tag{3.17}$$

where $T(\xi) := \sqrt{\xi^2+m^2}-m$ is the kinetic energy and $q=2$ for electrons. The density is

$$\begin{aligned}\rho(x)&=\int đ\xi\gamma(x,\xi)=\frac{1}{(2\pi)^3}\int \mathrm{d}\xi\gamma(x,\xi)\\ &=\frac{4\pi q}{(2\pi)^3}\int_0^{\sqrt{\varphi^2(x)+2m\varphi(x)}}\mathrm{d}\xi\xi^2=\gamma_{TF}^{-\frac{3}{2}}(\varphi^2(x)+2m\varphi(x))^{\frac{3}{2}}.\end{aligned} \tag{3.18}$$

Solve the equation of φ, since we need φ positive, we have

$$\varphi=\frac{-2m+\sqrt{4m^2+4\gamma_{TF}\rho^{\frac{2}{3}}}}{2}=\sqrt{\gamma_{TF}\rho^{\frac{2}{3}}+m^2}-m. \tag{3.19}$$

We use local Fermi momentum [10]

$$p = \gamma_{TF}^{\frac{1}{2}} \rho^{\frac{1}{3}}. \tag{3.20}$$

So the massive TF term is

$$\begin{aligned}
&\int \mathrm{đ}\xi \gamma(x,\xi) T(\xi) \\
&= \frac{4\pi q}{(2\pi)^3} \int_0^{\sqrt{\varphi^2(x)+2m\varphi(x)}} \mathrm{d}\xi \xi^2 T(\xi) = \frac{4\pi q}{(2\pi)^3} \int_0^{p} \mathrm{d}\xi \xi^2 T(\xi) \\
&= \frac{q}{16\pi^2} \left(p\sqrt{p^2+m^2}(2p^2+m^2) - m^4 \ln\left(\frac{p+\sqrt{p^2+m^2}}{m}\right) - \frac{8}{3} m p^3 \right) \\
&=: f(p).
\end{aligned} \tag{3.21}$$

This can also be found in Engel and Dreizler [9]. We solve the variational problem

$$\begin{aligned}
&\frac{\mathrm{d}}{\mathrm{d}\varepsilon} f\left(\gamma_{TF}^{\frac{1}{2}} (\rho+\varepsilon\eta)^{\frac{1}{3}}\right)\Big|_{\varepsilon=0} \\
=&\frac{\gamma_{TF}^{\frac{3}{2}}}{3} \frac{\gamma_{TF}\rho^{\frac{2}{3}} - m\sqrt{\gamma_{TF}\rho^{\frac{2}{3}}+m^2} + m^2}{\sqrt{\gamma_{TF}\rho^{\frac{2}{3}}+m^2}} \eta =: g(\rho)\eta.
\end{aligned} \tag{3.22}$$

So the term $\frac{\gamma_{TF}}{2}\rho_t^{\frac{2}{3}}$ in (3.4) is replaced by $g(\rho_t)$ here. In L. Chen and Siedentop's proof, there is a term

$$R_2 := \left\langle \int \mathrm{d}x \rho_t \nabla g_R \cdot \nabla \frac{\gamma_{TF}}{2} \rho_t^{\frac{2}{3}} \right\rangle_\infty \leq 0. \tag{3.23}$$

Now R_2 is

$$R_2 := \left\langle \int \mathrm{d}x \rho \nabla g_R \cdot \nabla g(\rho) \right\rangle_\infty. \tag{3.24}$$

We need to find a function $h(\rho)$, such that

$$\nabla h(\rho) = \rho \nabla g(\rho). \tag{3.25}$$

It means

$$h'(\rho)\nabla\rho = \rho g'(\rho)\nabla\rho. \tag{3.26}$$

We also need $\lim_{x\to\infty} h(\rho)(x) = 0$. This means $h(0)$ should be 0. So we choose

$$\begin{aligned}
h(t) &= \int_0^t h'(s)\mathrm{d}s = \int_0^t s g'(s)\mathrm{d}s \\
&= \int_0^t s \frac{\gamma_{TF}^3}{9\sqrt{\gamma_{TF}s^{\frac{2}{3}}+m^2}\gamma_{TF}^{\frac{1}{2}} s^{\frac{1}{3}}} \mathrm{d}s \\
&= \frac{\gamma_{TF}^{\frac{3}{2}} t}{12}\sqrt{\gamma_{TF}t^{\frac{2}{3}}+m^2} - \frac{m^2\gamma_{TF}^{\frac{1}{2}} t^{\frac{1}{3}}}{8}\sqrt{\gamma_{TF}t^{\frac{2}{3}}+m^2} \\
&\quad + \frac{m^4}{8} \ln\left(\frac{\gamma_{TF}^{\frac{1}{2}} t^{\frac{1}{3}} + \sqrt{\gamma_{TF}t^{\frac{2}{3}}+m^2}}{m}\right) \geq 0,
\end{aligned} \tag{3.27}$$

which satisfies (3.25). Then we have

$$\begin{aligned} R_2 &= \left\langle \int \mathrm{d}x \rho \nabla g_R \cdot \nabla g(\rho) \right\rangle_\infty = \left\langle \int \mathrm{d}x \nabla h(\rho) \cdot \nabla g_R \right\rangle_\infty \\ &= -\left\langle \int \mathrm{d}x h(\rho) \Delta g_R \right\rangle_\infty \le 0. \end{aligned} \tag{3.28}$$

The non-positivity of R_2 is kept. So the result is the same as before.

3.3 Bounded from below by N

From now we focus on the time-independent relativistic TFW model. We want to prove the energy $\mathcal{E}_Z^{rTFW}(p)$ given in (1.19) is bounded from below by N in this section.

Theorem 5. *For $p \in L^3 \cap P$ and $\alpha Z \le \sqrt{\frac{27\lambda}{8}}$, there is a constant c, such that*

$$\mathcal{E}_Z^{rTFW}(p) > cN. \tag{3.29}$$

The idea to prove this theorem is using the positive terms, and the kinetic energy, i.e., TF and Weizsäcker term, to control the negative Coulomb term.

Proof. For the TF term, from (3.21), we have

$$\begin{aligned} &\frac{1}{8\pi^2} \int \mathrm{d}x \left(p\sqrt{p^2+m^2}(2p^2+m^2) - m^4 \ln\left(\frac{p+\sqrt{p^2+m^2}}{m}\right) - \frac{8}{3}mp^3 \right) \\ &= \frac{8\pi}{(2\pi)^3} \int \mathrm{d}x \int_0^p \mathrm{d}\xi \xi^2 T(\xi) \ge \frac{8\pi}{(2\pi)^3} \int \mathrm{d}x \int_0^p \mathrm{d}\xi \xi^2 (\xi - m) \\ &= \frac{8\pi}{(2\pi)^3} \int \mathrm{d}x \left(\frac{1}{4}p^4 - m\frac{1}{3}p^3 \right) = \frac{1}{4\pi^2} \int \mathrm{d}x p^4 - mN. \end{aligned} \tag{3.30}$$

For the Weizsäcker term, there exists a function $F(p)$, such that

$$\begin{aligned} &\int \mathrm{d}x |\nabla p(x)|^2 \frac{p(x)}{\sqrt{p^2(x)+m^2}} \left(1 + 2\frac{p(x)}{\sqrt{p^2(x)+m^2}} \operatorname{arsinh}\left(\frac{p(x)}{m}\right) \right) \\ &= \int \mathrm{d}x |\nabla F(p(x))|^2 \ge \frac{1}{4} \int \mathrm{d}x \frac{|F(p(x))|^2}{|x|^2}. \end{aligned} \tag{3.31}$$

We will give the expression of F later. For the Coulomb term we use the Schwarz inequality

$$\int \mathrm{d}x \frac{p^3(x)}{|x|} \le \frac{1}{2} \left(\varepsilon \int \mathrm{d}x \frac{|F(p(x))|^2}{|x|^2} + \frac{1}{\varepsilon} \int \mathrm{d}x \frac{p^6(x)}{|F(p(x))|^2} \right). \tag{3.32}$$

The first term can be bounded by the Weizsäcker term. Then we want to bound the second term as following

$$\frac{p^6(x)}{|F(p(x))|^2} \le C_1 p^4(x) + C_2 p^3(x), \tag{3.33}$$

where $C_1, C_2 \geq 0$. To prove the existence of C_1, C_2. We want to find a lower estimate of $F(p)$. We have

$$\frac{p(x)}{\sqrt{p^2(x)+m^2}}\left(1+2\frac{p(x)}{\sqrt{p^2(x)+m^2}}\operatorname{arsinh}\left(\frac{p(x)}{m}\right)\right) \geq \frac{mp(x)+2p^2(x)\operatorname{arsinh}\left(\frac{p(x)}{m}\right)}{p^2(x)+m^2}. \tag{3.34}$$

It is not hard to prove

$$\frac{mp+2p^2\operatorname{arsinh}\left(\frac{p}{m}\right)}{p^2+m^2} \geq \frac{p}{m}, \qquad p<4m. \tag{3.35}$$

Since

$$\begin{aligned}&\frac{\mathrm{d}}{\mathrm{d}p}\frac{p}{\sqrt{p^2+m^2}}\left(1+2\frac{p}{\sqrt{p^2+m^2}}\operatorname{arsinh}\left(\frac{p}{m}\right)\right)\\ =&\frac{m^2(\sqrt{p^2+m^2}+2p\operatorname{arsinh}\left(\frac{p}{m}\right))}{(p^2+m^2)^2}>0.\end{aligned} \tag{3.36}$$

We have

$$\frac{mp+2p^2\operatorname{arsinh}\left(\frac{p}{m}\right)}{p^2+m^2} \geq 4, \qquad p \geq 4m. \tag{3.37}$$

Then we have

$$\begin{aligned}&\frac{p}{\sqrt{p^2+m^2}}\left(1+2\frac{p}{\sqrt{p^2+m^2}}\operatorname{arsinh}\left(\frac{p}{m}\right)\right)\\ \geq&\begin{cases}\frac{p}{m} & p<4m\\ 4 & p\geq 4m\end{cases} = \left(\begin{cases}\sqrt{\frac{p}{m}} & p<4m\\ 2 & p\geq 4m\end{cases}\right)^2 =: \tilde{f}^2(p).\end{aligned} \tag{3.38}$$

From this we know

$$\begin{aligned}F(p) &= \int_0^p \mathrm{d}t\sqrt{\frac{t}{\sqrt{t^2+m^2}}\left(1+2\frac{t}{\sqrt{t^2+m^2}}\operatorname{arsinh}\left(\frac{t}{m}\right)\right)}\\ &\geq \int_0^p \mathrm{d}t\tilde{f}(t) = \begin{cases}\frac{2}{3}p\sqrt{\frac{p}{m}} & p<4m\\ 2p-\frac{8}{3}m & p\geq 4m\end{cases} =: \tilde{F}(p).\end{aligned} \tag{3.39}$$

It is not hard to prove that

$$\frac{p^6(x)}{|F(p(x))|^2} < \frac{p^6(x)}{|\tilde{F}(p(x))|^2} \leq \frac{1}{4}p^4(x)+\frac{9m}{4}p^3(x). \tag{3.40}$$

So we have

$$\int \mathrm{d}x\frac{p^3(x)}{|x|} \leq \frac{\varepsilon}{2}\int \mathrm{d}x\frac{|F(p(x))|^2}{|x|^2}+\frac{1}{8\varepsilon}\int \mathrm{d}xp^4(x)+\frac{27\pi^2 m}{8\varepsilon}N. \tag{3.41}$$

If we want to use the TF and Weizsäcker term to bound this Coulomb term, we should have

$$2 \geq \frac{\alpha Z}{3\varepsilon}, \quad \frac{3\lambda}{4} \geq \frac{4\alpha Z \varepsilon}{3}. \tag{3.42}$$

So when $\alpha Z \leq \sqrt{\frac{27\lambda}{8}}$, the energy $\mathcal{E}_Z^{rTFW}$ can be bounded by N from below. □

Now we also take the Dirac term into account. It is

$$\mathcal{E}^D(p) := \frac{\alpha}{8\pi^3} \int \mathrm{d}x \left(-2p^4(x) + 3\left(p(x)\sqrt{p^2(x)+m^2} - m^2 \operatorname{arsinh}\left(\frac{p(x)}{m}\right)\right)^2 \right). \tag{3.43}$$

We consider

$$\begin{aligned} & p^4 - (-2p^4 + 3\left(p\sqrt{p^2+m^2} - m^2 \operatorname{arsinh}\left(\frac{p}{m}\right)\right)^2) \\ = & -3m^2\left(p^2 - 2p\sqrt{p^2+m^2}\operatorname{arsinh}\left(\frac{p}{m}\right) + m^2 \operatorname{arsinh}^2\left(\frac{p}{m}\right)\right) =: f_d(p). \end{aligned} \tag{3.44}$$

We can see $f_d(0) = 0$. It is not hard to prove that $\lim\limits_{p\to\infty} \frac{f_d(p)}{p^3} = 0$. So there exists a constant $C > 0$, such that

$$-2p^4 + 3\left(p\sqrt{p^2+m^2} - m^2 \operatorname{arsinh}\left(\frac{p}{m}\right)\right)^2) \geq p^4 - Cp^3, \tag{3.45}$$

numerically, this C is about 2.56. So we know that when $\alpha Z \leq \sqrt{\frac{27\lambda}{8}}$, $\mathcal{E}^{rTFDW} := \mathcal{E}_Z^{rTFW} + \mathcal{E}^D$ is bounded by N from below.

3.4 Bounded from below by $D[\rho]$

In this section, we want to bound $\mathcal{E}_Z^{rTFW}$ by $D[\rho]$ instead of N.

Theorem 6. *For $p \in P$ and $\alpha Z \leq \frac{\sqrt{4.35\lambda}}{2}$, there is a constant c, such that*

$$\mathcal{E}_Z^{rTFW}(p) > cD[\rho]. \tag{3.46}$$

Proof. We use the decomposition of Coulomb potential (Simon [34, p. 51])

$$\frac{1}{|x|} = V_1 + V_2, \tag{3.47}$$

where $V_2 := \frac{3}{4\pi R^3}\mathbb{1}_{B_R(0)} * \frac{1}{|\cdot|}$, $R > 0$. Since $\mathbb{1}_{B_R(0)}$ is spherical symmetric, we can use Newton's theorem [26]. We have

$$\begin{aligned} V_2 = & \frac{3}{4\pi R^3}\int_{|y|<R} \mathrm{d}y \frac{1}{|x-y|} = \frac{3}{4\pi R^3}\int_{|y|<R}\mathrm{d}y \frac{1}{\max(|x|,|y|)} \\ = & \begin{cases} \dfrac{3}{2R} - \dfrac{|x|^2}{2R^3} & |x| < R \\ \dfrac{1}{|x|} & |x| \geq R \end{cases}. \end{aligned} \tag{3.48}$$

We compute

$$
\begin{aligned}
&\frac{1}{8\pi^2}\int \mathrm{d}x\left(-\frac{8\alpha Z p^3(x)}{3}V_2+\frac{4\alpha}{9\pi^2}\int \mathrm{d}y\frac{p^3(x)p^3(y)}{|x-y|}\right)\\
=&\frac{1}{8\pi^2}\left(-\frac{4\alpha Z}{\pi R^3}D(p^3,\mathbb{1}_{B_R(0)})+\frac{8\alpha}{9\pi^2}D(p^3,p^3)\right)\\
\geq&\frac{\alpha}{9\pi^4}\left(-\frac{9\pi Z}{2R^3}D(p^3,p^3)^{\frac{1}{2}}D(\mathbb{1}_{B_R(0)},\mathbb{1}_{B_R(0)})^{\frac{1}{2}}+D(p^3,p^3)\right)\\
\geq&\frac{\alpha}{9\pi^4}\left(\left(D(p^3,p^3)^{\frac{1}{2}}-\frac{9\pi Z}{4R^3}D(\mathbb{1}_{B_R(0)},\mathbb{1}_{B_R(0)})^{\frac{1}{2}}\right)^2-\left(\frac{9\pi Z}{4R^3}\right)^2D(\mathbb{1}_{B_R(0)},\mathbb{1}_{B_R(0)})\right)\\
\geq&-\frac{9\alpha Z^2}{16\pi^2R^6}D(\mathbb{1}_{B_R(0)},\mathbb{1}_{B_R(0)})=-\frac{3\alpha Z^2}{5R}.
\end{aligned}
\tag{3.49}
$$

By (3.48), we know

$$
V_1=\begin{cases}\frac{1}{|x|}-\frac{3}{2R}+\frac{|x|^2}{2R^3} & |x|<R\\ 0 & |x|\geq R\end{cases}.
\tag{3.50}
$$

Obviously, $V_1<\frac{1}{|x|}$. Now we want to control the V_1 part. We define a set

$$
A:=\{x|p(x)<4m\}.
\tag{3.51}
$$

By (3.39), we have

$$
p(x)\leq\frac{3}{4}F(p),\quad x\in A^c.
\tag{3.52}
$$

Then we compute

$$
\begin{aligned}
&-\frac{1}{8\pi^2}\int \mathrm{d}x\frac{8\alpha Z p^3(x)}{3}V_1>-\frac{\alpha Z}{3\pi^2}\int_{|x|<R}\mathrm{d}x\frac{p^3(x)}{|x|}\\
=&-\frac{\alpha Z}{3\pi^2}\int_{|x|<R,\ x\in A}\mathrm{d}x\frac{p^3(x)}{|x|}-\frac{\alpha Z}{3\pi^2}\int_{|x|<R,\ x\in A^c}\mathrm{d}x\frac{p^3(x)}{|x|}\\
\geq&-\frac{\alpha Z}{3\pi^2}\int_{|x|<R,\ x\in A}\mathrm{d}x\frac{(4m)^3}{|x|}-\frac{\alpha Z}{6\pi^2}\left(\varepsilon\int_{|x|<R,\ x\in A^c}\mathrm{d}x\frac{p^2(x)}{|x|^2}+\frac{1}{\varepsilon}\int_{|x|<R,\ x\in A^c}\mathrm{d}x p^4(x)\right)\\
\geq&-\frac{128m^3R^2\alpha Z}{3\pi}-\frac{\alpha Z}{6\pi^2}\left(\varepsilon\int_{|x|<R,\ x\in A^c}\mathrm{d}x\frac{\left(\frac{3}{4}F(p)\right)^2}{|x|^2}+\frac{1}{\varepsilon}\int_{|x|<R,\ x\in A^c}\mathrm{d}x p^4(x)\right).
\end{aligned}
\tag{3.53}
$$

We want to use the TF term to bound this p^4 term. We compute the derivative of the quotient of them:

$$
\begin{aligned}
&\frac{\mathrm{d}}{\mathrm{d}p}\frac{p\sqrt{p^2+m^2}(2p^2+m^2)-m^4\operatorname{arsinh}\left(\frac{p}{m}\right)-\frac{8}{3}mp^3}{p^4}\\
=&\frac{4m\left(2p^3+3m^3\operatorname{arsinh}\left(\frac{p}{m}\right)-3mp\sqrt{p^2+m^2}\right)}{3p^5}.
\end{aligned}
\tag{3.54}
$$

Then we compute the derivative of this numerator:

$$\begin{aligned}&\frac{\mathrm{d}}{\mathrm{d}p}\left(2p^3+3m^3\operatorname{arsinh}\left(\frac{p}{m}\right)-3mp\sqrt{p^2+m^2}\right)\\=&\frac{6p^2(\sqrt{p^2+m^2}-m)}{\sqrt{p^2+m^2}}\geq 0.\end{aligned}\tag{3.55}$$

So for $p\geq 0$,

$$\frac{\mathrm{d}}{\mathrm{d}p}\frac{p\sqrt{p^2+m^2}(2p^2+m^2)-m^4\operatorname{arsinh}\left(\frac{p}{m}\right)-\frac{8}{3}mp^3}{p^4}\geq 0.\tag{3.56}$$

So this function is increasing for $p\geq 0$. The value at $p>4m$ is greater than the value at $p=4m$. So we have

$$\begin{aligned}&\frac{p\sqrt{p^2+m^2}(2p^2+m^2)-m^4\operatorname{arsinh}\left(\frac{p}{m}\right)-\frac{8}{3}mp^3}{p^4}\\>&\frac{33}{64}\sqrt{17}-\frac{1}{256}\operatorname{arsinh}(4)-\frac{2}{3}=:c_R\approx 1.45.\end{aligned}\tag{3.57}$$

We want to use the TF and Weizsäcker term to bound the negative term in (3.53). So the coefficient should satisfy

$$\frac{c_R}{8\pi^2}\geq\frac{\alpha Z}{6\pi^2\varepsilon},\quad\frac{3\lambda}{32\pi^2}\geq\frac{3\alpha Z\varepsilon}{32\pi^2}.\tag{3.58}$$

So when $\alpha Z\leq\frac{\sqrt{3\lambda c_R}}{2}$, the energy $\mathcal{E}_Z^{rTFW}$ has a lower bound. □

We can get a rough lower bound which is $-\alpha Z\min\left(\frac{3Z}{5R}+\frac{128m^3R^2}{3\pi}\right)=\frac{-6(60)^{1/3}m\alpha Z^{5/3}}{5\pi^{1/3}}$. To improve the bound of αZ, we replace the set A by

$$B_r:=\{x|p(x)<mr\}.\tag{3.59}$$

Use L'Hôpital's rule, we have

$$\begin{aligned}&\lim_{p\to\infty}\frac{F(p)}{p}=\lim_{p\to\infty}F'(p)\\=&\lim_{p\to\infty}\sqrt{\frac{p}{\sqrt{p^2+m^2}}\left(1+2\frac{p}{\sqrt{p^2+m^2}}\operatorname{arsinh}\left(\frac{p}{m}\right)\right)}=\infty.\end{aligned}\tag{3.60}$$

Similarly, $\lim_{p\to 0}\frac{F(p)}{p}=0$. We compute

$$\frac{\mathrm{d}}{\mathrm{d}p}\frac{F(p)}{p}=\frac{pF'(p)-F(p)}{p^2}\geq 0.\tag{3.61}$$

The last inequality is from (3.120). Then we compare the TF term and p^5.

$$\begin{aligned}&\frac{\mathrm{d}}{\mathrm{d}p}\frac{p\sqrt{p^2+m^2}(2p^2+m^2)-m^4\operatorname{arsinh}\left(\frac{p}{m}\right)-\frac{8}{3}mp^3}{p^5}\\=&\frac{16mp^3+15m^4\operatorname{arsinh}\left(\frac{p}{m}\right)-3p(5m^2+2p^2)\sqrt{p^2+m^2}}{3p^6}.\end{aligned}\tag{3.62}$$

We compute the derivative of this numerator:

$$\begin{aligned}&\frac{\mathrm{d}}{\mathrm{d}p}\left(16mp^3+15m^4\operatorname{arsinh}\left(\frac{p}{m}\right)-3p(5m^2+2p^2)\sqrt{p^2+m^2}\right)\\=&-\frac{24p^2(\sqrt{p^2+m^2}-m)^2}{\sqrt{p^2+m^2}}\leq 0.\end{aligned}\tag{3.63}$$

So for $p\geq 0$,

$$\frac{\mathrm{d}}{\mathrm{d}p}\frac{p\sqrt{p^2+m^2}(2p^2+m^2)-m^4\operatorname{arsinh}\left(\frac{p}{m}\right)-\frac{8}{3}mp^3}{p^5}\leq 0.\tag{3.64}$$

By (3.56), (3.61), and (3.64), for $p>rm$,

$$\begin{aligned}&\frac{p\sqrt{p^2+m^2}(2p^2+m^2)-m^4\operatorname{arsinh}\left(\frac{p}{m}\right)-\frac{8}{3}mp^3}{p^4}\\\geq&\frac{r\sqrt{r^2+1}(2r^2+1)-\operatorname{arsinh}(r)-\frac{8}{3}r^3}{r^4}:=q_{TF}(r),\\&\frac{F(p)}{p}\geq\frac{F(rm)}{rm}:=q_F(r).\end{aligned}\tag{3.65}$$

For $p<rm$,

$$\begin{aligned}&\frac{p\sqrt{p^2+m^2}(2p^2+m^2)-m^4\operatorname{arsinh}\left(\frac{p}{m}\right)-\frac{8}{3}mp^3}{p^5}\\\geq&\frac{r\sqrt{r^2+1}(2r^2+1)-\operatorname{arsinh}(r)-\frac{8}{3}r^3}{r^5}=\frac{q_{TF}(r)}{r}.\end{aligned}\tag{3.66}$$

It is easy to prove that $\frac{F(rm)}{rm}$ does not depend on m. (Note that F has also an explicit dependence on m.) Using the Schwarz inequality, we rewrite (3.53) as following

$$
\begin{aligned}
&-\frac{1}{8\pi^2}\int \mathrm{d}x\frac{8\alpha Zp^3(x)}{3}V_1\\
\geq&-\frac{\alpha Z}{6\pi^2}\left(\frac{3q_{TF}(r)}{4\alpha Zr}\int_{|x|<R,\ x\in B_r}\mathrm{d}xp^5+\frac{4\alpha Zr}{3q_{TF}(r)}\int_{|x|<R,\ x\in B_r}\mathrm{d}x\frac{p}{|x|^2}\right)\\
&-\frac{\alpha Z}{6\pi^2}\left(\frac{\varepsilon}{q_F^2(r)}\int_{|x|<R,\ x\in B_r^c}\mathrm{d}x\frac{(F(p))^2}{|x|^2}\right.\\
&\left.+\frac{1}{\varepsilon q_{TF}(r)}\int_{|x|<R,\ x\in B_r^c}\mathrm{d}x(p\sqrt{p^2+m^2}(2p^2+m^2)-m^4\operatorname{arsinh}\left(\frac{p}{m}\right)-\frac{8}{3}mp^3)\right) \qquad (3.67)\\
\geq&-\frac{q_{TF}(r)}{8\pi^2 r}\int_{|x|<R,\ x\in B_r}\mathrm{d}xp^5-\frac{8mr^2R(\alpha Z)^2}{9\pi q_{TF}(r)}\\
&-\frac{\alpha Z}{6\pi^2}\left(\frac{\varepsilon}{q_F^2(r)}\int_{|x|<R,\ x\in B_r^c}\mathrm{d}x\frac{(F(p))^2}{|x|^2}\right.\\
&\left.+\frac{1}{\varepsilon q_{TF}(r)}\int_{|x|<R,\ x\in B_r^c}\mathrm{d}x(p\sqrt{p^2+m^2}(2p^2+m^2)-m^4\operatorname{arsinh}\left(\frac{p}{m}\right)-\frac{8}{3}mp^3)\right).
\end{aligned}
$$

So (3.58) is changed to

$$\frac{1}{8\pi^2}\geq\frac{\alpha Z}{6\pi^2 q_{TF}(r)\varepsilon},\quad \frac{3\lambda}{32\pi^2}\geq\frac{\alpha Z\varepsilon}{6\pi^2 q_F^2(r)}. \tag{3.68}$$

So we have $\alpha Z\leq\sqrt{\frac{27\lambda q_{TF}(r)q_F^2(r)}{64}}$. It is easy to see that $q_{TF}(0)q_F^2(0)=0$. We can also prove that $\lim_{r\to\infty}q_{TF}(r)q_F^2(r)=\infty$ and $q_{TF}(r)q_F^2(r)$ is increasing. So there always is a r_Z satisfied $\alpha Z=\sqrt{\frac{27\lambda q_{TF}(r_Z)q_F^2(r_Z)}{64}}$. It means that there is no constraint on αZ any more. The energy always has a lower bound. So

$$\mathcal{E}_Z^{rTFW}\geq\ -\frac{3\alpha Z^2}{5R}-\frac{8mr_Z^2R(\alpha Z)^2}{9\pi q_{TF}(r_Z)}. \tag{3.69}$$

Optimizing this in R, we get

$$\mathcal{E}_Z^{rTFW}\geq-\min_{R>0}\left(\frac{3\alpha Z^2}{5R}+\frac{8mr_Z^2R(\alpha Z)^2}{9\pi q_{TF}(r_Z)}\right)=-\frac{8r_Zm^{\frac{1}{2}}\alpha^{\frac{3}{2}}Z^2}{\sqrt{40\pi q_{TF}(r_Z)}}. \tag{3.70}$$

Now we change our setting of c. It is not a constant any more. We set $\alpha=\frac{1}{c}$ and fix $\kappa=\frac{Z}{c}$.

Then our functional becomes

$$
\begin{aligned}
&\mathcal{E}^{TFW}_{\kappa,c}(p) = \\
&\frac{c}{8\pi^2}\int \mathrm{d}x \Bigg(p(x)\sqrt{p^2(x)+m^2c^2}(2p^2(x)+m^2c^2) - m^4c^4 \operatorname{arsinh}\left(\frac{p(x)}{mc}\right) - \frac{8}{3}mcp^3(x) \\
&+ 3\lambda|\nabla p(x)|^2 \frac{p(x)}{\sqrt{p^2(x)+m^2c^2}}\left(1+2\frac{p(x)}{\sqrt{p^2(x)+m^2c^2}}\operatorname{arsinh}\left(\frac{p(x)}{mc}\right)\right) \\
&-\frac{8Zp^3(x)}{3c|x|} + \frac{4}{9c\pi^2}\int \mathrm{d}y \frac{p^3(x)p^3(y)}{|x-y|}\Bigg) \\
&= \frac{mc^2}{8\pi^2}\int \mathrm{d}x \Bigg(\tilde{p}(x)\sqrt{\tilde{p}^2(x)+1}(2\tilde{p}^2(x)+1) - \operatorname{arsinh}(\tilde{p}(x)) - \frac{8}{3}\tilde{p}^3(x) \\
&+ 3\lambda|\nabla \tilde{p}(x)|^2 \frac{\tilde{p}(x)}{\sqrt{\tilde{p}^2(x)+1}}\left(1+2\frac{\tilde{p}(x)}{\sqrt{\tilde{p}^2(x)+1}}\operatorname{arsinh}(\tilde{p}(x))\right) \\
&-\frac{8\kappa\tilde{p}^3(x)}{3|x|} + \frac{4}{9c\pi^2}\int \mathrm{d}y \frac{\tilde{p}^3(x)\tilde{p}^3(y)}{|x-y|}\Bigg) =: \tilde{\mathcal{E}}^{TFW}_{\kappa,c}(\tilde{p}),
\end{aligned}
\tag{3.71}
$$

where $\tilde{p}(x) := \frac{1}{m}p(\frac{x}{m})$, and we scale x to $\frac{x}{m}$. Similar as (3.49),

$$
\frac{mc^2}{8\pi^2}\int \mathrm{d}x \left(-\frac{8\kappa p^3(x)}{3}V_2 + \frac{4}{9c\pi^2}\int \mathrm{d}y \frac{p^3(x)p^3(y)}{|x-y|}\right) \geq -\frac{3mc^3\kappa^2}{5R}. \tag{3.72}
$$

Similar as (3.67),

$$
\begin{aligned}
&-\frac{mc^2}{8\pi^2}\int \mathrm{d}x \frac{8\kappa p^3(x)}{3}V_1 \\
\geq &-\frac{mc^2 q_{TF}(r)}{8\pi^2 r}\int_{|x|<R,\ x\in\tilde{B}_r} \mathrm{d}x p^5 - \frac{8mc^2r^2R\kappa^2}{9\pi q_{TF}(r)} \\
&-\frac{mc^2\kappa}{6\pi^2}\Bigg(\frac{\varepsilon}{q_F^2(r)}\int_{|x|<R,\ x\in\tilde{B}_r^c} \mathrm{d}x \frac{(F(p))^2}{|x|^2} \\
&+\frac{1}{\varepsilon q_{TF}(r)}\int_{|x|<R,\ x\in\tilde{B}_r^c} \mathrm{d}x (p\sqrt{p^2+1}(2p^2+1) - \operatorname{arsinh}(p) - \frac{8}{3}p^3)\Bigg)
\end{aligned}
\tag{3.73}
$$

where $\tilde{B}_r := \{x|p(x)<r\}$. The same as before, there is a r_κ satisfied $\kappa = \sqrt{\frac{27\lambda q_{TF}(r_\kappa)q_F^2(r_\kappa)}{64}}$. So we have

$$
\mathcal{E}^{TFW}_{\kappa,c} \geq -\min_{R>0}\left(\frac{3mc^3\kappa^2}{5R} + \frac{8mc^2r_\kappa^2R\kappa^2}{9\pi q_{TF}(r_\kappa)}\right) = -\frac{8r_\kappa mc^{\frac{5}{2}}\kappa^2}{\sqrt{30\pi q_{TF}(r_\kappa)}} = -\frac{8r_\kappa mZ^{\frac{5}{2}}}{\sqrt{30\pi\kappa q_{TF}(r_\kappa)}}. \tag{3.74}
$$

3.5 Existence of the minimizer

Since $\mathcal{E}^{rTFW}_Z$ has a lower bounded, there is a finite infimum of it. We claim that the infimum is also the minimum and there is a global minimizer.

Theorem 7. *For $p \in P$, there is a p_0, such that*

$$\mathcal{E}_Z^{rTFW}(p_0) = \inf \mathcal{E}_Z^{rTFW}(p). \tag{3.75}$$

Proof. $\mathcal{E}_Z^{rTFW}$ has a lower bounded, so there is a minimizing sequence p_j, such that

$$\lim_{j\to\infty} \mathcal{E}_Z^{rTFW}(p_j) = \inf_p \mathcal{E}_Z^{rTFW}(p). \tag{3.76}$$

To prove the existence of the minimizer, we need to prove the lower semicontinuity of each term of $\mathcal{E}_Z^{rTFW}$. First we consider the TF term. We define

$$f_{TF}(\eta) := \eta^{\frac{1}{3}}\sqrt{\eta^{\frac{2}{3}} + m^2}(2\eta^{\frac{2}{3}} + m^2) - m^4 \operatorname{arsinh}\left(\frac{\eta^{\frac{1}{3}}}{m}\right) - \frac{8}{3}m\eta, \quad \eta \geq 0. \tag{3.77}$$

So we have

$$f_{TF}(\eta_1) = f_{TF}(\eta_2) + f'_{TF}(\eta_2)(\eta_1 - \eta_2) + \frac{1}{2}f''_{TF}(\eta_\delta)(\eta_1 - \eta_2)^2, \tag{3.78}$$

where η_δ is between η_1 and η_2. We compute the derivatives of f_{TF}, and have

$$\begin{aligned} f'_{TF}(\eta) &= \frac{8}{3}(\sqrt{\eta^{\frac{2}{3}} + m^2} - m), \\ f''_{TF}(\eta) &= \frac{8}{9\sqrt{\eta^{\frac{2}{3}} + m^2}\eta^{\frac{1}{3}}} \geq 0. \end{aligned} \tag{3.79}$$

So we have

$$f_{TF}(\eta_1) \geq f_{TF}(\eta_2) + f'_{TF}(\eta_2)(\eta_1 - \eta_2). \tag{3.80}$$

We take a weak convergent subsequence of p_j^3 in $L^{\frac{4}{3}}$. The weak limit is p_{TF}^3. We still call this sequence p_j^3. So we have

$$\int \mathrm{d}x f_{TF}(p_j^3(x)) \geq \int \mathrm{d}x (f_{TF}(p_{TF}^3(x)) + f'_{TF}(p_{TF}^3(x))(p_j(x) - p_{TF}^3(x))). \tag{3.81}$$

Since $p_{TF}^3 \in L^{\frac{4}{3}}$ and $f'_{TF}(p^3) = \frac{8}{3}(\sqrt{p^2 + m^2} - m) \leq \frac{8}{3}p$, we have $f'_{TF}(p_{TF}^3) \in L^4$. So we have

$$\begin{aligned} &\underline{\lim} \int \mathrm{d}x f_{TF}(p_j^3(x)) \\ \geq &\lim \int \mathrm{d}x (f_{TF}(p_{TF}^3(x)) + f'_{TF}(p_{TF}^3(x))(p_j^3(x) - p_{TF}^3(x))) \\ = &\int \mathrm{d}x f_{TF}(p_{TF}^3(x)). \end{aligned} \tag{3.82}$$

Now we consider the Weizsäcker term. We know $\|\nabla F(p_j)\|_2$ is bounded. Since $F(0) = 0$, it is easy to prove that $F(p_j)$ vanish at infinity. So we know $F(p_j) \in D^1$. D^1 consists of functions that vanishes at infinity with gradient in L^2. Since $\|\nabla F(p_j)\|_2$ is uniformly bounded, we have a subsequence still called $\nabla F(p_j)$, which converges weakly in L^2 to

$\nabla\nu$, $\nu \in D^1$ and $\nu \geq 0$ (Lieb and Loss [20, Theorem 8.6]). From (3.39), we know $F(p)$ is increasing in p and $\lim_{p\to\infty} F(p) = \infty$, so F^{-1} exists. We define $p_W := F^{-1}(\nu)$. So $\nabla F(p_j)$ converges weakly to $\nabla F(p_W)$. So we have

$$\begin{aligned}&\int \mathrm{d}x|\nabla F(p_W)|^2 = \lim \int \mathrm{d}x \nabla F(p_j)\cdot\nabla F(p_W)\\ &\leq \|\nabla F(p_W)\|_2 \underline{\lim}\|\nabla F(p_j)\|_2.\end{aligned} \tag{3.83}$$

It implies

$$\underline{\lim}\|\nabla F(p_j)\|_2 \geq \|\nabla F(p_W)\|_2. \tag{3.84}$$

Then we consider the Coulomb term. From (3.38), we know $\|\nabla\tilde{F}(p_j)\|_2$ is also uniformly bounded. Similar as above, we have a subsequence still called $\nabla\tilde{F}(p_j)$ and a p_C. The sequence converges weakly in L^2 to $\nabla\tilde{F}(p_C)$. By Lieb and Loss [20, Theorem 8.6], we have, for any set A of finite measure,

$$\chi_A\tilde{F}(p_j) \to \chi_A\tilde{F}(p_C) \textit{ strongly in } L^p \tag{3.85}$$

for every $1 \leq p < 6$. We define $q_j := \tilde{F}(p_j),\ q_C := \tilde{F}(p_C)$. From the definition of $\tilde{F}$, we have

$$p_j = \tilde{F}^{-1}(q_j) = \begin{cases} m^{\frac{1}{3}}\left(\frac{3}{2}q_j\right)^{\frac{2}{3}} & q_j < \frac{16}{3}m \\ \frac{1}{2}q_j + \frac{4}{3}m & q_j \geq \frac{16}{3}m \end{cases}. \tag{3.86}$$

We compute $\frac{p_j^3 - p_C^3}{q_j - q_C}$. If $q_j,\ q_C \leq \frac{16}{3}m$, we have

$$\frac{p_j^3 - p_C^3}{q_j - q_C} = \frac{m\left(\frac{3}{2}q_j\right)^2 - m\left(\frac{3}{2}q_C\right)^2}{q_j - q_C} = \frac{9}{4}m(q_j + q_C). \tag{3.87}$$

If $q_j,\ q_C > \frac{16}{3}m$, we have

$$\begin{aligned}&\frac{p_j^3 - p_C^3}{q_j - q_C} = \frac{\left(\frac{1}{2}q_j + \frac{4}{3}m\right)^3 - \left(\frac{1}{2}q_C + \frac{4}{3}m\right)^3}{q_j - q_C}\\ &= \frac{1}{2}\left(\left(\frac{1}{2}q_j + \frac{4}{3}m\right)^2 + \left(\frac{1}{2}q_C + \frac{4}{3}m\right)^2 + \left(\frac{1}{2}q_j + \frac{4}{3}m\right)\left(\frac{1}{2}q_C + \frac{4}{3}m\right)\right)\\ &\leq \frac{3}{4}\left(\left(\frac{1}{2}q_j + \frac{4}{3}m\right)^2 + \left(\frac{1}{2}q_C + \frac{4}{3}m\right)^2\right)\\ &\leq \frac{3}{2}\left(\left(\frac{1}{2}q_j\right)^2 + \left(\frac{4}{3}m\right)^2 + \left(\frac{1}{2}q_C\right)^2 + \left(\frac{4}{3}m\right)^2\right) \leq \frac{3}{8}\left(q_j^2 + q_C^2\right) + \frac{16}{3}m^2.\end{aligned} \tag{3.88}$$

Otherwise, we suppose $q_j > \frac{16}{3}m,\ q_C \leq \frac{16}{3}m$. Since $(\tilde{F}^{-1})^3$ is convex. We have

$$\begin{aligned}&\frac{p_j^3 - p_C^3}{q_j - q_C} \leq \frac{p_j^3 - \left(\tilde{F}^{-1}\left(\frac{16}{3}m\right)\right)^3}{q_j - \frac{16}{3}m}\\ &\leq \frac{3}{8}\left(q_j^2 + \left(\frac{16}{3}m\right)^2\right) + \frac{16}{3}m^2 \leq \frac{3}{8}q_j^2 + 16m^2 \leq \frac{3}{8}(q_j^2 + q_C^2) + 16m^2.\end{aligned} \tag{3.89}$$

For $1 < \gamma < 2$, using the convexity of x^γ, it is easy to prove $(a+b+c)^\gamma \le c_\gamma(a^\gamma+b^\gamma+c^\gamma),\ c_\gamma > 0$. So we have

$$\begin{aligned}
&\int_A \mathrm{d}x|p_j^3(x) - p_C^3(x)|^\gamma \\
\le& \int_A \mathrm{d}x|q_j(x) - q_C(x)|^\gamma \left|\frac{9}{4}m(q_j(x) + q_C(x)) + \frac{3}{8}\left(q_j^2(x) + q_C^2(x)\right) + \frac{16}{3}m^2\right. \\
&\left.+\frac{3}{8}(q_j^2(x) + q_C^2(x)) + 16m^2\right|^\gamma \\
\le& \left(\frac{64m^2}{3}\right)^\gamma c_\gamma \int_A \mathrm{d}x|q_j(x) - q_C(x)|^\gamma + \left(\frac{9m}{4}\right)^\gamma c_\gamma \int_A \mathrm{d}x|q_j(x) - q_C(x)|^\gamma|q_j(x) + q_C(x)|^\gamma \\
&+ \left(\frac{4}{3}\right)^\gamma c_\gamma \int_A \mathrm{d}x|q_j(x) - q_C(x)|^\gamma|q_j^2(x) + q_C^2(x)|^\gamma. \\
\le& \left(\frac{64m^2}{3}\right)^\gamma c_\gamma \int_A \mathrm{d}x|q_j(x) - q_C(x)|^\gamma \\
&+ \left(\frac{9m}{4}\right)^\gamma c_\gamma \left(\int_A \mathrm{d}x|q_j(x) - q_C(x)|^{2\gamma}\right)^{\frac{1}{2}} \left(\int_A \mathrm{d}x|q_j(x) + q_C(x)|^{2\gamma}\right)^{\frac{1}{2}} \\
&+ \left(\frac{4}{3}\right)^\gamma c_\gamma \left(\int_A \mathrm{d}x|q_j(x) - q_C(x)|^{3\gamma}\right)^{\frac{1}{3}} \left(\int_A \mathrm{d}x|q_j^2(x) + q_C^2(x)|^{\frac{3\gamma}{2}}\right)^{\frac{2}{3}}.
\end{aligned} \tag{3.90}$$

Since $\chi_A q_j$ converges strongly to $\chi_A q_C$ in L^p for every $1 \le p < 6$. It converges strongly in $L^\gamma,\ L^{2\gamma}$, and $L^{3\gamma}$. The norms $\|\chi_A q_j\|_{2\gamma},\ \|\chi_A q_j\|_{3\gamma}$ are uniformly bounded. So we have

$$\lim \int_A \mathrm{d}x|p_j^3(x) - p_C^3(x)|^\gamma = 0. \tag{3.91}$$

By Lieb and Loss [20, Theorem 11.4], we have

$$\lim \int \mathrm{d}x \frac{p_j^3(x)}{|x|} = \int \mathrm{d}x \frac{p_C^3(x)}{|x|}. \tag{3.92}$$

For the $D[\rho]$ term, it is easy to prove that $D(\rho, \phi)$ is a scaler product. So the space $H_D := \{\rho | D[\rho] < \infty\}$ is a Hilbert space, and is reflexive. Since $D[p_j^3]$ is bounded. There is a subsequence still called $\{p_j^3\}$ which converges weakly in H_D to p_D^3. So we know

$$D(p_D^3, p_D^3) = \lim D(p_j^3, p_D^3) \le \sqrt{D(p_D^3, p_D^3)}\,\underline{\lim}\sqrt{D(p_j^3, p_j^3)}. \tag{3.93}$$

It means

$$\underline{\lim} D(p_j^3, p_j^3) \ge D(p_D^3, p_D^3). \tag{3.94}$$

Now we need to prove the limits in different senses are the same. We prove $p_W = p_C$ first. By Lieb and Loss [20, Theorem 8.7], there is a subsequence of $\{F(p_j)\}$ still called $\{F(p_j)\}$, that converges to $F(p_W)$ almost everywhere. By the continuity of F^{-1}, we know that p_j converges to p_W almost everywhere. Using the proof of Lieb and Loss [20, Theorem 8.7], p_j converges to p_C almost everywhere. It means $p_W = p_C$ almost everywhere.

We know that $\{p_j^3\}$ converges weakly in H_D to p_D^3. For any $\phi \in C_0^\infty$, $\psi := \frac{-\Delta}{4\pi}\phi$ is also in C_0^∞. So we have

$$\lim \iint \mathrm{d}x\mathrm{d}y \frac{p_j^3(x)\psi(y)}{|x-y|} = \iint \mathrm{d}x\mathrm{d}y \frac{p_D^3(x)\psi(y)}{|x-y|}. \tag{3.95}$$

It means

$$\lim \int \mathrm{d}x p_j^3(x)\phi(x) = \int \mathrm{d}x p_D^3(x)\phi(x). \tag{3.96}$$

From (3.91), p_j^3 converges to p_C^3 strongly in L^γ on A. It implies weak convergence. We choose $A = supp(\phi)$. So we have

$$\lim \int \mathrm{d}x p_j^3(x)\phi(x) = \int \mathrm{d}x p_C^3(x)\phi(x). \tag{3.97}$$

Since p_j^3 converges to p_{TF}^3 weakly in $L^{\frac{4}{3}}$. we have

$$\lim \int \mathrm{d}x p_j^3(x)\phi(x) = \int \mathrm{d}x p_{TF}^3(x)\phi(x). \tag{3.98}$$

By (3.96), (3.97), and (3.98), p_j^3 converges to p_D^3, p_C^3, and p_{TF}^3 in the sense of distribution. Since functions are uniquely determined by distributions, $p_D^3 = p_C^3 = p_{TF}^3$ almost everywhere. So $p_D = p_C = p_{TF}$ almost everywhere. We proved $p_W = p_C$ before. So we have $p_D = p_C = p_{TF} = p_W$. So it is the minimizer of $\mathcal{E}_Z^{rTFW}$. □

Now we want to prove $\inf\{\mathcal{E}_Z^{rTFW}(p) : p \geq 0,\ \int p^3(x)\mathrm{d}x = c_{TF}N\} = \inf\{\mathcal{E}_Z^{rTFW}(p) : p \geq 0,\ \int p^3(x)\mathrm{d}x \leq c_{TF}N\}$. The corresponding equation for the non-relativistic TFW theory is proved by Benguria, Brézis, and Lieb [2]. We follow their proof and deal with the different terms. Let $p \geq 0$ be such that $\int p^3(x)\mathrm{d}x < c_{TF}N$. We only need to prove: There is a sequence $p_n \geq 0$ such that $\int p_n^3(x)\mathrm{d}x = c_{TF}N$ and $\liminf \mathcal{E}_Z^{rTFW}(p_n) \leq \mathcal{E}_Z^{rTFW}(p)$. We choose

$$p_n(x) = \left(p^3(x) + \frac{k}{n^3}\zeta_n^2(x)\right)^{\frac{1}{3}} \tag{3.99}$$

where $\zeta_n(x) = \zeta_0(\frac{x}{n})$ ($\zeta_0 \in C_0^\infty$ is any function $\zeta_0 \not\equiv 0$) and $k = \frac{c_{TF}N - \int p^3(x)\mathrm{d}x}{\int \zeta_0^2(x)\mathrm{d}x}$, so that $\int p_n^3(x)\mathrm{d}x = c_{TF}N$. Comparing to the non-relativistic case, the differences are the TF and Weizsäcker term. Using the convexity of f_{TF}, we have

$$\begin{aligned}\mathcal{E}_Z^{TF}(p_n) &:= \frac{1}{8\pi^2}\int \mathrm{d}x f_{TF}(p_n^3(x)) \\ &\leq \mathcal{E}_Z^{TF}(p) + \frac{k}{8\pi^2 n^3}\int \mathrm{d}x f'_{TF}(p_n^3(x))\zeta_n^2(x).\end{aligned} \tag{3.100}$$

Using (3.79) and by Hölder's inequality

$$\begin{aligned}&\frac{k}{8\pi^2 n^3}\int \mathrm{d}x f'_{TF}(p_n^3(x))\zeta_n^2(x) = \frac{k}{3\pi^2 n^3}\int \mathrm{d}x(\sqrt{p_n^2(x)+m^2} - m)\zeta_n^2(x) \\ \leq &\frac{k}{3\pi^2 n^3}\int \mathrm{d}x p_n(x)\zeta_n^2(x) \leq \frac{k}{3\pi^2 n^3}\left(\int \mathrm{d}x p_n^3(x)\right)^{\frac{1}{3}}\left(\int \mathrm{d}x \zeta_n^3(x)\right)^{\frac{2}{3}} \\ = &\frac{k(c_{TF}N)^{\frac{1}{3}}}{3\pi^2 n}\left(\int \mathrm{d}x\zeta_0^3(x)\right)^{\frac{2}{3}} \to 0.\end{aligned} \tag{3.101}$$

We consider the Weizsäcker term:

$$\begin{aligned}
&\mathcal{E}_Z^W(p) := \\
&\frac{3\lambda}{8\pi^2}\int \mathrm{d}x |\nabla p(x)|^2 \frac{p(x)}{\sqrt{p^2(x)+m^2}}\left(1+2\frac{p(x)}{\sqrt{p^2(x)+m^2}}\operatorname{arsinh}\left(\frac{p(x)}{m}\right)\right) \\
&=\frac{3\lambda}{8\pi^2}\int \mathrm{d}x |\nabla p^3(x)|^2 f_W(p^3(x)),
\end{aligned} \tag{3.102}$$

where $f_W(\eta) := \frac{1}{\eta\sqrt{\eta^{\frac{2}{3}}+m^2}}\left(1+2\frac{\eta^{\frac{1}{3}}}{\sqrt{\eta^{\frac{2}{3}}+m^2}}\operatorname{arsinh}\left(\frac{\eta^{\frac{1}{3}}}{m}\right)\right)$. It is not hard to prove that $f_W'(\eta) < 0$. Using this and the Schwarz inequality

$$\begin{aligned}
\mathcal{E}_Z^W(p_n) \le &(1+\varepsilon)\frac{3\lambda}{8\pi^2}\int \mathrm{d}x |\nabla p^3(x)|^2 f_W(p_n^3(x)) \\
&+(1+\frac{1}{\varepsilon})\frac{3\lambda}{8\pi^2}\int \mathrm{d}x |\nabla \frac{k}{n^3}\zeta_n^2(x)|^2 f_W(p_n^3(x)) \\
\le &(1+\varepsilon)\mathcal{E}_Z^W(p) + (1+\frac{1}{\varepsilon})\mathcal{E}_Z^W\left(\frac{k}{n^3}\zeta_n^2(x)\right).
\end{aligned} \tag{3.103}$$

We have

$$\begin{aligned}
&\mathcal{E}_Z^W\left(\frac{k}{n^3}\zeta_n^2(x)\right) \\
=&\frac{3\lambda}{8\pi^2}\int \mathrm{d}x \frac{|\frac{k}{n^3}\zeta_n^2(x)|^2}{\frac{k}{n^3}\zeta_n^2(x)\sqrt{\frac{k^{\frac{2}{3}}}{n^2}\zeta_n^{\frac{4}{3}}(x)+m^2}}\left(1+2\frac{\frac{k^{\frac{1}{3}}}{n}\zeta_n^{\frac{2}{3}}(x)}{\sqrt{\frac{k^{\frac{2}{3}}}{n^2}\zeta_n^{\frac{4}{3}}(x)+m^2}}\operatorname{arsinh}\left(\frac{\frac{k^{\frac{1}{3}}}{n}\zeta_n^{\frac{2}{3}}(x)}{m}\right)\right) \\
=&\frac{3\lambda k}{8\pi^2 n^2}\int \mathrm{d}x \frac{|\zeta_0^2(x)|^2}{\zeta_0^2(x)\sqrt{\frac{k^{\frac{2}{3}}}{n^2}\zeta_0^{\frac{4}{3}}(x)+m^2}}\left(1+2\frac{k^{\frac{1}{3}}\zeta_0^{\frac{2}{3}}(x)}{\sqrt{k^{\frac{2}{3}}\zeta_0^{\frac{4}{3}}(x)+m^2n^2}}\operatorname{arsinh}\left(\frac{\frac{k^{\frac{1}{3}}}{n}\zeta_0^{\frac{2}{3}}(x)}{m}\right)\right) \to 0.
\end{aligned} \tag{3.104}$$

Since $\mathcal{E}_Z^W(p)$ is finite, let $\varepsilon \to 0$ first, then let $n \to \infty$. We have $\varepsilon\mathcal{E}_Z^W(p)+(1+\frac{1}{\varepsilon})\mathcal{E}_Z^W\left(\frac{k}{n^3}\zeta_n^2(x)\right) \to 0$. That difference of other terms go to 0, is proved by Benguria, Brézis, and Lieb [2]. So we proved $\liminf \mathcal{E}_Z^{rTFW}(p_n) \le \mathcal{E}_Z^{rTFW}(p)$. Then we consider the TFW variational problem

$$E_Z^{TFW}(N) := \inf\{\mathcal{E}_Z^{rTFW}(p) : p \ge 0, \int p^3(x)\mathrm{d}x = c_{TF}N\}. \tag{3.105}$$

We just proved $E_Z^{TFW}(N) = \inf\{\mathcal{E}_Z^{rTFW}(p) : p \ge 0, \int p^3(x)\mathrm{d}x \le c_{TF}N\}$. Obviously, $E_Z^{TFW}(N)$ is a decreasing function of N.

3.6 The excess charge problem

Proof of Theorem 2. We consider the global minimizer p_0. Let $\int p_0^3(x)\mathrm{d}x = c_{TF}N$. To make the Weizsäcker term simpler, we consider the energy as a functional of $\psi_0(x) := \sqrt{F(p_0(x))}$. So we have

$$\mathcal{E}_Z^{rTFW}(F^{-1}(\psi_0^2)) = \inf_{\psi}\{\mathcal{E}_Z^{rTFW}(F^{-1}(\psi^2))\}. \tag{3.106}$$

ψ_0 satisfies the Euler-Lagrange equation

$$\begin{aligned}&\frac{\psi(x)}{4\pi^2}\Bigg(\frac{8(F^{-1}(\psi^2))^2(x)(\sqrt{(F^{-1}(\psi^2))^2(x)+m^2}-m)}{F'(F^{-1}(\psi^2))(x)}-6\lambda\Delta\psi^2(x)\\&-\frac{8\alpha Z(F^{-1}(\psi^2))^2(x)}{|x|F'(F^{-1}(\psi^2))(x)}+\frac{8\alpha}{3\pi^2}\int\mathrm{d}y\frac{(F^{-1}(\psi^2))^2(x)(F^{-1}(\psi^2))^3(y)}{|x-y|F'(F^{-1}(\psi^2))(x)}\Bigg)=0.\end{aligned}\tag{3.107}$$

Rewriting this equation in p yields

$$\begin{aligned}&\frac{8p^2(x)(\sqrt{p^2(x)+m^2}-m)}{F'(p)(x)}-6\lambda\Delta F(p)(x)-\frac{8\alpha Zp^2(x)}{|x|F'(p)(x)}\\&+\frac{8\alpha}{3\pi^2}\int\mathrm{d}y\frac{p^2(x)p^3(y)}{|x-y|F'(p)(x)}=0.\end{aligned}\tag{3.108}$$

We prove $N\geq Z$ first. In the non-relativistic case, this is proved by Benguria, Brézis, and Lieb [2]. Our case is not so different. So we follow their proof. We choose $\zeta_o\in C_o^\infty$ the same as in Benguria, Brézis, and Lieb [2]. It is a spherically symmetric function such that $\zeta_0\not\equiv 0$, $\zeta_0(x)=0$ for $|x|<1$ and for $|x|>2$. Set $\zeta_n(x)=\zeta_0(\frac{x}{n})$. By (3.108) we have,

$$\begin{aligned}&\int\mathrm{d}x\zeta_n^2(x)\Bigg(8(\sqrt{p^2(x)+m^2}-m)-\frac{6\lambda F'(p)(x)\Delta F(p)(x)}{p^2(x)}-\frac{8\alpha Z}{|x|}\\&+\frac{8\alpha}{3\pi^2}\int\mathrm{d}y\frac{p^3(y)}{|x-y|}\Bigg)=0.\end{aligned}\tag{3.109}$$

Integrating by parts and using the Schwarz inequality, we have

$$\begin{aligned}&-\int\mathrm{d}x\zeta_n^2\frac{F'(p)\Delta F(p)}{p^2}\\&=\int\mathrm{d}x\left(2\zeta_n\nabla\zeta_n\frac{F'(p)}{p^2}+\zeta_n^2\left(\frac{F'(p)}{p^2}\right)'\nabla p\right)F'(p)\nabla p\\&\leq\frac{1}{\varepsilon}\int\mathrm{d}x|\nabla\zeta_n|^2+\int\mathrm{d}x\left(\varepsilon\left(\frac{F'^2(p)}{p^2}\right)^2+\left(\frac{F'(p)}{p^2}\right)'F'(p)\right)\zeta_n^2|\nabla p|^2.\end{aligned}\tag{3.110}$$

Using the definition of $F(p)$, we get

$$\left(\frac{F'(p)}{p^2}\right)'=-\frac{(2p^2+3m^2)\sqrt{p^2+m^2}+4(2p^2+m^2)p\operatorname{arsinh}\left(\frac{p}{m}\right)}{2p^{\frac{5}{2}}(p^2+m^2)^{\frac{3}{2}}\sqrt{\sqrt{p^2+m^2}+2p\operatorname{arsinh}\left(\frac{p}{m}\right)}}<0.\tag{3.111}$$

Define

$$g(p):=-\frac{\left(\frac{F'(p)}{p^2}\right)'F'(p)}{\left(\frac{F'^2(p)}{p^2}\right)^2}>0.\tag{3.112}$$

We easily get $g(0)=\frac{3}{2}m$ and $\lim_{p\to\infty} g(p)=\infty$. So $c_g := \min_{p\geq 0} g(p) > 0$. Choose $\varepsilon = c_g$. Then

$$-\int \mathrm{d}x \zeta_n^2 \frac{F'(p)\Delta F(p)}{p^2} \leq \frac{1}{c_g}\int \mathrm{d}x |\nabla \zeta_n|^2 \leq Cn. \tag{3.113}$$

Next, we compute

$$\int \mathrm{d}x \zeta_n^2 (\sqrt{p^2+m^2}-m) < \int \mathrm{d}x \zeta_n^2 p \leq \varepsilon_n n^2, \tag{3.114}$$

where $\varepsilon_n \to 0$ as $n\to\infty$. The last inequality is proved by Benguria, Brézis, and Lieb [2]. About the rest terms, it is proved by Benguria, Brézis, and Lieb [2] that for large n

$$\int \mathrm{d}x \zeta_n^2(x)\left(-\frac{8\alpha Z}{|x|}+\frac{8\alpha}{3\pi^2}\int \mathrm{d}y \frac{p^3(y)}{|x-y|}\right) \leq c(N-Z)n^2. \tag{3.115}$$

Combining (3.109), (3.113), (3.114), and (3.116), we find

$$\varepsilon_n n^2 + Cn + c(N-Z)n^2 \geq 0. \tag{3.116}$$

As $n\to\infty$, we have that $Z \leq N$.

To find the upper bound of N. We multiply (3.108) by $|x|F(p)$ and integrate,

$$\begin{aligned}\int \mathrm{d}x F(p)(x)|x| \Bigg(&\frac{8p^2(x)(\sqrt{p^2(x)+m^2}-m)}{F'(p)(x)} - 6\lambda \Delta F(p)(x) \\ &-\frac{8\alpha Z p^2(x)}{|x|F'(p)(x)} + \frac{8\alpha}{3\pi^2}\int \mathrm{d}y \frac{p^2(x)p^3(y)}{|x-y|F'(p)(x)}\Bigg) = 0.\end{aligned} \tag{3.117}$$

Lieb [19] proved that the operator $-\mathfrak{R}|x|\Delta > 0$. So we discard the term $-\int \mathrm{d}x F(p)(x)|x|\Delta F(p)(x)$.

From the definition of $F(p)$, we know $F(p)\geq 0$ and $F'(p)\geq 0$. The first term on the LHS is positive. So we have

$$-Z\int \mathrm{d}x \frac{p^2(x)F(p)(x)}{F'(p)(x)} + \frac{1}{3\pi^2}\iint \mathrm{d}x\mathrm{d}y \frac{|x|p^2(x)F(p)(x)p^3(y)}{|x-y|F'(p)(x)} < 0. \tag{3.118}$$

We want to compare the first term with $\int \mathrm{d}x p^3(x)$. So we need a estimate of $\frac{F(p)}{pF'(p)}$. We compute

$$F''(p) = \frac{(2p^2+m^2)\sqrt{p^2+m^2}+4m^2 p \operatorname{arsinh}\left(\frac{p}{m}\right)}{2(p^2+m^2)^{\frac{3}{2}}\sqrt{p\sqrt{p^2+m^2}+2p^2\operatorname{arsinh}\left(\frac{p}{m}\right)}} > 0. \tag{3.119}$$

So $F'(p)$ is an increasing function. We have

$$F(p) = \int_0^p F'(t)\mathrm{d}t \leq \int_0^p F'(p)\mathrm{d}t = pF'(p). \tag{3.120}$$

Use L'Hôpital's rule, we have

$$\begin{aligned}&\lim_{p\to\infty}\frac{F(p)}{pF'(p)}=\lim_{p\to\infty}\frac{F'(p)}{F'(p)+pF''(p)}=\lim_{p\to\infty}\frac{1}{1+\frac{pF''(p)}{F'(p)}}\\=&\frac{1}{1+\lim\limits_{p\to\infty}\frac{pF''(p)}{F'(p)}}\end{aligned}\tag{3.121}$$

and

$$\begin{aligned}&\lim_{p\to\infty}\frac{pF''(p)}{F'(p)}=\lim_{p\to\infty}\frac{\frac{p(2p^2+m^2)\sqrt{p^2+m^2}+4m^2p^2\operatorname{arsinh}\left(\frac{p}{m}\right)}{2(p^2+m^2)^{\frac{3}{2}}\sqrt{p\sqrt{p^2+m^2}+2p^2\operatorname{arsinh}\left(\frac{p}{m}\right)}}}{\sqrt{\frac{p}{\sqrt{p^2+m^2}}\left(1+2\frac{p}{\sqrt{p^2+m^2}}\operatorname{arsinh}\left(\frac{p}{m}\right)\right)}}\\=&\lim_{p\to\infty}\frac{\frac{2p^4}{2\sqrt{2p^4}\sqrt{\ln p}}}{\sqrt{2\ln p}}=0.\end{aligned}\tag{3.122}$$

So we have

$$\lim_{p\to\infty}\frac{F(p)}{pF'(p)}=1.\tag{3.123}$$

Similarly,

$$\lim_{p\to 0}\frac{F(p)}{pF'(p)}=\frac{1}{1+\lim\limits_{p\to 0}\frac{pF''(p)}{F'(p)}}\tag{3.124}$$

and

$$\begin{aligned}&\lim_{p\to 0}\frac{pF''(p)}{F'(p)}=\lim_{p\to 0}\frac{\frac{p(2p^2+m^2)\sqrt{p^2+m^2}+4m^2p^2\operatorname{arsinh}\left(\frac{p}{m}\right)}{2(p^2+m^2)^{\frac{3}{2}}\sqrt{p\sqrt{p^2+m^2}+2p^2\operatorname{arsinh}\left(\frac{p}{m}\right)}}}{\sqrt{\frac{p}{\sqrt{p^2+m^2}}\left(1+2\frac{p}{\sqrt{p^2+m^2}}\operatorname{arsinh}\left(\frac{p}{m}\right)\right)}}\\=&\lim_{p\to 0}\frac{\frac{1}{2}\sqrt{\frac{p}{m}}}{\sqrt{\frac{p}{m}}}=\frac{1}{2}.\end{aligned}\tag{3.125}$$

So we have

$$\lim_{p\to 0}\frac{F(p)}{pF'(p)}=\frac{2}{3}.\tag{3.126}$$

Obviously, $\frac{F(p)}{pF'(p)}$ is a positive continuous function of p. By (3.123) and (3.126), $\frac{F(p)}{pF'(p)}$ has a positive minimum

$$0<c_F=\min_{p\geq 0}\frac{F(p)}{pF'(p)}.\tag{3.127}$$

Numerically, $c_F=0.612$. Using (3.127) for the second term in (3.118), then symmetrizing it and using triangle inequality yields

$$\begin{aligned}&\frac{1}{3\pi^2}\iint\mathrm{d}x\mathrm{d}y\frac{|x|p^2(x)F(p)(x)p^3(y)}{|x-y|F'(p)(x)}\geq\frac{c_F}{3\pi^2}\iint\mathrm{d}x\mathrm{d}y\frac{|x|p^3(x)p^3(y)}{|x-y|}\\=&\frac{c_F}{6\pi^2}\iint\mathrm{d}x\mathrm{d}y\frac{(|x|+|y|)p^3(x)p^3(y)}{|x-y|}\geq\frac{c_F}{6\pi^2}\left(\int\mathrm{d}xp^3(x)\right)^2.\end{aligned}\tag{3.128}$$

Similarly, using (3.120) for the y part in the same term yields

$$\begin{aligned}&\frac{1}{3\pi^2}\iint \mathrm{d}x\mathrm{d}y\frac{|x|p^2(x)F(p)(x)p^3(y)}{|x-y|F'(p)(x)}\\ \geq&\frac{1}{3\pi^2}\iint \mathrm{d}x\mathrm{d}y\frac{|x|p^2(x)F(p)(x)p^2(y)F(p)(y)}{|x-y|F'(p)(x)F'(p)(y)}\\ \geq&\frac{1}{6\pi^2}\left(\int \mathrm{d}x\frac{p^2(x)F(p)(x)}{F'(p)(x)}\right)^2.\end{aligned} \tag{3.129}$$

Combining (3.128) and (3.129), we have

$$\begin{aligned}&\frac{1}{3\pi^2}\iint \mathrm{d}x\mathrm{d}y\frac{|x|p^2(x)F(p)(x)p^3(y)}{|x-y|F'(p)(x)}\\ \geq&\frac{1}{2}\left(\frac{c_F}{6\pi^2}\left(\int \mathrm{d}xp^3(x)\right)^2+\frac{1}{6\pi^2}\left(\int \mathrm{d}x\frac{p^2(x)F(p)(x)}{F'(p)(x)}\right)^2\right)\\ \geq&\frac{\sqrt{c_F}}{6\pi^2}\int \mathrm{d}xp^3(x)\int \mathrm{d}x\frac{p^2(x)F(p)(x)}{F'(p)(x)}.\end{aligned} \tag{3.130}$$

Using it in (3.118), we have

$$Z\int \mathrm{d}x\frac{p^2(x)F(p)(x)}{F'(p)(x)} > \frac{\sqrt{c_F}}{6\pi^2}\int \mathrm{d}xp^3(x)\int \mathrm{d}x\frac{p^2(x)F(p)(x)}{F'(p)(x)}. \tag{3.131}$$

So it means

$$Z > \frac{\sqrt{c_F}}{6\pi^2}\int \mathrm{d}xp^3(x) = \frac{\sqrt{c_F}}{2}N, \tag{3.132}$$

i.e.,

$$N < \frac{2}{\sqrt{c_F}}Z \approx 2.56Z. \tag{3.133}$$

□

3.7 Improvement

We follow the idea of Frank, Nam, and van den Bosch [15] to improve the result.

Lemma 4. *Let $\{f_i\}_{i=1..n}$ be a partition of unity, satisfies $\nabla(f_i^{\frac{2}{3}}) \in L^\infty$, $\Delta(f_i^{\frac{4}{3}}) \in L^\infty$. Then*

$$\begin{aligned}&\sum_{i=1}^n \tilde{\mathcal{E}}^{TFW}_{\kappa,c}(f_i^{\frac{2}{3}}p) - \tilde{\mathcal{E}}^{TFW}_{\kappa,c}(p)\\ \leq&2C\lambda mc^2\left(\sum_{i=1}^n \|\nabla(f_i^{\frac{2}{3}})\|^2_{L^\infty}+\sum_{i=1}^n \|\Delta(f_i^{\frac{4}{3}})\|_{L^\infty}\right)\int_A p^3\\ &+\frac{3(n-1)\lambda mc^2}{8\pi^2}\int_A|\nabla p|^2 f_W(p)+\frac{mc}{9\pi^4}\left(\sum_{i=1}^n D[f_i^2p^3]-D[p^3]\right),\end{aligned} \tag{3.134}$$

where $A = \bigcup_{i=1}^{n} \{x \in \mathbb{R}^3 | 0 < f_i(x) < 1\}$.

Proof. For the Thomas-Fermi term, it is easy to prove that $f''''_{TF}(p)$ are positive for $p > 0$, and $f_{TF}(0) = f'_{TF}(0) = f''_{TF}(0) = 0$. Since $f_i \le 1$, we have $f'''_{TF}(f_i^{\frac{2}{3}} p) \le f'''_{TF}(p)$. Using $f''_{TF}(0) = f'_{TF}(0) = f_{TF}(0) = 0$ successively, we obtain $f''_{TF}(f_i^{\frac{2}{3}} p) \le f_i^{\frac{2}{3}} f''_{TF}(p)$, $f'_{TF}(f_i^{\frac{2}{3}} p) \le f_i^{\frac{4}{3}} f'_{TF}(p)$, and $f_{TF}(f_i^{\frac{2}{3}} p) \le f_i^2 f_{TF}(p)$. So we have

$$\sum_{i=1}^{n} \int f_{TF}(f_i^{\frac{2}{3}} p) - \int f_{TF}(p) \le \int \left(\sum_{i=1}^{n} f_i^2 - 1 \right) f_{TF}(p) = 0. \tag{3.135}$$

For the gradient term, it is easy to prove that $\lim_{p \to 0} \frac{f_W(p)}{p} = 1$ and $\lim_{p \to \infty} \frac{f_W(p)}{p} = 0$. So $f_W(p) \le Cp$ for $p \ge 0$. Since f_W is an increasing function and $f_i \le 1$, this gives $f_W(f_i^{\frac{2}{3}} p) \le f_W(p)$. Thus we have

$$\begin{aligned}
&\sum_{i=1}^{n} \int |\nabla (f_i^{\frac{2}{3}} p)|^2 f_W(f_i^{\frac{2}{3}} p) - \int |\nabla p|^2 f_W(p) \\
=&\sum_{i=1}^{n} \int_A \left(|\nabla f_i^{\frac{2}{3}}|^2 p^2 + f_i^{\frac{4}{3}} |\nabla p|^2 + 2 f_i^{\frac{2}{3}} \nabla (f_i^{\frac{2}{3}}) \cdot p \nabla p \right) f_W(f_i^{\frac{2}{3}} p) - \int_A |\nabla p|^2 f_W(p) \\
\le&\sum_{i=1}^{n} \int_A \left(|\nabla f_i^{\frac{2}{3}}|^2 p^2 + f_i^{\frac{4}{3}} |\nabla p|^2 + 2 f_i^{\frac{2}{3}} \nabla (f_i^{\frac{2}{3}}) \cdot p \nabla p \right) f_W(p) - \int_A |\nabla p|^2 f_W(p) \\
\le& C \sum_{i=1}^{n} \|\nabla f_i^{\frac{2}{3}}\|_{L^\infty}^2 \int_A p^3 + (n-1) \int_A |\nabla p|^2 f_W(p) + 2 \sum_{i=1}^{n} \int_A f_i^{\frac{2}{3}} \nabla (f_i^{\frac{2}{3}}) \cdot p (\nabla p) f_W(p).
\end{aligned} \tag{3.136}$$

For the last term, we have

$$\begin{aligned}
&2 \sum_{i=1}^{n} \int_A f_i^{\frac{2}{3}} \nabla (f_i^{\frac{2}{3}}) \cdot p (\nabla p) f_W(p) \le C \sum_{i=1}^{n} \int_A \nabla (f_i^{\frac{4}{3}}) \cdot \nabla p^3 \\
=& -C \sum_{i=1}^{n} \int_A \Delta (f_i^{\frac{4}{3}}) p^3 \le C \sum_{i=1}^{n} \|\Delta (f_i^{\frac{4}{3}})\|_{L^\infty} \int_A p^3.
\end{aligned} \tag{3.137}$$

Thus (3.137) implies that

$$\begin{aligned}
&\sum_{i=1}^{n} \int |\nabla (f_i^{\frac{2}{3}} p)|^2 f_W(f_i^{\frac{2}{3}} p) - \int |\nabla (p)|^2 f_W(p) \\
\le& C \left(\sum_{i=1}^{n} \|\nabla (f_i^{\frac{2}{3}})\|_{L^\infty}^2 + \sum_{i=1}^{n} \|\Delta (f_i^{\frac{4}{3}})\|_{L^\infty} \right) \int_A p^3 + (n-1) \int_A |\nabla p|^2 f_W(p).
\end{aligned} \tag{3.138}$$

□

Now we give the estimate of the minimizer p.

Lemma 5. *For all $s > 0$, we have*

$$\begin{aligned}&\frac{1}{24\pi^2}\left(\int p^3\right)^2 - \frac{2s}{3\pi^2}D[p^3]\\ \leq&\left(C\lambda c s^{-1} + \frac{Z}{4}\right)\int p^3 + \frac{9s\lambda c}{8}\int |\nabla p|^2 f_W(p).\end{aligned} \tag{3.139}$$

Proof. The non-relativistic version of this lemma is proved by Frank, Nam, and van den Bosch [15]. We follow their method and deal with the different parts. We choose a similar partition of unity as them, but with some different restrictions. For every $l > 0$, $\nu \in \mathbb{S}^2$, we choose

$$\chi_1(x) = g_1\left(\frac{\nu\cdot x - l}{s}\right), \quad \chi_2(x) = g_2\left(\frac{\nu\cdot x - l}{s}\right) \tag{3.140}$$

where $g_1,\ g_2 : \mathbb{R}\to\mathbb{R}$ satisfy

$$\begin{aligned}&g_1^2 + g_2^2 = 1, \quad g_1(t) = 1 \text{ if } t \leq 0, \quad g_1(t) = 0 \text{ if } t \geq 1,\\ &|(g_1^{\frac{2}{3}})'| + |(g_2^{\frac{2}{3}})'| + |(g_1^{\frac{4}{3}})'| + |(g_2^{\frac{4}{3}})'| + |(g_1^{\frac{4}{3}})''| + |(g_2^{\frac{4}{3}})''| \leq C.\end{aligned} \tag{3.141}$$

In Frank, Nam, and van den Bosch [15], they choose $\chi_1(x) = g_1\left(\frac{\nu\cdot\theta(x)-l}{s}\right)$, $\chi_2(x) = g_2\left(\frac{\nu\cdot\theta(x)-l}{s}\right)$, and $\theta : \mathbb{R}^3\to\mathbb{R}^3$ satisfying $|\theta(x)| \leq |x|$, $\theta(x) = 0$ if $|x| \leq r$, $\theta(x) = x$ if $|x| \geq (1+\mu)r$, $|\nabla\theta| \leq C\mu^{-1}$. But in our case, we set $r = 0$ simply, i.e., $\theta(x) = x$. There are two reasons for this choice. On the one hand, to get the non-relativistic version of Theorem 3, they let $r \to 0$. This is equivalent to setting $r = 0$ at the beginning. On the other hand, if $\Delta\theta$ is not 0, we will have a extra Z order term. This is not what we want to have. θ should be linear in our case, so we choose $\theta(x) = x$. This implies

$$\begin{aligned}|\nabla(\chi_i^{\frac{2}{3}}(x))| &= \left|(g_1^{\frac{2}{3}})'\left(\frac{\nu\cdot x - l}{s}\right)\nabla\frac{\nu\cdot x - l}{s}\right| \leq Cs^{-1},\\ |\Delta(\chi_i^{\frac{4}{3}}(x))| &= \left|(g_1^{\frac{4}{3}})''\left(\frac{\nu\cdot x - l}{s}\right)\left|\nabla\frac{\nu\cdot x - l}{s}\right|^2\right.\\ &\qquad\left.+(g_1^{\frac{4}{3}})'\left(\frac{\nu\cdot x - l}{s}\right)\Delta\frac{\nu\cdot x - l}{s}\right| \leq Cs^{-2}.\end{aligned} \tag{3.142}$$

Since p is the minimizer, we have

$$\tilde{\mathcal{E}}_{\kappa,c}^{TFW}(\chi_1^{\frac{2}{3}}p) + \tilde{\mathcal{E}}_{0,c}^{TFW}(\chi_2^{\frac{2}{3}}p) - \tilde{\mathcal{E}}_{\kappa,c}^{TFW}(p) \geq 0. \tag{3.143}$$

By Lemma 4, we have

$$\begin{aligned}&\tilde{\mathcal{E}}_{\kappa,c}^{TFW}(\chi_1^{\frac{2}{3}}p) + \tilde{\mathcal{E}}_{0,c}^{TFW}(\chi_2^{\frac{2}{3}}p) - \tilde{\mathcal{E}}_{\kappa,c}^{TFW}(p)\\ \leq&\frac{mc^2\kappa}{3\pi^2}\int \mathrm{d}x\frac{\chi_2^2(x)p^3(x)}{|x|} + 2C\lambda mc^2 s^{-2}\int_{\nu\cdot x - s\leq l\leq \nu\cdot x}\mathrm{d}x p^3(x)\\ &+\frac{3\lambda mc^2}{8\pi^2}\int_{\nu\cdot x - s\leq l\leq\nu\cdot x}\mathrm{d}x|\nabla p(x)|^2 f_W(p)(x) + \frac{qmc}{9\pi^4}\left(D[\chi_1^2p^3] + D[\chi_2^2p^3] - D[p^3]\right).\end{aligned} \tag{3.144}$$

The same as the non-relativistic case (Frank, Nam, and van den Bosch [15]), we have

$$\begin{aligned}&\frac{mc^2\kappa}{3\pi^2}\int \mathrm{d}x\frac{\chi_2^2(x)p^3(x)}{|x|}+\frac{mc}{9\pi^4}\left(D[\chi_1^2p^3]+D[\chi_2^2p^3]-D[p^3]\right)\\ \leq&\frac{mcZ}{3\pi^2}\int_{l\leq\nu\cdot x}\mathrm{d}x\frac{p^3(x)}{|x|}-\frac{mc}{9\pi^4}\iint_{\nu\cdot y\leq l\leq\nu\cdot x-s}\mathrm{d}x\mathrm{d}y\frac{p^3(x)p^3(y)}{|x-y|}.\end{aligned}\tag{3.145}$$

Thus (3.143) implies that

$$\begin{aligned}&\frac{1}{3\pi^2}\iint_{\nu\cdot y\leq l\leq\nu\cdot x-s}\mathrm{d}x\mathrm{d}y\frac{p^3(x)p^3(y)}{|x-y|}\leq C\lambda cs^{-2}\int_{\nu\cdot x-s\leq l\leq\nu\cdot x}\mathrm{d}xp^3(x)\\ &+\frac{9\lambda c}{8}\int_{\nu\cdot x-s\leq l\leq\nu\cdot x}\mathrm{d}x|\nabla p(x)|^2f_W(p)(x)+Z\int_{l\leq\nu\cdot x}\mathrm{d}x\frac{p^3(x)}{|x|}.\end{aligned}\tag{3.146}$$

Integrating (3.146) over $l\in(0,\infty)$, we have

$$\begin{aligned}&\frac{1}{3\pi^2}\int_0^\infty\mathrm{d}l\left(\iint_{\nu\cdot y\leq l\leq\nu\cdot x-s}\mathrm{d}x\mathrm{d}y\frac{p^3(x)p^3(y)}{|x-y|}\right)\\ \leq&C\lambda cs^{-1}\int p^3+\frac{9s\lambda c}{8}\int|\nabla p|^2f_W(p)+Z\int\mathrm{d}x[\nu\cdot x]_+\frac{p^3(x)}{|x|}.\end{aligned}\tag{3.147}$$

Then we average over $\nu\in\mathbb{S}^2$ and use the proof of Frank, Nam, and van den Bosch [15]. We obtain

$$\begin{aligned}&\frac{1}{3\pi^2}\left(\frac{1}{8}\left(\int p^3\right)^2-2sD[p^3]\right)\\ \leq&\left(C\lambda cs^{-1}+\frac{Z}{4}\right)\int p^3+\frac{9s\lambda c}{8}\int|\nabla p|^2f_W(p).\end{aligned}\tag{3.148}$$

□

Using (3.148), we can prove Theorem 3 now:

Proof of Theorem 3. We use $\int p^3=3\pi^2N$. This implies

$$N^2\leq\frac{16s}{9\pi^4}D[p^3]+\left(C\lambda cs^{-1}+2Z\right)N+\frac{3s\lambda c}{\pi^2}\int|\nabla p|^2f_W(p)\tag{3.149}$$

for all $s>0$. We optimize over $s>0$, then we have

$$N\leq 2Z+CN^{-\frac{1}{2}}\sqrt{\frac{16\lambda c}{9\pi^4}D[p^3]+\frac{3\lambda^2c^2}{\pi^2}\int|\nabla p|^2f_W(p)}.\tag{3.150}$$

Since p is the minimizer and using (3.74), we have

$$\begin{aligned}
0 \geq \tilde{\mathcal{E}}^{TFW}_{\kappa,c}(p) = &\frac{mc^2}{8\pi^2}\int \mathrm{d}x \left(f_{TF}(p) + 3\lambda|\nabla p(x)|^2 f_W(p) - \frac{8\kappa p^3(x)}{3|x|} + \frac{4}{9c\pi^2}\int \mathrm{d}y \frac{p^3(x)p^3(y)}{|x-y|}\right)\\
= &\frac{mc^2}{8\pi^2}\int \mathrm{d}x \left(f_{TF}(p) + \frac{3}{4}\lambda|\nabla p(x)|^2 f_W(p) - \frac{8\kappa p^3(x)}{3|x|} + \frac{2}{9c\pi^2}\int \mathrm{d}y \frac{p^3(x)p^3(y)}{|x-y|}\right)\\
&+ \frac{mc^2}{8\pi^2}\int \mathrm{d}x \left(\frac{9}{4}\lambda|\nabla p(x)|^2 f_W(p) + \frac{2}{9c\pi^2}\int \mathrm{d}y \frac{p^3(x)p^3(y)}{|x-y|}\right)\\
\geq &-CZ^{\frac{5}{2}} + \frac{mc^2}{8\pi^2}\int \mathrm{d}x \left(\frac{3}{4}\lambda|\nabla p(x)|^2 f_W(p) + \frac{2}{9c\pi^2}\int \mathrm{d}y \frac{p^3(x)p^3(y)}{|x-y|}\right).
\end{aligned} \tag{3.151}$$

Thus

$$\frac{16\lambda c}{9\pi^4}D[p^3] + \frac{3\lambda^2 c^2}{\pi^2}\int |\nabla p|^2 f_W(p) \leq CZ^{\frac{5}{2}}. \tag{3.152}$$

This implies the theorem. □

Appendix A

Proof of the Positivity of $\Re F_l$

To prove the positivity, we need

Lemma 6. *The function $O_l(x)$ decreases in l when x is greater than 1, i.e.,*

$$O_l(x) > O_{l+1}(x), \;\; x > 1. \tag{A.1}$$

Proof. In this proof, x is always greater than 1. We know

$$\frac{\mathrm{d}}{\mathrm{d}x} Q_l(x) = \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}x}\int_{-1}^{1} \mathrm{d}u \frac{P_l(u)}{x-u} = -\frac{1}{2}\int_{-1}^{1} \mathrm{d}u \frac{P_l(u)}{(x-u)^2} = -O_l(x). \tag{A.2}$$

We use the positivity of Q_l (Whittaker and Watson [37, p. 305]),

$$Q_l(x) = \frac{1}{2^{l+1}}\int_{-1}^{1} (1-u^2)^l (x-u)^{-l-1} \mathrm{d}t > 0. \tag{A.3}$$

Then we know

$$O_l(x) = -\frac{\mathrm{d}}{\mathrm{d}x}\frac{1}{2^{l+1}}\int_{-1}^{1} (1-u^2)^l (x-u)^{-l-1} \mathrm{d}t = \frac{l+1}{2^{l+1}}\int_{-1}^{1} (1-u^2)^l (x-u)^{-l-2} \mathrm{d}t > 0. \tag{A.4}$$

We integrate by parts,

$$O_{l+1}(x) = \frac{1}{2}\int_{-1}^{1} \mathrm{d}u \frac{P_{l+1}(u)}{(x-u)^2} = \frac{1}{2}\frac{P_{l+1}(u)}{x-u}\bigg|_{u=-1}^{1} - \frac{1}{2}\int_{-1}^{1} \mathrm{d}u \frac{P'_{l+1}(u)}{x-u} \tag{A.5}$$

and use the properties of P_l (Whittaker and Watson [37, p. 305])

$$\begin{aligned} &P'_{l+1}(x) - xP'_l(x) = (l+1)P_l(x), \\ &(l+1)P_{l+1}(x) - (2l+1)xP_l(x) + lP_{l-1}(x) = 0, \\ &P_l(1) = 1, \;\; P_l(-1) = (-1)^l. \end{aligned} \tag{A.6}$$

We have

$$O_{l+1}(x) = \frac{l+1}{2l+1}O_{l+1}(x) + \frac{l}{2l+1}O_{l-1}(x) - lQ_l(x). \tag{A.7}$$

It implies

$$O_{l-1}(x) - O_{l+1}(x) = (2l+1)Q_l(x) > 0 \tag{A.8}$$

and

$$\frac{1}{2}\int_{-1}^{1} \mathrm{d}u \frac{P_{l+1}(u) + (2l+1)(x-u)P_l(u) - P_{l-1}(u)}{(x-u)^2} = 0. \tag{A.9}$$

From (A.6) and (A.9), we have

$$\frac{1}{2}\int_{-1}^{1} \mathrm{d}u \frac{lP_{l+1}(u) - (2l+1)xP_l(u) + (l+1)P_{l-1}(u)}{(x-u)^2} = 0. \tag{A.10}$$

Using the definition of O_l, (A.10) is equivalent to

$$lO_{l+1}(x) = (2l+1)xO_l(x) - (l+1)O_{l-1}(x). \tag{A.11}$$

So we get

$$\begin{aligned} &l(O_l(x) - O_{l+1}(x)) < l(xO_l(x) - O_{l+1}(x)) \\ =&(l+1)(O_{l-1}(x) - xO_l(x)) < (l+1)(O_{l-1}(x) - O_l(x)). \end{aligned} \tag{A.12}$$

If for some l,

$$O_{l-1}(x) - O_l(x) \leq 0. \tag{A.13}$$

Then from (A.12), we have

$$O_l(x) - O_{l+1}(x) \leq 0. \tag{A.14}$$

Then

$$O_{l-1}(x) - O_{l+1}(x) = O_{l-1}(x) - O_l(x) + O_l(x) - O_{l+1}(x) \leq 0. \tag{A.15}$$

There is a contradiction to (A.8). So for all l,

$$O_{l-1}(x) - O_l(x) > 0. \tag{A.16}$$

□

Now we can prove the positivity of $\Re F_l$. By the definition, the imaginary part is

$$\Im f_l(r,r) = -\int_0^\infty \frac{\mathrm{d}q}{q} O_l(\frac{1}{2}(\frac{1}{q}+q))\left(q^{\frac{1}{2}}\sin(r\ln q) + \frac{1}{q^{\frac{1}{2}}}\sin(-r\ln q)\right). \tag{A.17}$$

Using Lemma 6, we have

$$\begin{aligned}
\mathfrak{R} f_l(r,r) &= \int_0^\infty \frac{\mathrm{d}q}{q} \left(O_0(\frac{1}{2}(\frac{1}{q}+q)) \left(q+\frac{1}{q}\right) - O_l(\frac{1}{2}(\frac{1}{q}+q)) \left(q^{\frac{1}{2}} \cos(r \ln q) + \frac{1}{q^{\frac{1}{2}}} \cos(r \ln q) \right) \right) \\
&> \int_0^\infty \frac{\mathrm{d}q}{q} \left(O_0(\frac{1}{2}(\frac{1}{q}+q)) \left(q+\frac{1}{q}\right) - O_l(\frac{1}{2}(\frac{1}{q}+q)) \left(q^{\frac{1}{2}} + \frac{1}{q^{\frac{1}{2}}} \right) \right) \\
&> \int_0^\infty \frac{\mathrm{d}q}{q} O_0(\frac{1}{2}(\frac{1}{q}+q)) \left(q + \frac{1}{q} - q^{\frac{1}{2}} - \frac{1}{q^{\frac{1}{2}}} \right) \\
&= \int_0^\infty \frac{\mathrm{d}q}{q} O_0(\frac{1}{2}(\frac{1}{q}+q)) (q^{\frac{1}{2}} + \frac{1}{q^{\frac{1}{2}}} - 2)(q^{\frac{1}{2}} + \frac{1}{q^{\frac{1}{2}}} + 1) > 0.
\end{aligned} \tag{A.18}$$

So the positivity is proved.

Appendix B

Proof of the Positivity of $\Re G_l$

We start from the definition of G_l

$$\begin{aligned}
&\int_0^\infty \mathrm{d}k Q_l(\frac{1}{2}(\frac{1}{k}+k))\frac{1}{k^{\frac{1}{2}}}e^{ir\ln k} \\
=&\int_0^\infty \mathrm{d}k Q_l(\frac{1}{2}(\frac{1}{k}+k))\frac{1}{k^{\frac{1}{2}}}(\cos(r\ln k)+i\sin(r\ln k)).
\end{aligned} \tag{B.1}$$

Then we focus on the real part and change the variable k to e^k,

$$\begin{aligned}
&\Re\int_0^\infty \mathrm{d}k Q_l(\frac{1}{2}(\frac{1}{k}+k))\frac{1}{k^{\frac{1}{2}}}e^{ir\ln k} = \int_0^\infty \mathrm{d}k Q_l(\frac{1}{2}(\frac{1}{k}+k))\frac{1}{k^{\frac{1}{2}}}\cos(r\ln k) \\
=&\int_{-\infty}^\infty \mathrm{d}k e^k Q_l(\frac{1}{2}(e^{-k}+e^k))e^{-\frac{1}{2}k}\cos(rk) = \frac{2}{r}\int_0^\infty \mathrm{d}k \cosh\frac{k}{2r}Q_l(\cosh\frac{k}{r})\cos k.
\end{aligned} \tag{B.2}$$

We define

$$h_l(k) := \cosh\frac{k}{2r}Q_l(\cosh\frac{k}{r}). \tag{B.3}$$

Then (B.2) can be rewritten as

$$\begin{aligned}
&\Re\int_0^\infty \mathrm{d}k Q_l(\frac{1}{2}(\frac{1}{k}+k))\frac{1}{k^{\frac{1}{2}}}e^{ir\ln k} \\
=&\frac{2}{r}\sum_{n=0}^\infty \int_{2n\pi}^{2(n+1)\pi} \mathrm{d}k h_l(k)\cos k \\
=&\frac{2}{r}\sum_{n=0}^\infty \int_{2n\pi}^{2n\pi+\frac{\pi}{2}} \mathrm{d}k (h_l(k)-h_l((4n+1)\pi-k)-h_l(k+\pi)+h_l((4n+2)\pi-k)\cos k.
\end{aligned} \tag{B.4}$$

Now we need the positivity of the second derivative of $h_l(k)$, for $k > 0$. We compute it directly

$$\begin{aligned} h_l''(k) =& \frac{\mathrm{d}^2}{\mathrm{d}k^2}\left(\cosh\frac{k}{2r}Q_l(\cosh\frac{k}{r})\right) \\ =& \frac{1}{r^2}\cosh\frac{k}{2r}\left(\frac{1}{4}Q_l(\cosh\frac{k}{r}) + \left(2\cosh\frac{k}{r}-1\right)Q_l'(\cosh\frac{k}{r}) + (\cosh^2\frac{k}{r}-1)Q_l''(\cosh\frac{k}{r})\right). \end{aligned} \tag{B.5}$$

We know $\frac{1}{r^2}\cosh\frac{k}{2r} > 0$, $Q_l(\cosh\frac{k}{r}) > 0$, and $\cosh\frac{k}{r} > 1$ for $k > 0$. So we only need to prove

$$(2x-1)Q_l'(x) + (x^2-1)Q_l''(x) > 0, \ x > 1. \tag{B.6}$$

Because $Q_l(x)$ is a solution of Legendre's differential equation (Erdélyi et al. [11]), we know

$$(1-x^2)Q_l''(x) - 2xQ_l'(x) + l(l+1)Q_l(x) = 0. \tag{B.7}$$

So we have

$$\begin{aligned} &(2x-1)Q_l'(x) + (x^2-1)Q_l''(x) = -Q_l'(x) + l(l+1)Q_l(x) \\ &= O_l(x) + l(l+1)Q_l(x) > 0, \ x > 1. \end{aligned} \tag{B.8}$$

The positivity of $h_l''(k)$ is proved

$$h_l''(k) > 0, \ k > 0. \tag{B.9}$$

From this, we know

$$h_l(k) - h_l((4n+1)\pi - k) - h_l(k+\pi) + h_l((4n+2)\pi - k) > 0. \tag{B.10}$$

Since $\cos k > 0$, for $k \in (2n\pi, 2n\pi + \frac{\pi}{2})$, Equality (B.4) is positive. So the positivity of $\Re G_l$ is proved.

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Eidesstattliche Versicherung

Hiermit erkläre ich an Eides statt, dass die Dissertation von mir selbständig, ohne unerlaubte Beihilfe angefertigt ist.

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