# STATISTICAL THEORY OF THE ATOM IN MOMENTUM SPACE

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**Zusammenfassung**

Im Jahre 1992 führte Englert [3] ein Impuls-Energie-Funktional für Atome ein und erörterte seinen Zusammenhang mit dem Thomas-Fermi-Funktional (Lenz [8]). Wir integrieren dieses Modell in eine mathematische Umgebung. Unter unseren Resultaten findet sich ein Beweis für die Existenz und Eindeutigkeit einer minimierenden Impulsdichte für dieses Impuls-Energie-Funktional; des Weiteren untersuchen wir einige Eigenschaften des Minimierers, darunter auch den Zusammenhang mit der Euler-Gleichung.

Wir verknüpfen die Minimierer des Thomas-Fermi-Funktionals mit dem Impuls-Energie-Funktional von Englert durch explizite Transformationen. Wie sich herausstellt, können auf diese Weise bekannte Ergebnisse aus dem Thomas-Fermi-Modell direkt auf das von uns betrachtete Modell übertragen werden. Wir erhalten sogar die Äquivalenz der beiden Funktionale bezüglich ihrer Minima.

Abschließend betrachten wir impulsabhängige Störungen. Insbesondere zeigen wir, dass die atomare Impulsdichte für große Kernladung in einem bestimmten Sinne gegen den Minimierer des Impuls-Energie-Funktionals konvergiert.

Die vorliegende Arbeit basiert auf Zusammenarbeit mit Prof. Dr. Heinz Siedentop. Wesentliche Inhalte werden ebenfalls in einer gemeinsamen Publikation [27] erscheinen.

**Abstract**

In 1992, Englert [3] found a momentum energy functional for atoms and discussed the relation to the Thomas-Fermi functional (Lenz [8]). We place this model in a mathematical setting. Our results include a proof of existence and uniqueness of a minimizing momentum density for this momentum energy functional. Further, we investigate some properties of this minimizer, among them the connection with Euler's equation.

We relate the minimizers of the Thomas-Fermi functional and the momentum energy functional found by Englert by explicit transforms. It turns out that in this way results well-known in the Thomas-Fermi model can be transferred directly to the model under consideration. In fact, we gain equivalence of the two functionals upon minimization.

Finally, we consider momentum dependent perturbations. In particular, we show that the atomic momentum density converges to the minimizer of the momentum energy functional as the total nuclear charge becomes large in a certain sense.

This thesis is based on joint work with Prof. Dr. Heinz Siedentop and the main contents will also appear in a joint article [27].

# Contents

**Introduction** **3**

**1. The Momentum Energy Functional** **7**
1.1. The Quantum Mechanical Setting . . . . . . . . . . . . . . . 7
1.2. Basic Properties of the Energy Functional . . . . . . . . . 8

**2. The Functional $\mathcal{E}_s$** **11**

**3. Thomas-Fermi and the Momentum Energy Functional** **15**
3.1. A Few Results on the Thomas-Fermi Functional . . . . . . 15
3.2. Transforms between Position and Momentum Functional . 17

**4. Results on the Minimal Energy and the Minimizer** **23**
4.1. Existence and Uniqueness Results . . . . . . . . . . . . . . . 23
4.2. Properties of the Minimizing Density and Euler's Equation 25
4.3. The Virial Theorem . . . . . . . . . . . . . . . . . . . . . . . 31

**5. Asymptotic Exactness of Englert's Statistical Model of the Atom** **33**

**Appendix** **46**

**A. Existence and Uniqueness of the Minimizer: An Alternative Proof** **47**

**B. Supplemental Material** **55**

**Bibliography** **57**

# Introduction

Density functional theory is a method to investigate properties of physical systems, such as atoms, molecules or solids. The ground state of these systems is of particular interest. The approach of this theory is to consider a functional depending on the one-particle electron density where the minimum of this functional yields an approximation for the ground state energy and the minimizer yields an approximation for the ground state density. So, dealing with the variational problem of minimizing an energy functional which depends only on the one-particle density reduces an initially multi-particle problem to a one-particle problem. There exists a huge literature for the theory of energy functionals of the spatial density, whereas the theory of energy functionals of the momentum density gained by far less attention.

In the field of spatial density functionals the Thomas-Fermi model is of outstanding importance. This statistical method of Thomas [26] and Fermi [6, 7] was set on a mathematical footing by Lieb and Simon [10, 12, 13]. Their results include a proof that the Thomas-Fermi energy, the minimum of the Thomas-Fermi functional (Lenz [8]), is asymptotic to the ground state energy for large physical systems. More precisely, if the total nuclear charge $Z$ becomes large and the number of electrons $N$ increases simultaneously such that the ratio $N/Z$ is fixed, then these two energies are equal up to an error of order $o(Z^{7/3})$. Moreover, the Thomas-Fermi model provides the opportunity to determine the linear response to perturbations that are local in position space since Lieb and Simon [10, 12, 13] also show that the quantum mechanical density converges weakly to the Thomas-Fermi minimizer for large physical systems. Since then results on the Thomas-Fermi functional were refined, e. g., by corrections to the asymptotic behavior of the leading order (see, e. g., Siedentop and Weikard [20, 21, 22, 23, 24]). Further the validity of the Thomas-Fermi theory was extended, e. g., to magnetic fields (Lieb, Solovej, and Yngvason [14, 15] and Erdős and

Solovej [4, 5]).

For the treatment of momentum dependent perturbations the Thomas-Fermi model does not apply to. In fact, it is well-known that the momentum density is not merely the Fourier transform of the spatial density and although there are techniques to deduce momentum densities from the spatial ones, these rules are quite limited in their applicability, as remarked by Englert [3] already. To pursue a self-consistent determination of the momentum density Englert [3] introduced a momentum energy functional for atoms. This allows – in a natural way – for the treatment of purely momentum dependent perturbations. He also discussed the relation to the Thomas-Fermi functional.

The aim of this thesis is to place the model found by Englert [3] in a mathematical setting. We shall prove the existence and uniqueness of a minimizing density and furthermore that this density is asymptotically exact to the quantum mechanical ground state density.

To start with, Chapter 1 contains some basic properties of the momentum functional introduced by Englert [3]. Among them we are concerned with the question of convexity of this particular functional which we denote by $\mathcal{E}_{\mathrm{mTF}}$.

In Chapter 2 we introduce a new functional which emerged from the original one simply by substitution. This new functional is strictly convex and ensures therefrom uniqueness of a minimizing momentum density, as far as it exists. Later, this will also entail the uniqueness of any minimizer of $\mathcal{E}_{\mathrm{mTF}}$, the momentum energy functional originally introduced in the first chapter.

Chapter 3 covers the relation between the Thomas-Fermi functional in position space and the energy functional $\mathcal{E}_{\mathrm{mTF}}$ in momentum space by explicit transforms. This is extensively used in the next chapter where we finally answer the question of existence of the minimizer.

In Chapter 4 we use the relation shown in the previous chapter to gain equivalence of the two functionals upon minimization. This allows us to transfer results from the Thomas-Fermi model directly to the one under consideration. In particular, this implies that the infimum of the momentum energy functional agrees with the ground state energy up to the same order as the Thomas-Fermi energy does. Further, we establish bounds on the minimizer and its connection with Euler's equation.

Finally, in Chapter 5 we consider momentum dependent perturbations. To be more precise, we prove that the atomic momentum density converges on the scale $Z^{2/3}$ to the minimizer of the momentum energy functional. Hence, the momentum density functional gives the right appropriate linear response to momentum dependent forces. The proof uses coherent states. Schrödinger [19] derived these states as Gaussian wave functions parametrized by points in phase space satisfying minimal uncertainty. There exist various generalizations and the concept of coherent states has become a topic of self-contained interest.

Enclosed, in the appendix we also give an alternative proof for the existence of the minimizer. There, we do not rely on the relation discussed in Chapter 3 and the known results from the Thomas-Fermi model. Instead, we use variational methods on Banach spaces equipped with the weak topology together with semicontinuity of the functional in this weak topology in the spirit of Weierstrass. This is a fairly standard strategy in the calculus of variations which has also been used in the article of Lieb and Simon [13].

At the end of this introduction, we would like to briefly indicate a difference regarding the general structure of energy functionals of the one-particle density in position space and the one-particle density in momentum space. For example, if we compare the Hamiltonian of an atom with the Hamiltonian related to a molecule in position space then we observe that in both cases the external potential appears as a sum of one-particle multiplication operators. This suggests that a one-particle spatial density functional corresponding to an atom should have essentially the same general structure as a one-particle spatial density functional corresponding to a molecule. On the other hand, in momentum space we observe one-particle multiplication operators in the kinetic term of the Hamiltonian but not in the potential terms. Consequently, a one-particle momentum density functional suitable for atoms is not necessarily easily adapted to molecules. However, in the context of this thesis, we concentrate on the momentum energy functional $\mathcal{E}_{\mathrm{mTF}}$ which is associated with an atom. Besides this, we also want to refer to an article of Cinal and Englert [2] which is closely related to the one of Englert [3]. They found the momentum energy functional $\mathcal{E}_{\mathrm{mTF}}$ to be applicable in deriving a further momentum energy functional which improves the approximation of the ground state energy in higher order than $o(Z^{7/3})$. In fact, they incorporate the correction corresponding to the strongly bound electrons, the so-called Scott correction, into the existing momentum functional.

♢

The main part of this thesis is related to the article [27] which will be published co-authored with Prof. Dr. Heinz Siedentop. We give references for the corresponding propositions in the article. The formulation of the associated proofs is taken mostly from that article with more details and some intermediate steps where this seems appropriate.

♢

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# 1. The Momentum Energy Functional

## 1.1. The Quantum Mechanical Setting

The quantum mechanical system we will be concerned with is an atom with $N$ electrons of mass $m$ and charge $-e < 0$ moving about one fixed positive charge of magnitude $eZ$. This system is described by the Hamiltonian

$$H_N := \sum_{n=1}^{N}\Big(-\frac{\hbar^2}{2m}\Delta_n - \frac{Ze^2}{|x_n|}\Big) + \sum_{1\leq n<m\leq N}\frac{e^2}{|x_n - x_m|} \tag{1.1}$$

where $\hbar$ is Planck's constant divided by $2\pi$. This operator $H_N$ is self-adjoint on the Hilbert space $\bigwedge_{n=1}^{N} L^2(\mathbb{R}^3 : \mathbb{C}^q)$, the anti-symmetric subspace of square integrable functions on $\mathbb{R}^3$ with values in $\mathbb{C}^q$, where $q$ denotes the number of spin states. The corresponding ground state energy is defined to be $\inf \sigma(H_N)$, the infimum of the spectrum of $H_N$.

Englert [3] derived an energy functional depending on the momentum density $\tau$ for the ground state energy associated with $H_N$. It reads

$$\begin{aligned}\mathcal{E}_{\mathrm{mTF}}(\tau) := &\int_{\mathbb{R}^3}\mathrm{d}\xi\, \tfrac{\xi^2}{2m}\tau(\xi) - \tfrac{3}{2}\gamma_{\mathrm{TF}}^{-1/2}Ze^2\int_{\mathbb{R}^3}\mathrm{d}\xi\,\tau(\xi)^{\frac{2}{3}}\\ &+ \tfrac{3}{4}\gamma_{\mathrm{TF}}^{-1/2}e^2\int_{\mathbb{R}^3}\mathrm{d}\xi\int_{\mathbb{R}^3}\mathrm{d}\eta\,\big(\tau_<(\xi,\eta)\tau_>(\xi,\eta)^{\frac{2}{3}} - \tfrac{1}{5}\tau_<(\xi,\eta)^{\frac{5}{3}}\big)\end{aligned} \tag{1.2}$$

where $\gamma_{\mathrm{TF}} := (6\pi^2/q)^{2/3}\frac{\hbar^2}{2m}$ is the Thomas-Fermi constant, $\tau_<(\xi,\eta) := \min\{\tau(\xi),\tau(\eta)\}$, and $\tau_>(\xi,\eta) := \max\{\tau(\xi),\tau(\eta)\}$.

From now on we will use units where $\hbar = 2m = |e| = 1$. We will refer to the Hamiltonian in the new convention

$$H_N = \sum_{n=1}^{N}\Big(-\Delta_n - \frac{Z}{|x_n|}\Big) + \sum_{1\leq n<m\leq N}\frac{1}{|x_n - x_m|}. \tag{1.3}$$

With our choice of units $\gamma_{\mathrm{TF}} = (6\pi^2/q)^{2/3}$ and the energy functional has the following form:

$$\begin{aligned}\mathcal{E}_{\mathrm{mTF}}(\tau) &=: \mathcal{K}_m(\tau) - \mathcal{A}_m(\tau) + \mathcal{R}_m(\tau)\\ &= \int_{\mathbb{R}^3} \mathrm{d}\xi\, \xi^2 \tau(\xi) - \tfrac{3}{2}\gamma_{\mathrm{TF}}^{-1/2} Z \int_{\mathbb{R}^3} \mathrm{d}\xi\, \tau(\xi)^{\frac{2}{3}}\\ &\quad + \tfrac{3}{4}\gamma_{\mathrm{TF}}^{-1/2} \int_{\mathbb{R}^3} \mathrm{d}\xi \int_{\mathbb{R}^3} \mathrm{d}\eta\, \big(\tau_<(\xi,\eta)\tau_>(\xi,\eta)^{\frac{2}{3}} - \tfrac{1}{5}\tau_<(\xi,\eta)^{\frac{5}{3}}\big). \end{aligned} \tag{1.4}$$

## 1.2. Basic Properties of the Energy Functional

For the purpose of defining the functional $\mathcal{E}_{\mathrm{mTF}}$ it is sufficient to require $\tau \in L^1(\mathbb{R}^3, (1+\xi^2)\mathrm{d}\xi)$:

**Theorem 1.1** (Conta and Siedentop [27, Theorem 1])**.** *The functional $\mathcal{E}_{\mathrm{mTF}}$ is well-defined on real-valued functions in $L^1(\mathbb{R}^3, (1+\xi^2)\mathrm{d}\xi)$.*

*Proof.* The first summand of $\mathcal{E}_{\mathrm{mTF}}(\tau)$, the kinetic energy $\mathcal{K}_m$, is obviously well-defined. The claim for the attraction $\mathcal{A}_m$ follows from

$$\int_{\mathbb{R}^3} \mathrm{d}\xi\, |\tau(\xi)|^{\frac{2}{3}} \leq \Big(\int_{\mathbb{R}^3} \frac{\mathrm{d}\xi}{(1+\xi^2)^2}\Big)^{\frac{1}{3}} \Big(\int_{\mathbb{R}^3} \mathrm{d}\xi\, (1+\xi^2)|\tau(\xi)|\Big)^{\frac{2}{3}} < \infty \tag{1.5}$$

by Hölder's inequality. The repulsion $\mathcal{R}_m$ consists of two parts. Now,

$$\begin{aligned}\int_{\mathbb{R}^3} \mathrm{d}\xi \int_{\mathbb{R}^3} \mathrm{d}\eta\, |\tau_<(\xi,\eta)|^{\frac{5}{3}} &\leq \int_{\mathbb{R}^3} \mathrm{d}\xi \int_{\mathbb{R}^3} \mathrm{d}\eta\, |\tau_>(\xi,\eta)|^{\frac{2}{3}} |\tau_<(\xi,\eta)|\\ &\leq 2 \int_{\mathbb{R}^3} \mathrm{d}\xi\, |\tau(\xi)|^{\frac{2}{3}} \int_{\mathbb{R}^3} \mathrm{d}\eta\, |\tau(\eta)| \end{aligned} \tag{1.6}$$

which is finite by the previous argument. □

For densities in momentum space we define the sets

$$\begin{aligned}\mathcal{J} &:= \big\{\tau \in L^1(\mathbb{R}^3, (1+\xi^2)\mathrm{d}\xi) \mid \tau \geq 0\big\},\\ \mathcal{J}_N &:= \big\{\tau \in \mathcal{J} \mid \textstyle\int_{\mathbb{R}^3} \mathrm{d}\xi\, \tau(\xi) \leq N\big\},\\ \mathcal{J}_{\partial N} &:= \big\{\tau \in \mathcal{J} \mid \textstyle\int_{\mathbb{R}^3} \mathrm{d}\xi\, \tau(\xi) = N\big\}.\end{aligned}$$

In view of approximating the ground state energy via the minimal energy of the functional for large atoms, i. e., in the simultaneous limit $Z \to \infty$, $N \to \infty$ with the ratio $N/Z$ fixed, the following scaling law is of particular interest. It is implicitly given in the article [27].

**Theorem 1.2.** *Let $\tau \in \mathcal{J}$. Let $Z > 0$ and $\tau_Z(\xi) = Z^{-1}\tau(Z^{-2/3}\xi)$. Then*

$$\int_{\mathbb{R}^3} \mathrm{d}\xi\, \tau_Z(\xi) = Z \int_{\mathbb{R}^3} \mathrm{d}\xi\, \tau(\xi) \tag{1.7}$$

*and*

$$\mathcal{E}_{\mathrm{mTF}}(\tau_Z) = Z^{7/3}\mathcal{E}_{\mathrm{mTF,Z=1}}(\tau) \tag{1.8}$$

*where* $\mathcal{E}_{\mathrm{mTF,Z=1}}(\tau) := \mathcal{K}_m(\tau) - \frac{3}{2}\gamma_{\mathrm{TF}}^{-1/2} \int_{\mathbb{R}^3} \mathrm{d}\xi\, \tau(\xi)^{\frac{2}{3}} + \mathcal{R}_m(\tau)$.

*Proof.* The assertion (1.7) follows by a direct change of the integration variable. Likewise, we proceed in each term of (1.4) to get (1.8). □

We are interested in results pertaining to the existence of a minimizer of the functional $\mathcal{E}_{\mathrm{mTF}}$. For that reason convexity, and even more strict convexity, would be a desirable property of $\mathcal{E}_{\mathrm{mTF}}$. Clearly, $\mathcal{K}_m$ and $-\mathcal{A}_m$ are convex in $\tau$ but the interaction term $\mathcal{R}_m$ of $\mathcal{E}_{\mathrm{mTF}}$ is not. For example, consider the family of functions $(\tau_a)_{a\geq 1}$ on $\mathbb{R}^3$ given by

$$\tau_a(\xi) := \begin{cases} \frac{1}{a^3} & |\xi| \leq a \\ 0 & |\xi| > a \end{cases} \tag{1.9}$$

and set $\tau \equiv \tau_1$. Obviously, $\int_{\mathbb{R}^3} \mathrm{d}\xi\, \tau_a(\xi) = \int_{\mathbb{R}^3} \mathrm{d}\xi\, \tau(\xi)$ holds for all $a \geq 1$. Moreover, define

$$d(a) := c^{-1}\Big[\mathcal{R}_m\Big(\frac{\tau + \tau_a}{2}\Big) - \tfrac{1}{2}\big(\mathcal{R}_m(\tau) + \mathcal{R}_m(\tau_a)\big)\Big] \tag{1.10}$$

where $c := \frac{3}{4}\gamma_{\mathrm{TF}}^{-1/2} \cdot \frac{4}{5} \cdot \left(\frac{4\pi}{3}\right)^2$.

By an easy computation we get, on the one hand, that

$$\tfrac{1}{2}\big(\mathcal{R}_m(\tau) + \mathcal{R}_m(\tau_a)\big) = c\, \tfrac{1+a}{2}.$$

On the other hand, since

$$(\tau+\tau_a)(\xi) = \begin{cases} 1+\frac{1}{a^3} & |\xi| \le 1 \\ \frac{1}{a^3} & 1 < |\xi| \le a \\ 0 & a < |\xi| \end{cases}$$

we find

$$\mathcal{R}_m\Big(\frac{\tau+\tau_a}{2}\Big) \\ = 2^{-5/3}\, c\Big[\big(1+\tfrac{1}{a^3}\big)^{5/3}+\tfrac{5}{2}\Big(\tfrac{1}{a^3}\big(1+\tfrac{1}{a^3}\big)^{2/3}-\tfrac{1}{5}\big(\tfrac{1}{a^5}\big)\Big)(a^3-1)+\big(\tfrac{1}{a^3}\big)^{5/3}(a^3-1)^2\Big].$$

All together, this leads to

$$d(a) = 2^{-5/3}\Big[\big(1+\tfrac{1}{a^3}\big)^{5/3}+\tfrac{5}{2}\big(1-\tfrac{1}{a^3}\big)\Big(\big(1+\tfrac{1}{a^3}\big)^{2/3}-\tfrac{1}{5a^2}\Big)+\tfrac{(a^3-1)^2}{a^5}\Big]-\tfrac{1+a}{2}$$

for any $a \ge 1$. Therefrom, $d(2) > 0$ can be verified immediately which implies that $\mathcal{R}_m$ is not convex in $\tau$.

# 2. The Functional $\mathcal{E}_s$

We introduce a further functional. It is strictly convex and so closely related to $\mathcal{E}_{\mathrm{mTF}}$ that we may treat this new functional instead of $\mathcal{E}_{\mathrm{mTF}}$ when investigating the existence and uniqueness of a minimizing density.

Let the functional $\mathcal{E}_s$ of the momentum density $\tilde{\tau} \geq 0$ be given by

$$\begin{aligned}\mathcal{E}_s(\tilde{\tau}) := &\int_{\mathbb{R}^3} \mathrm{d}\xi\, \xi^2 \tilde{\tau}(\xi)^{\frac{3}{2}} - \tfrac{3}{2}\gamma_{\mathrm{TF}}^{-1/2} Z \int_{\mathbb{R}^3} \mathrm{d}\xi\, \tilde{\tau}(\xi) \\ &+ \tfrac{3}{4}\gamma_{\mathrm{TF}}^{-1/2} \int_{\mathbb{R}^3} \mathrm{d}\xi \int_{\mathbb{R}^3} \mathrm{d}\eta\, \left(\tilde{\tau}_<(\xi,\eta)^{\frac{3}{2}} \tilde{\tau}_>(\xi,\eta) - \tfrac{1}{5}\tilde{\tau}_<(\xi,\eta)^{\frac{5}{2}}\right) \end{aligned} \tag{2.1}$$

where $\tilde{\tau}_<$ and $\tilde{\tau}_>$ are defined analogously to $\tau_<$ and $\tau_>$, respectively. Indeed, $\mathcal{E}_s$ is derived from $\mathcal{E}_{\mathrm{mTF}}(\tau)$ by substituting $\tau \to \tilde{\tau}^{3/2}$, i. e.,

$$\mathcal{E}_s(\tilde{\tau}) := \mathcal{E}_{\mathrm{mTF}}(\tilde{\tau}^{3/2}). \tag{2.2}$$

In analogy to $\mathcal{E}_{\mathrm{mTF}}$ we define the sets

$$\begin{aligned}\mathcal{J}^s &:= \left\{\tilde{\tau} \in L^{3/2}(\mathbb{R}^3, (1+\xi^2)\mathrm{d}\xi) \mid \tilde{\tau} \geq 0\right\}, \\ \mathcal{J}^s_N &:= \left\{\tilde{\tau} \in \mathcal{J}^s \mid \textstyle\int_{\mathbb{R}^3} \mathrm{d}\xi\, \tilde{\tau}(\xi)^{\frac{3}{2}} \leq N\right\}, \\ \mathcal{J}^s_{\partial N} &:= \left\{\tilde{\tau} \in \mathcal{J}^s \mid \textstyle\int_{\mathbb{R}^3} \mathrm{d}\xi\, \tilde{\tau}(\xi)^{\frac{3}{2}} = N\right\}.\end{aligned}$$

**Theorem 2.1** (Conta and Siedentop [27])**.** *$\mathcal{E}_s$ is well-defined on $\mathcal{J}^s$. In particular, $\tilde{\tau} \in \mathcal{J}^s$ implies $\tilde{\tau} \in L^1(\mathbb{R}^3, \mathrm{d}\xi)$.*

*Proof.* By construction (Eq. (2.2)) the finiteness of $\mathcal{E}_s$ follows from the same estimates as in the proof of Theorem 1.1 when substituting $\tau \to \tilde{\tau}^{3/2}$. □

Uniqueness of a minimizer, given that it exists, is an important consequence of strict convexity. The treatment of the functional $\mathcal{E}_s$ is highly motivated by this particular property.

**Lemma 2.2** (Conta and Siedentop [27, Lemma 1]). *The functional $\mathcal{E}_s$ is strictly convex on all of $\mathcal{J}^s$ and on any convex subset of $\mathcal{J}^s$.*

*Proof.* Let $\tilde\tau \in \mathcal{J}^s_\#$ where $\mathcal{J}^s_\#$ denotes $\mathcal{J}^s$ or any convex subset of $\mathcal{J}^s$, e. g., $\mathcal{J}^s_N$ or $\mathcal{J}^s_{\partial N}$. Obviously, the first term of $\mathcal{E}_s$ is strictly convex, the second is linear. Thus, it suffices to show convexity of the repulsion term. Let $\theta$ denote the Heaviside function, i. e., $\theta(x) = 1$ if $x \geq 0$ and $\theta(x) = 0$ otherwise, and define the positive part for $x \in \mathbb{R}$ by $[x]_+ := \max\{0, x\}$. Then, we get

$$\begin{aligned}
&\int_0^\infty \mathrm{d}r \left(\int_{\mathbb{R}^3} \mathrm{d}\xi\, [\tilde\tau(\xi) - r^2]_+\right)^2 \\
&= \int_{\mathbb{R}^3} \mathrm{d}\xi \int_{\mathbb{R}^3} \mathrm{d}\eta \int_0^\infty \mathrm{d}r\, [\tilde\tau(\xi) - r^2][\tilde\tau(\eta) - r^2]\theta(\tilde\tau(\xi) - r^2)\theta(\tilde\tau(\eta) - r^2) \\
&= \int_{\mathbb{R}^3} \mathrm{d}\xi \int_{\mathbb{R}^3} \mathrm{d}\eta \int_0^{\tilde\tau_<(\xi,\eta)^{1/2}} \mathrm{d}r \left(\tilde\tau(\xi)\tilde\tau(\eta) - \tilde\tau(\xi)r^2 - \tilde\tau(\eta)r^2 + r^4\right) \\
&= \int_{\mathbb{R}^3} \mathrm{d}\xi \int_{\mathbb{R}^3} \mathrm{d}\eta \left(\tilde\tau(\xi)\tilde\tau(\eta)\tilde\tau_<(\xi,\eta)^{\frac12} - \tfrac13\tilde\tau(\xi)\tilde\tau_<(\xi,\eta)^{\frac32}\right. \\
&\qquad\qquad \left. - \tfrac13\tilde\tau(\eta)\tilde\tau_<(\xi,\eta)^{\frac32} + \tfrac15\tilde\tau_<(\xi,\eta)^{\frac52}\right) \\
&= \int_{\mathbb{R}^3} \mathrm{d}\xi \int_{\mathbb{R}^3} \mathrm{d}\eta \left(\tilde\tau_>(\xi,\eta)\tilde\tau_<(\xi,\eta)^{\frac32} - \tfrac13\tilde\tau_>(\xi,\eta)\tilde\tau_<(\xi,\eta)^{\frac32}\right. \\
&\qquad\qquad \left. - \tfrac13\tilde\tau_<(\xi,\eta)^{\frac52} + \tfrac15\tilde\tau_<(\xi,\eta)^{\frac52}\right) \\
&= \tfrac23 \int_{\mathbb{R}^3} \mathrm{d}\xi \int_{\mathbb{R}^3} \mathrm{d}\eta \left(\tilde\tau_<(\xi,\eta)^{\frac32}\tilde\tau_>(\xi,\eta) - \tfrac15\tilde\tau_<(\xi,\eta)^{\frac52}\right).
\end{aligned}$$

The assertion follows from this identity since the term in the first line is obviously convex. ☐

**Corollary 2.3** (Conta and Siedentop [27]). *Let $\mathcal{J}^s_\#$ denote $\mathcal{J}^s$ or any convex subset of $\mathcal{J}^s$, e. g., $\mathcal{J}^s_N$ or $\mathcal{J}^s_{\partial N}$. Then there is at most one $\tilde\tau \in \mathcal{J}^s_\#$ such that*

$$\mathcal{E}_s(\tilde\tau) = \inf_{\tilde\sigma \in \mathcal{J}^s_\#} \mathcal{E}_s(\tilde\sigma).$$

*Proof.* Let $\tilde\tau_1, \tilde\tau_2 \in \mathcal{J}^s_\#$. Suppose $\tilde\tau_1 \neq \tilde\tau_2$ were minimizers of the functional, i. e., $\mathcal{E}_s(\tilde\tau_1) = \mathcal{E}_s(\tilde\tau_2) = \inf_{\tilde\tau \in \mathcal{J}^s_\#} \mathcal{E}_s(\tilde\tau)$. This contradicts $\mathcal{E}_s(\frac{\tilde\tau_1 + \tilde\tau_2}{2}) < \inf_{\tilde\tau \in \mathcal{J}^s_\#} \mathcal{E}_s(\tilde\tau)$, and therefore the strict convexity of $\mathcal{E}_s$. ☐

The proof of Lemma 2.2 offers an expedient integral representation for the electron-electron interaction term of $\mathcal{E}_s$:

**Definition 2.4.** We write the electron-electron interaction term of $\mathcal{E}_s$ in the following convention:

$$\mathcal{R}^s_m(\tilde{\tau}) = \tfrac{9}{8}\gamma_{\mathrm{TF}}^{-1/2} \int_0^\infty \mathrm{d}r \, \Big( \int_{\mathbb{R}^3} \mathrm{d}\xi \, [\tilde{\tau}(\xi) - r^2]_+ \Big)^2.$$

# 3. Thomas-Fermi and the Momentum Energy Functional

We wish to relate the momentum energy functional given in the first chapter with the Thomas-Fermi functional. To this end, we first briefly recall the definition of the Thomas-Fermi functional and some results we will refer to in the sequel. Then, we define explicit transforms which, eventually, the relation of the two functionals emerges from.

## 3.1. A Few Results on the Thomas-Fermi Functional

In the chosen units where $\hbar = 2m = |e| = 1$ the well-known Thomas-Fermi functional (Lenz [8]) reads

$$\begin{aligned} \mathcal{E}_{\mathrm{TF}}(\rho) &:= \mathcal{K}(\rho) - \mathcal{A}(\rho) + \mathcal{R}(\rho) && (3.1)\\ &= \tfrac{3}{5}\gamma_{\mathrm{TF}} \int_{\mathbb{R}^3} \mathrm{d}x\, \rho(x)^{\frac{5}{3}} - \int_{\mathbb{R}^3} \mathrm{d}x\, \frac{Z}{|x|}\rho(x) + D[\rho] && (3.2) \end{aligned}$$

where $D[\rho]$ is the quadratic form of

$$D(\rho,\sigma) := \tfrac{1}{2} \int_{\mathbb{R}^3} \mathrm{d}x \int_{\mathbb{R}^3} \mathrm{d}y\, \frac{\rho(x)\sigma(y)}{|x-y|} \tag{3.3}$$

for one-particle electron densities $\rho$ and $\sigma$ in position space. The Thomas-Fermi constant is given as before by $\gamma_{\mathrm{TF}} = (6\pi^2/q)^{2/3}$. Mathematically this functional has been studied in detail by Lieb and Simon [12, 13] and Lieb [10]. The Thomas-Fermi functional is well-defined for functions in $L^1(\mathbb{R}^3) \cap L^{5/3}(\mathbb{R}^3)$ and we write

$$\begin{aligned} \mathcal{I} &:= \left\{\rho \in L^1(\mathbb{R}^3) \cap L^{5/3}(\mathbb{R}^3) \mid \rho \geq 0\right\},\\ \mathcal{I}_N &:= \left\{\rho \in \mathcal{I} \mid \textstyle\int_{\mathbb{R}^3} \mathrm{d}x\, \rho(x) \leq N\right\},\\ \mathcal{I}_{\partial N} &:= \left\{\rho \in \mathcal{I} \mid \textstyle\int_{\mathbb{R}^3} \mathrm{d}x\, \rho(x) = N\right\} \end{aligned}$$

for densities in position space.

In the following we will use the notion of spherically symmetric rearrangement, namely,

**Definition 3.1.** Let $A \subset \mathbb{R}^3$ and let $|A|$ denote its Lebesgue measure. If $|A| < \infty$ then $A^*$ is defined to be the closed ball centered at the origin which has the same volume as $A$. We call $A^*$ the spherically symmetric rearrangement of $A$.

For any function $\rho \in L^p(\mathbb{R}^3)$, $1 \le p < \infty$ its spherically symmetric rearrangement $\rho^*$ is given by

$$\rho^*(x) := \int_0^\infty \mathrm{d}t\, \chi_{\{x \in \mathbb{R}^3 || \rho(x)| > t\}}(x)$$

where $\chi_A$ denotes the characteristic function of the set $A$.

Now, the property of the Thomas-Fermi functional we want to mention first is that it decreases under spherically symmetric rearrangement, i. e.,

**Lemma 3.2** (Lieb [10, Theorem 2.12])**.** *Let $\rho \in \mathcal{I}$ and let $\rho^*$ denote its spherically symmetric rearrangement. Then*

$$\mathcal{E}_{\mathrm{TF}}(\rho^*) \le \mathcal{E}_{\mathrm{TF}}(\rho). \tag{3.4}$$

Other important results we will employ are collected in the following theorem:

**Theorem 3.3** (Lieb and Simon [13, Theorems II.14, II.17, II.18, II.20])**.** *Let $Z \ge 0$.*

1. *For all $0 \le N \le Z$ there exists a unique minimizer $\rho_N$ of $\mathcal{E}_{\mathrm{TF}}$ on $\mathcal{I}_{\partial N}$.*
2. *For $N > Z$ there exists no minimizer of $\mathcal{E}_{\mathrm{TF}}$ on $\mathcal{I}_{\partial N}$.*
3. *For each $N \ge 0$ there exists a unique minimizer $\rho_N$ of $\mathcal{E}_{\mathrm{TF}}$ on $\mathcal{I}_N$. Moreover, $\rho_N \in \mathcal{I}_{\partial \min\{N,Z\}}$.*
4. *Let $\rho_Z$ be the unique minimizer of $\mathcal{E}_{\mathrm{TF}}$ on $\mathcal{I}_{\partial Z}$. Then, for all $\rho \in \mathcal{I}$,*
$$\mathcal{E}_{\mathrm{TF}}(\rho) \ge \mathcal{E}_{\mathrm{TF}}(\rho_Z).$$

The minimum of the Thomas-Fermi functional is an approximation of the ground state energy. More precisely, suppose the ratio $N/Z$ is fixed, then

$$\inf \sigma(H_N) = \inf_{\rho \in \mathcal{I}_N} \mathcal{E}_{\mathrm{TF}}(\rho) + o(Z^{7/3}).$$

Moreover, there is a quantum mechanical limit for the density as well. For the case of a neutral atom, i. e., $N = Z$, we have that

$$Z^{-2} \rho_{\psi_Z}(\,\cdot\, Z^{-1/3}) \to Z^{-2} \rho_Z(\,\cdot\, Z^{-1/3}) = \rho_1 \tag{3.5}$$

weakly in the limit $Z \to \infty$. Here, $\rho_{\psi_Z}$ denotes the one-particle density of the quantum atom of charge $Z$ and $\rho_Z$ is the Thomas-Fermi minimizer. These results, among others, assert Thomas-Fermi theory in the regime of quantum mechanics and give rise to determine the linear response of atoms to perturbations that are local in position space.

We aim to prove some basic mathematical properties of $\mathcal{E}_{\mathrm{mTF}}$. In fact, we show equivalent results to Lemma 3.2 and Theorem 3.3 for the momentum functional $\mathcal{E}_{\mathrm{mTF}}$. This will establish the functional $\mathcal{E}_{\mathrm{mTF}}$ in the regime of quantum mechanics. We will consider momentum dependent perturbations as well.

## 3.2. Transforms between Position and Momentum Functional

Now, we define the explicit transforms which transfer each term of $\mathcal{E}_{\mathrm{mTF}}$ to the associated term of $\mathcal{E}_{\mathrm{TF}}$ as long as spherically symmetric decreasing densities are concerned. We set

$$\begin{aligned} S : L^1(\mathbb{R}^3) &\to L^1(\mathbb{R}^3) \\ \tau &\mapsto \rho \end{aligned} \tag{3.6}$$

where $\rho$ is given by

$$\rho(x) := \tfrac{q}{(2\pi)^3} \int_{|x| < \gamma_{\mathrm{TF}}^{1/2} |\tau(\xi)|^{1/3}} \mathrm{d}\xi \tag{3.7}$$

for all $x \in \mathbb{R}^3$.

For any function $\rho \in L^1(\mathbb{R}^3)$ and for any $s \geq 0$ we define the Fermi radius $r$ by

$$r(s) := 0 \quad \text{if } \gamma_{\mathrm{TF}}^{1/2}|\rho(x)|^{1/3} \leq s \text{ for a.e. } x \in \mathbb{R}^3,$$
$$r(s) := \inf\big\{K \mid \gamma_{\mathrm{TF}}^{1/2}|\rho(x)|^{1/3} > s \text{ for a.e. } |x| \leq K\big\} \quad \text{otherwise.} \tag{3.8}$$

This infimum can be understood, in some sense, as an essential supremum of the set $\{|x| \mid \gamma_{\mathrm{TF}}^{1/2}|\rho(x)|^{1/3} > s\}$, especially if $\rho$ is spherically symmetric. Now, based on the definition of the Fermi radius $r$ we set

$$T : L^1(\mathbb{R}^3) \to L^1(\mathbb{R}^3)$$
$$\rho \mapsto \tau \tag{3.9}$$

where $\tau$ is given by

$$\tau(\xi) := \gamma_{\mathrm{TF}}^{-3/2} r(|\xi|)^3 \tag{3.10}$$

for all $\xi \in \mathbb{R}^3$.

The first operator will be used to transfer a momentum density into a position density and the second to transfer a position into a momentum density. With this in view we prove the following results on the operators $S$ and $T$.

**Lemma 3.4** (Conta and Siedentop [27, Lemma 4])**.**

1. *The operator $S$ is isometric on $L^1(\mathbb{R}^3)$.*
2. *If $\rho \in L^1(\mathbb{R}^3)$ and $|\rho|$ spherically symmetric decreasing then*

$$\|T(\rho)\|_1 = \|\rho\|_1.$$

3. *All elements in the image of $S$ are spherically symmetric, nonnegative, and decreasing.*
4. *For every spherically symmetric $\rho \in L^1(\mathbb{R}^3)$, its image $T(\rho)$ is spherically symmetric, nonnegative, and decreasing.*

*Proof.* 1. The claim follows easily by direct computation interchanging the integration with respect to $x$ and the integration with respect to $\xi$.

2. To treat $T$ we may, without loss of generality, assume $\rho \geq 0$. Let $\xi \in \mathbb{R}^3$. By definition of $r$ and since $\rho$ is spherically symmetric decreasing

$$|x| < r(|\xi|) \Rightarrow \gamma_{\mathrm{TF}}^{1/2} \rho(x)^{1/3} > |\xi| \tag{3.11}$$

for almost every $x \in \mathbb{R}^3$, in the sense that almost every $x \in \mathbb{R}^3$ with $|x| < r(|\xi|)$ satisfies $\gamma_{\mathrm{TF}}^{1/2} \rho(x)^{1/3} > |\xi|$. Likewise, the definition of $r$ provides that

$$|x| \leq r(|\xi|) \Leftarrow \gamma_{\mathrm{TF}}^{1/2} \rho(x)^{1/3} > |\xi| \tag{3.12}$$

for almost every $x \in \mathbb{R}^3$.

We have

$$\|T(\rho)\|_1 = \tfrac{3}{4\pi\gamma_{\mathrm{TF}}^{3/2}} \int \mathrm{d}\xi \int_{|x|<r(|\xi|)} \mathrm{d}x. \tag{3.13}$$

By (3.11) we get the estimate

$$\begin{aligned} \|T(\rho)\|_1 &\leq \tfrac{3}{4\pi\gamma_{\mathrm{TF}}^{3/2}} \int \mathrm{d}\xi \int_{\gamma_{\mathrm{TF}}^{1/2} \rho(x)^{1/3} > |\xi|} \mathrm{d}x \\ &= \tfrac{3}{4\pi\gamma_{\mathrm{TF}}^{3/2}} \int \mathrm{d}x \int_{\gamma_{\mathrm{TF}}^{1/2} \rho(x)^{1/3} > |\xi|} \mathrm{d}\xi = \int \mathrm{d}x\, \rho(x). \end{aligned} \tag{3.14}$$

On the other hand, if we allow for $\leq$ instead of strict inequality on the integration constraints in (3.13) we can also reverse the inequality in (3.14) using (3.12).

3. and 4. The claims follow directly from the definitions. □

Now, we will see how the functionals $\mathcal{E}_{\mathrm{TF}}$ and $\mathcal{E}_{\mathrm{mTF}}$ are related via the operators $S$ and $T$, namely,

**Lemma 3.5** (Conta and Siedentop [27, Lemma 4]).

1. *For every spherically symmetric decreasing $\tau \in \mathcal{J}$*

$$\mathcal{E}_{\mathrm{mTF}}(\tau) = \mathcal{E}_{\mathrm{TF}} \circ S(\tau).$$

2. *For every spherically symmetric decreasing $\rho \in \mathcal{I}$*

$$\mathcal{E}_{\mathrm{mTF}} \circ T(\rho) = \mathcal{E}_{\mathrm{TF}}(\rho).$$

*Proof.* 1. We treat each term of the energy functional individually. We start with the potential terms, actually with the external potential which is an easy variant of the interaction potential. Both follow by explicit calculation.

We have

$$\mathcal{A}(S(\tau)) = \int \mathrm{d}x\, \frac{Z}{|x|} S(\tau)(x) = Z \int \mathrm{d}x\, \tfrac{q}{(2\pi)^3} \int_{|x|<\gamma_{\mathrm{TF}}^{1/2}\tau(\xi)^{1/3}} \mathrm{d}\xi\, \frac{1}{|x|}$$

$$= Z \int \mathrm{d}\xi\, \tfrac{q}{(2\pi)^3}\, \tfrac{4\pi}{2}\, \gamma_{\mathrm{TF}}\, \tau(\xi)^{\frac{2}{3}} = \tfrac{3}{2}\gamma_{\mathrm{TF}}^{-1/2} Z \int \mathrm{d}\xi\, \tau(\xi)^{\frac{2}{3}}. \quad (3.15)$$

Now we exhibit the calculation for the interaction potential. Given a radius $a > 0$ we set $K_a := \chi_{\{x\in\mathbb{R}^3 | |x|<a\}}$ to be the characteristic function of the open ball of radius $a$ centered at the origin. We get

$$\mathcal{R}(S(\tau)) = \tfrac{1}{2} \int \mathrm{d}x \int \mathrm{d}y\, \frac{1}{|x-y|}$$

$$\left(\tfrac{q}{(2\pi)^3}\right)^2 \int_{|x|<\gamma_{\mathrm{TF}}^{1/2}\tau(\xi)^{1/3}} \mathrm{d}\xi \int_{|y|<\gamma_{\mathrm{TF}}^{1/2}\tau(\eta)^{1/3}} \mathrm{d}\eta \quad (3.16)$$

$$= \left(\tfrac{q}{(2\pi)^3}\right)^2 \iint \mathrm{d}\xi \mathrm{d}\eta\, D(K_{\gamma_{\mathrm{TF}}^{1/2}\tau(\xi)^{1/3}}, K_{\gamma_{\mathrm{TF}}^{1/2}\tau(\eta)^{1/3}}) \quad (3.17)$$

$$= \left(\tfrac{3}{4\pi}\right)^2 \gamma_{\mathrm{TF}}^{-1/2} \iint \mathrm{d}\xi \mathrm{d}\eta\, D(K_{\sqrt[3]{\tau_<(\xi,\eta)}}, K_{\sqrt[3]{\tau_>(\xi,\eta)}}) \quad (3.18)$$

$$= \tfrac{9}{(4\pi)^2}\gamma_{\mathrm{TF}}^{-1/2}\Big(\iint \mathrm{d}\xi \mathrm{d}\eta\, D[K_{\sqrt[3]{\tau_<(\xi,\eta)}}]$$

$$+ \iint \mathrm{d}\xi \mathrm{d}\eta\, D(K_{\sqrt[3]{\tau_<(\xi,\eta)}}, K_{\sqrt[3]{\tau_>(\xi,\eta)}} - K_{\sqrt[3]{\tau_<(\xi,\eta)}})\Big) \quad (3.19)$$

$$= \tfrac{9}{(4\pi)^2}\gamma_{\mathrm{TF}}^{-1/2}\Big(\iint \mathrm{d}\xi \mathrm{d}\eta\, D[K_{\sqrt[3]{\tau_<(\xi,\eta)}}]$$

$$+ \iint \mathrm{d}\xi \mathrm{d}\eta\, \tfrac{1}{2} \int_{|x|<\sqrt[3]{\tau_<(\xi,\eta)}} \mathrm{d}x \int_{\sqrt[3]{\tau_<(\xi,\eta)}\le|y|<\sqrt[3]{\tau_>(\xi,\eta)}} \mathrm{d}y\, \frac{1}{|y|}\Big) \quad (3.20)$$

$$= \tfrac{9}{(4\pi)^2}\gamma_{\mathrm{TF}}^{-1/2}\Big(\iint \mathrm{d}\xi \mathrm{d}\eta\, D[K_1]\tau_<(\xi,\eta)^{\frac{5}{3}}$$

$$+ \iint \mathrm{d}\xi \mathrm{d}\eta\, \tfrac{4\pi}{2\cdot 3}\, \tau_<(\xi,\eta) 2\pi \big(\tau_>(\xi,\eta)^{\frac{2}{3}} - \tau_<(\xi,\eta)^{\frac{2}{3}}\big)\Big) \quad (3.21)$$

$$= \tfrac{3}{4}\gamma_{\mathrm{TF}}^{-1/2} \iint \mathrm{d}\xi \mathrm{d}\eta\, \tau_<(\xi,\eta)\tau_>(\xi,\eta)^{\frac{2}{3}} - \tfrac{1}{5}\tau_<(\xi,\eta)^{\frac{5}{3}} \quad (3.22)$$

where we used the scaling properties of $D$ in (3.18) and Newton's Theorem B.5 to get (3.20). In particular, $D[K_1] = \frac{(4\pi)^2}{15}$ follows by a simple computation.

Now we turn to the remaining term, the kinetic energy. It transforms as

$$\mathcal{K}(S(\tau)) = \tfrac{3}{5}\gamma_{\mathrm{TF}} \int \mathrm{d}x\, S(\tau)(x)^{\frac{5}{3}} = 3\gamma_{\mathrm{TF}} \int \mathrm{d}x \int_{0\le t\le S(\tau)(x)^{1/3}} \mathrm{d}t\, t^4$$

$$= \tfrac{3}{4\pi}\gamma_{\mathrm{TF}} \int \mathrm{d}\xi \xi^2 \int_{|\xi|^3\le S(\tau)(x)} \mathrm{d}x. \tag{3.23}$$

Given that $S(\tau)(x) \ge |\xi|^3$ implies $\gamma_{\mathrm{TF}}^{1/2}\tau(\gamma_{\mathrm{TF}}^{1/2}\xi)^{1/3} \ge |x|$, which is equivalent to the statement that $\frac{3}{4\pi}\int_{|x|<\tau(\eta)^{1/3}} \mathrm{d}\eta \ge |\xi|^3$ implies $\tau(\xi)^{1/3} \ge |x|$, we have

$$\tfrac{3}{5}\gamma_{\mathrm{TF}} \int \mathrm{d}x\, S(\tau)(x)^{\frac{5}{3}} \le \tfrac{3}{4\pi}\gamma_{\mathrm{TF}} \int \mathrm{d}\xi\, \xi^2 \int_{|x|\le\gamma_{\mathrm{TF}}^{1/2}\tau(\gamma_{\mathrm{TF}}^{1/2}\xi)^{1/3}} \mathrm{d}x \tag{3.24}$$

$$= \int \mathrm{d}\xi\, \xi^2 \tau(\xi). \tag{3.25}$$

Suppose $\frac{3}{4\pi}\int_{|x|<\tau(\eta)^{1/3}} \mathrm{d}\eta \ge |\xi|^3$ would not imply $\tau(\xi)^{1/3} \ge |x|$. Then

$$|\xi|^3 \le \tfrac{3}{4\pi} \int_{|x|<\tau(\eta)^{1/3}} \mathrm{d}\eta < \tfrac{3}{4\pi} \int_{\tau(\xi)<\tau(\eta)} \mathrm{d}\eta \le \tfrac{3}{4\pi} \int_{|\xi|>|\eta|} \mathrm{d}\eta = |\xi|^3 \tag{3.26}$$

where we used in the last inequality that $\tau$ is spherically symmetric and decreasing.

On the other hand, $\frac{3}{4\pi}\int_{|x|<\tau(\eta)^{1/3}} \mathrm{d}\eta \ge |\xi|^3$ follows from $\tau(\xi)^{1/3} > |x|$ as

$$|\xi|^3 = \tfrac{3}{4\pi} \int_{|\eta|\le|\xi|} \mathrm{d}\eta \le \tfrac{3}{4\pi} \int_{\tau(\xi)\le\tau(\eta)} \mathrm{d}\eta \le \tfrac{3}{4\pi} \int_{|x|<\tau(\eta)^{1/3}} \mathrm{d}\eta \tag{3.27}$$

using in the first inequality again that $\tau$ is spherically symmetric and decreasing. Thus we can reverse the inequality in (3.24), i. e.,

$$\tfrac{3}{5}\gamma_{\mathrm{TF}} \int \mathrm{d}x\, S(\tau)(x)^{\frac{5}{3}} \ge \tfrac{3}{4\pi}\gamma_{\mathrm{TF}} \int \mathrm{d}\xi\, \xi^2 \int_{|x|<\gamma_{\mathrm{TF}}^{1/2}\tau(\gamma_{\mathrm{TF}}^{1/2}\xi)^{1/3}} \mathrm{d}x \tag{3.28}$$

$$= \int \mathrm{d}\xi\, \xi^2 \tau(\xi). \tag{3.29}$$

2. To prove that $\mathcal{E}_{\mathrm{mTF}} \circ T(\rho) = \mathcal{E}_{\mathrm{TF}}(\rho)$ we proceed as in 1. We begin with the kinetic energy:

$$\begin{aligned}\mathcal{K}_m(T(\rho)) &= \int \mathrm{d}\xi\, \xi^2 \gamma_{\mathrm{TF}}^{-3/2} r(|\xi|)^3 = \tfrac{3}{4\pi}\gamma_{\mathrm{TF}}^{-3/2} \int \mathrm{d}\xi\, \xi^2 \int_{|x|<r(|\xi|)} \mathrm{d}x \\ &= \tfrac{3}{4\pi}\gamma_{\mathrm{TF}}^{-3/2} \int \mathrm{d}\xi\, \xi^2 \int_{|\xi|<\gamma_{\mathrm{TF}}^{1/2}\rho(x)^{1/3}} \mathrm{d}x = \mathcal{K}(\rho) \qquad (3.30)\end{aligned}$$

where we used (3.11) and (3.12) in the penultimate identity.

For the external potential we get

$$\begin{aligned}&\mathcal{A}_m(T(\rho)) = \tfrac{3}{2}\gamma_{\mathrm{TF}}^{-3/2} Z \int \mathrm{d}\xi\, r(|\xi|)^2 = 3\gamma_{\mathrm{TF}}^{-3/2} Z \int \mathrm{d}\xi \int_{0\le t<r(|\xi|)} \mathrm{d}t\, t \\ &= Z\tfrac{3}{4\pi}\gamma_{\mathrm{TF}}^{-3/2} \int \mathrm{d}\xi \int_{|x|<r(|\xi|)} \mathrm{d}x\, \tfrac{1}{|x|} = Z\tfrac{3}{4\pi}\gamma_{\mathrm{TF}}^{-3/2} \int \mathrm{d}x\, \tfrac{1}{|x|} \int_{|\xi|<\gamma_{\mathrm{TF}}^{1/2}\rho(x)^{1/3}} \mathrm{d}\xi \\ &= Z \int \mathrm{d}x\, \frac{1}{|x|}\rho(x) \qquad (3.31)\end{aligned}$$

using again (3.11) and (3.12) in the penultimate identity.

Finally we go to $\mathcal{R}_m$. Adapting the steps (3.22) to (3.16) yields

$$\begin{aligned}&\mathcal{R}_m(T(\rho)) = \tfrac{1}{2} \iint \mathrm{d}x\mathrm{d}y\, \frac{1}{|x-y|} \big(\tfrac{q}{(2\pi)^3}\big)^2 \int_{|x|<r(|\xi|)} \mathrm{d}\xi \int_{|y|<r(|\eta|)} \mathrm{d}\eta \\ &= \tfrac{1}{2}\big(\tfrac{q}{(2\pi)^3}\big)^2 \iint \mathrm{d}x\mathrm{d}y\, \frac{1}{|x-y|} \int_{|\xi|<\gamma_{\mathrm{TF}}^{1/2}\rho(x)^{1/3}} \mathrm{d}\xi \int_{|\eta|<\gamma_{\mathrm{TF}}^{1/2}\rho(y)^{1/3}} \mathrm{d}\eta \\ &= \mathcal{R}(\rho) \qquad (3.32)\end{aligned}$$

using (3.11) and (3.12) once more. □

# 4. Results on the Minimal Energy and the Minimizer

## 4.1. Existence and Uniqueness Results

The following theorem establishes $\mathcal{E}_{\mathrm{mTF}}$ as the momental analogue of the Thomas-Fermi functional (cf. Theorem 3.3).

**Theorem 4.1** (Conta and Siedentop [27, Theorem 2]). *Let $Z \geq 0$.*

1. *For all $N \geq 0$, we have $\inf_{\tau \in \mathcal{J}_{\partial N}} \mathcal{E}_{\mathrm{mTF}}(\tau) = \inf_{\rho \in \mathcal{I}_{\partial N}} \mathcal{E}_{\mathrm{TF}}(\rho)$.*
2. *Let $0 \leq N \leq Z$. If $\rho_N$ is the unique minimizer of $\mathcal{E}_{\mathrm{TF}}$ on $\mathcal{I}_{\partial N}$ then $T(\rho_N)$ is the unique minimizer of $\mathcal{E}_{\mathrm{mTF}}$ on $\mathcal{J}_{\partial N}$.*
3. *For $N > Z$ there exists no minimizer of $\mathcal{E}_{\mathrm{mTF}}$ on $\mathcal{J}_{\partial N}$.*
4. *For each $N \geq 0$ there exists a unique minimizer $\tau_N$ of $\mathcal{E}_{\mathrm{mTF}}$ on $\mathcal{J}_N$. Moreover, $\tau_N \in \mathcal{J}_{\partial \min\{N,Z\}}$.*
5. *Let $\tau_Z$ be the unique minimizer of $\mathcal{E}_{\mathrm{mTF}}$ on $\mathcal{J}_{\partial Z}$. Then, for all $\tau \in \mathcal{J}$,*
$$\mathcal{E}_{\mathrm{mTF}}(\tau) \geq \mathcal{E}_{\mathrm{mTF}}(\tau_Z).$$

The proof of Theorem 4.1 is based on the relation of the functionals $\mathcal{E}_{\mathrm{TF}}$ and $\mathcal{E}_{\mathrm{mTF}}$ that was indicated in Lemma 3.5. Thus, in order to apply this lemma we want to restrict the two functionals to spherically symmetric decreasing densities. We overcome this problem if we can ensure that $\mathcal{E}_{\mathrm{mTF}}$ decreases under spherically symmetric rearrangement since the same result holds for $\mathcal{E}_{\mathrm{TF}}$ (Lemma 3.2).

**Lemma 4.2** (Conta and Siedentop [27, Lemma 5]). *Let $\tau \in \mathcal{J}$ and let $\tau^*$ denote its spherically symmetric rearrangement (Definition 3.1). Then*
$$\mathcal{E}_{\mathrm{mTF}}(\tau^*) \leq \mathcal{E}_{\mathrm{mTF}}(\tau). \tag{4.1}$$

*Proof.* The attraction $\mathcal{A}_m$ is obviously invariant under rearrangement. The repulsion $\mathcal{R}_m$ is – by definition – a superposition of rearranged terms only, i. e., is also trivially invariant.

Let $|A|$ denote the Lebesgue measure of any subset $A$ of $\mathbb{R}^3$. Since $\mathcal{K}_m(\tau) = \int_0^\infty \mathrm{d}t \int \mathrm{d}\xi\, \xi^2 \chi_{\{\xi\in\mathbb{R}^3|\tau(\xi)>t\}}(\xi)$, it suffices to show that for any $A \subset \mathbb{R}^3$ with finite measure

$$\int \mathrm{d}\xi\, \xi^2 \chi_A(\xi) \geq \int \mathrm{d}\xi\, \xi^2 \chi_{A^*}(\xi) = \int_{|\xi|\leq R} \mathrm{d}\xi\, \xi^2$$

where $R$ is defined by $|A| = \frac{4\pi}{3}R^3$, i. e., the radius of the ball $A^* := B_R(0)$ centered at the origin which has the same volume as $A$. Now define the sets $B := B_R(0) \setminus A$, $C := A \setminus B_R(0)$, and $D := A \cap B_R(0)$. Then $|B| = |C|$, and thus

$$\begin{aligned}\int_{A^*} \mathrm{d}\xi\, \xi^2 = \int_B \mathrm{d}\xi\, \xi^2 + \int_D \mathrm{d}\xi\, \xi^2 &\leq R^2 \int_B \mathrm{d}\xi + \int_D \mathrm{d}\xi\, \xi^2 \\ &\leq \int_C \mathrm{d}\xi\, \xi^2 + \int_D \mathrm{d}\xi\, \xi^2 = \int_A \mathrm{d}\xi\, \xi^2.\end{aligned}$$

□

**Corollary 4.3** (Conta and Siedentop [27]). *Every minimizer $\tau \in \mathcal{J}$ of $\mathcal{E}_{\mathrm{mTF}}$ is spherically symmetric decreasing.*

Now, we can prove Theorem 4.1:

*Proof.* 1. The two functionals $\mathcal{E}_{\mathrm{TF}}$ and $\mathcal{E}_{\mathrm{mTF}}$ decrease under spherically symmetric rearrangement (Lemma 3.2 and Lemma 4.2). So, as far as minimization is concerned, we may restrict both functionals to spherically symmetric decreasing densities $\rho$ and $\tau$. Under this restriction $S$ and $T$ preserve the norm and hence Statement 1 of Lemma 3.5 implies that

$$\inf_{\tau\in\mathcal{J}_{\partial N}} \mathcal{E}_{\mathrm{mTF}}(\tau) \geq \inf_{\rho\in\mathcal{I}_{\partial N}} \mathcal{E}_{\mathrm{TF}}(\rho)$$

whereas Statement 2 implies the reverse inequality. This proves the first assertion of Theorem 4.1.

2. Since $\mathcal{E}_{\mathrm{TF}}$ has a unique minimizer $\rho_N$ on $\mathcal{I}_{\partial N}$ if $N \leq Z$ (Theorem 3.3), it follows from the preceding step and Lemma 3.5, Statement 2 that $T(\rho_N)$ minimizes $\mathcal{E}_{\mathrm{mTF}}$ on $\mathcal{J}_{\partial N}$.

It remains to show that there is no other minimizer of the momentum functional. This follows from the strict convexity of $\mathcal{E}_s$ (Lemma 2.2). Indeed, suppose that $\tau_N \neq \tau'_N$ were two different minimizers of $\mathcal{E}_{\mathrm{mTF}}$ on $\mathcal{J}_{\partial N}$. Then, since $\inf_{\tau\in\mathcal{J}_{\partial N}} \mathcal{E}_{\mathrm{mTF}}(\tau) = \inf_{\tau\in\mathcal{J}^s_{\partial N}} \mathcal{E}_s(\tau)$ (Eq. (2.2)), we obtain two different minimizers $\tilde{\tau}_N \neq \tilde{\tau}'_N$ of $\mathcal{E}_s$ on $\mathcal{J}^s_{\partial N}$ from the substitutions $\tilde{\tau}_N^{3/2} = \tau_N$ and $(\tilde{\tau}'_N)^{3/2} = \tau'_N$. But this contradicts Corollary 2.3.

3. Suppose $\tau_N$ is a minimizer of $\mathcal{E}_{\mathrm{mTF}}$ on $\mathcal{J}_{\partial N}$ for some $N > Z$. Then $S(\tau_N)$ has to be a minimizer of $\mathcal{E}_{\mathrm{TF}}$ by Statement 1 and Lemma 3.5, Statement 1 but this does not exist (Theorem 3.3).

4. Again, if $\tau_N$ minimizes $\mathcal{E}_{\mathrm{mTF}}$ on $\mathcal{J}_N$ then $S(\tau_N)$ minimizes $\mathcal{E}_{\mathrm{TF}}$ on $\mathcal{I}_N$. Thus, $\int \tau_N = \int S(\tau_N) = \min\{Z, N\}$. Uniqueness of $\tau_N$ follows from the strict convexity of $\mathcal{E}_s$ as in the proof of Statement 2.

5. The claim follows from Statement 2 and Statement 4. □

## 4.2. Properties of the Minimizing Density and Euler's Equation

We start with a bound on the minimizer. By the definition of $T$, the relation between $r$ and $\tau$ as given by (3.10), and Theorem 4.1 any bound on the position space density implies a corresponding bound on the momentum space density.

**Lemma 4.4** (Conta and Siedentop [27]). *Let $\tau$ be the minimizer of $\mathcal{E}_{\mathrm{mTF}}$ on $\mathcal{J}$, then*

$$\tau(\xi) \leq \gamma_{\mathrm{TF}}^{-3/2} \frac{Z^3}{|\xi|^6} \tag{4.2}$$

*for almost every $\xi \in \mathbb{R}^3$. Furthermore, there exists $\xi_0 \in \mathbb{R}^3 \setminus \{0\}$ such that*

$$\tau(\xi) \leq \left(\tfrac{3}{\pi}\right)^{\frac{3}{2}} \gamma_{\mathrm{TF}}^{-3/2} \frac{1}{|\xi|^{3/2}} \tag{4.3}$$

*for almost every $\xi \in \mathbb{R}^3$ satisfying $|\xi| < |\xi_0|$.*

*Proof.* Let $\rho$ be the Thomas-Fermi minimizer on $\mathcal{I}$. Then $\rho$ obeys

$$\rho(x) \leq \gamma_{\mathrm{TF}}^{-3/2} \frac{Z^{3/2}}{|x|^{3/2}}$$

for almost every $x \in \mathbb{R}^3$ as a consequence of the corresponding Euler equation in position space (see, e. g., Lieb and Simon [13]). This implies the first bound in the proposition since $\tau$ can be represented in terms of $\rho$ by means of $T$ as defined in Eq. (3.10). In this case,

$$\begin{aligned}
\tau(\xi) &= T(\rho)(\xi) \\
&= \gamma_{\mathrm{TF}}^{-3/2}\big(\inf\{K \mid \gamma_{\mathrm{TF}}^{1/2}|\rho(x)|^{1/3} > |\xi| \text{ for a.e. } |x| \le K\}\big)^3 \\
&= \gamma_{\mathrm{TF}}^{-3/2}\Big(\inf\Big\{K \mid \frac{Z^{1/2}}{|x|^{1/2}} \ge \gamma_{\mathrm{TF}}^{1/2}|\rho(x)|^{1/3} > |\xi| \text{ for a.e. } |x| \le K\Big\}\Big)^3 \\
&\le \gamma_{\mathrm{TF}}^{-3/2}\Big(\sup\Big\{|x| \mid \frac{Z^{1/2}}{|x|^{1/2}} > |\xi|\Big\}\Big)^3 \\
&= \gamma_{\mathrm{TF}}^{-3/2}\Big(\sup\Big\{|x| \mid \frac{Z}{|\xi|^2} > |x|\Big\}\Big)^3 \\
&\le \gamma_{\mathrm{TF}}^{-3/2}\Big(\frac{Z}{|\xi|^2}\Big)^3 = \gamma_{\mathrm{TF}}^{-3/2}\frac{Z^3}{|\xi|^6}
\end{aligned} \tag{4.4}$$

for almost every $\xi \in \mathbb{R}^3$. Indeed, the infimum exists as $\rho$ is unbounded (see, e. g., Lieb and Simon [13]).

Likewise, the second bound in the proposition is a consequence of the Sommerfeld bound [13, 25] concerning the asymptotics of $\rho$ at infinity. In position space there exists some $x_0 \in \mathbb{R}^3 \setminus \{0\}$ such that

$$\rho(x) \le 27\pi^{-3}\gamma_{\mathrm{TF}}^{-3/2}\frac{1}{|x|^6}$$

for almost every $x \in \mathbb{R}^3$ with $|x| \ge |x_0|$. Moreover, since $\rho$ is spherically symmetric decreasing (Lemma 3.2) we can find some $\xi_0 \in \mathbb{R}^3\setminus\{0\}$ such that $\gamma_{\mathrm{TF}}^{1/2}\rho(x)^{1/3} \ge |\xi_0|$ for almost every $|x| < |x_0|$. Thus, for almost every $\xi \in \mathbb{R}^3$ with $|\xi| < |\xi_0|$ we get

$$\begin{aligned}
\tau(\xi) &= \gamma_{\mathrm{TF}}^{-3/2}\big(\inf\{K \mid \gamma_{\mathrm{TF}}^{1/2}|\rho(x)|^{1/3} > |\xi| \text{ for a.e. } |x| \le K\}\big)^3 \\
&= \gamma_{\mathrm{TF}}^{-3/2}\big(\inf\{K \mid \gamma_{\mathrm{TF}}^{1/2}|\rho(x)|^{1/3} > |\xi| \text{ for a.e. } |x_0| \le |x| \le K\}\big)^3 \\
&\le \gamma_{\mathrm{TF}}^{-3/2}\Big(\sup\Big\{|x| \mid 3\pi^{-1}\frac{1}{|x|^2} > |\xi|\Big\}\Big)^3
\end{aligned}$$

$$
\begin{aligned}
&= \gamma_{\mathrm{TF}}^{-3/2}\Big(\sup\Big\{|x| \mid \big(\tfrac{3}{\pi}\big)^{1/2}\frac{1}{|\xi|^{1/2}} > |x|\Big\}\Big)^3 \\
&\le \big(\tfrac{3}{\pi}\big)^{3/2}\gamma_{\mathrm{TF}}^{-3/2}\frac{1}{|\xi|^{3/2}}. \qquad (4.5)
\end{aligned}
$$

Note that the second identity holds since $\rho$ is spherically symmetric decreasing. □

The following property of the minimizer will be applied for the derivation of the Euler equation hereafter.

**Lemma 4.5** (adapted from Conta and Siedentop [27, Lemma 2])**.** *The minimizer of $\mathcal{E}_{\mathrm{mTF}}$ on $\mathcal{J}$ is strictly positive almost everywhere. Moreover, the minimizer of $\mathcal{E}_{\mathrm{mTF}}$ on $\mathcal{J}_N$ for each $N > 0$ is strictly positive almost everywhere.*

*Proof.* Let $\tau$ be a minimizer of $\mathcal{E}_{\mathrm{mTF}}$. Suppose that the set $N_\tau := \{\xi \in \mathbb{R}^3 | \tau(\xi) = 0\}$, on which $\tau$ vanishes, would not be of measure zero. Then pick any function $\sigma \in \mathcal{J}$ with $\tau(\xi)\sigma(\xi) = 0$ for almost all $\xi \in \mathbb{R}^3$ which is not identical zero on $N_\tau$ and satisfies $\int_{\mathbb{R}^3} \mathrm{d}\xi\, \sigma(\xi) \le \int_{\mathbb{R}^3} \mathrm{d}\xi\, \tau(\xi)$.

For any $0 < \varepsilon \le 1$ we define the function

$$
\tau_\varepsilon := \tau + \varepsilon\big(\sigma - \tfrac{\int \sigma}{\int \tau}\,\tau\big).
$$

Note that $\tau_\varepsilon \in \mathcal{J}$ and $\int \tau_\varepsilon = \int \tau$. Then by the integral representation of the interaction term (Definition 2.4) together with the substitution $\tilde{\tau}^{3/2} = \tau$ we get

$$
\begin{aligned}
&\mathcal{E}_{\mathrm{mTF}}(\tau_\varepsilon) - \mathcal{E}_{\mathrm{mTF}}(\tau) \\
&= \tfrac{3}{2}\gamma_{\mathrm{TF}}^{-1/2} Z \int_{\mathbb{R}^3} \mathrm{d}\xi \left(1 - \big(1 - \varepsilon \tfrac{\int\sigma}{\int\tau}\big)^{\frac{2}{3}}\right)\tau(\xi)^{\frac{2}{3}} - \tfrac{3}{2}\gamma_{\mathrm{TF}}^{-1/2} Z \int_{\mathbb{R}^3} \mathrm{d}\xi\, \varepsilon^{2/3}\sigma(\xi)^{\frac{2}{3}} \\
&\quad + \tfrac{3}{2}\cdot\tfrac{3}{4}\gamma_{\mathrm{TF}}^{-1/2} \int_0^\infty \mathrm{d}r \left(\int_{\mathbb{R}^3} \mathrm{d}\xi \left[\big(1 - \varepsilon \tfrac{\int\sigma}{\int\tau}\big)^{\frac{2}{3}}\tau(\xi)^{\frac{2}{3}} - r^2\right]_+ \right. \\
&\qquad\qquad \left. + \int_{\mathbb{R}^3} \mathrm{d}\xi\, [\varepsilon^{2/3}\sigma(\xi)^{\frac{2}{3}} - r^2]_+\right)^2 \\
&\quad - \tfrac{3}{2}\cdot\tfrac{3}{4}\gamma_{\mathrm{TF}}^{-1/2} \int_0^\infty \mathrm{d}r \left(\int_{\mathbb{R}^3} \mathrm{d}\xi\, [\tau(\xi)^{\frac{2}{3}} - r^2]_+\right)^2 + O(\varepsilon) \qquad (4.6)
\end{aligned}
$$

$$
\begin{aligned}
&\le -\varepsilon^{2/3}\,\tfrac{3}{2}\gamma_{\mathrm{TF}}^{-1/2} Z \int_{\mathbb{R}^3} \mathrm{d}\xi\, \sigma(\xi)^{2/3} + O(\varepsilon) \\
&\quad + \tfrac{3}{2}\cdot\tfrac{3}{4}\gamma_{\mathrm{TF}}^{-1/2} \int_0^\infty \mathrm{d}r \Big( \int_{\mathbb{R}^3} \mathrm{d}\xi\, [\tau(\xi)^{\frac{2}{3}} - r^2]_+ \\
&\qquad\qquad + \int_{\mathbb{R}^3} \mathrm{d}\xi\, [\varepsilon^{2/3}\sigma(\xi)^{\frac{2}{3}} - r^2]_+ \Big)^2 \\
&\quad - \tfrac{3}{2}\cdot\tfrac{3}{4}\gamma_{\mathrm{TF}}^{-1/2} \int_0^\infty \mathrm{d}r \Big( \int_{\mathbb{R}^3} \mathrm{d}\xi\, [\tau(\xi)^{\frac{2}{3}} - r^2]_+ \Big)^2 \qquad (4.7) \\
&= -\varepsilon^{2/3}\,\tfrac{3}{2}\gamma_{\mathrm{TF}}^{-1/2} Z \int_{\mathbb{R}^3} \mathrm{d}\xi\, \sigma(\xi)^{\frac{2}{3}} + O(\varepsilon) \\
&\quad + 2\cdot\tfrac{3}{4}\cdot\tfrac{3}{2}\gamma_{\mathrm{TF}}^{-1/2} \int_0^\infty \mathrm{d}r \Big( \int_{\mathbb{R}^3} \mathrm{d}\xi\, [\tau(\xi)^{\frac{2}{3}} - r^2]_+ \Big) \\
&\qquad\qquad \times \Big( \int_{\mathbb{R}^3} \mathrm{d}\eta [\varepsilon^{2/3}\sigma(\eta)^{\frac{2}{3}} - r^2]_+ \Big) \qquad (4.8) \\
&\le -\varepsilon^{2/3}\,\tfrac{3}{2}\gamma_{\mathrm{TF}}^{-1/2} Z \int_{\mathbb{R}^3} \mathrm{d}\xi\, \sigma(\xi)^{\frac{2}{3}} + O(\varepsilon) \\
&\quad + \tfrac{9}{4}\gamma_{\mathrm{TF}}^{-1/2} \Big[ \int_0^\infty \mathrm{d}r \Big( \int_{\mathbb{R}^3} \mathrm{d}\xi\, [\tau(\xi)^{\frac{2}{3}} - r^2]_+ \Big)^2 \Big]^{\frac{1}{2}} \\
&\qquad \times \Big[ \int_0^\infty \mathrm{d}r \Big( \int_{\mathbb{R}^3} \mathrm{d}\eta\, [\varepsilon^{2/3}\sigma(\eta)^{\frac{2}{3}} - r^2]_+ \Big)^2 \Big]^{\frac{1}{2}} \\
&= -\varepsilon^{2/3}\,\tfrac{3}{2}\gamma_{\mathrm{TF}}^{-1/2} Z \int_{\mathbb{R}^3} \mathrm{d}\xi\, \sigma(\xi)^{\frac{2}{3}} + O(\varepsilon^{5/6}) \qquad (4.9)
\end{aligned}
$$

where in the first inequality we used that $1-\varepsilon\,\frac{\int\sigma}{\int\tau} \le \big(1-\varepsilon\,\frac{\int\sigma}{\int\tau}\big)^{2/3} \le 1$. In the second inequality we applied the Cauchy-Schwarz inequality. And finally, scaling the powers of $\varepsilon$ out yields the given estimate.

In fact, this implies that

$$\mathcal{E}_{\mathrm{mTF}}(\tau_\varepsilon) - \mathcal{E}_{\mathrm{mTF}}(\tau) < 0,$$

for sufficiently small $\varepsilon$. Hence, $\tau$ cannot be a minimizer. □

Now, we turn to the proof of Euler's equation.

**Lemma 4.6** (Conta and Siedentop [27, Lemma 3])**.** *The Euler equation which the minimizer of $\mathcal{E}_{\mathrm{mTF}}$ on $\mathcal{J}$ satisfies is*

$$\gamma_{\mathrm{TF}}^{1/2}|\xi|^2\tau(\xi)^{\frac{1}{3}} - Z + \int_{\mathbb{R}^3} \mathrm{d}\eta\, \big(\tfrac{3}{2}\tau(\eta)^{\frac{2}{3}}\tau_<(\xi,\eta)^{\frac{1}{3}} - \tfrac{1}{2}\tau_<(\xi,\eta)\big) = 0. \quad (4.10)$$

*Proof.* Instead of deriving the Euler equation for $\mathcal{E}_{\mathrm{mTF}}$ we use $\mathcal{E}_s$ (see Eq. (2.2)).

Let $\tilde{\tau}$ be the minimizer which is strictly positive almost everywhere because of Lemma 4.5. Thus we can pick any $\sigma \in L^{3/2}(\mathbb{R}^3, (1+\xi^2)\mathrm{d}\xi)$ with $|\sigma| \leq \tilde{\tau}$. Then, for $\varepsilon \in [-1,1]$, $\tilde{\tau} + \varepsilon\sigma$ is an allowed trial function and the function $F(\varepsilon) = \mathcal{E}_s(\tilde{\tau} + \varepsilon\sigma)$ has a minimum at zero. We show that $F$ is differentiable at zero.

The first two terms of $F$ are obviously differentiable. For the derivative of the kinetic term we obtain $\frac{3}{2}\int_{\mathbb{R}^3} \mathrm{d}\xi\, \xi^2\sigma(\xi)\tilde{\tau}(\xi)^{1/2}$ at $\varepsilon = 0$ and for the derivative of the external potential evaluated at the origin we get $\frac{3}{2}\gamma_{\mathrm{TF}}^{-1/2} Z \int_{\mathbb{R}^3} \mathrm{d}\xi\, \sigma(\xi)$. Thus, we concentrate on

$$\begin{aligned} T(\varepsilon) &:= \varepsilon^{-1} \int_0^\infty \mathrm{d}r \left[ \left( \int_{\mathbb{R}^3} \mathrm{d}\xi\, [\tilde{\tau}(\xi) + \varepsilon\sigma(\xi) - r^2]_+ \right)^2 \right. \\ &\qquad\qquad \left. - \left( \int_{\mathbb{R}^3} \mathrm{d}\xi\, [\tilde{\tau}(\xi) - r^2]_+ \right)^2 \right] \\ &= \int_0^\infty \mathrm{d}r \int_{\mathbb{R}^3} \mathrm{d}\xi \int_{\mathbb{R}^3} \mathrm{d}\eta\, \frac{[\tilde{\tau}(\xi) + \varepsilon\sigma(\xi) - r^2]_+ - [\tilde{\tau}(\xi) - r^2]_+}{\varepsilon} \\ &\qquad\qquad \times \left( [\tilde{\tau}(\eta) + \varepsilon\sigma(\eta) - r^2]_+ + [\tilde{\tau}(\eta) - r^2]_+ \right) \\ &=: \int_0^\infty \mathrm{d}r \int_{\mathbb{R}^3} \mathrm{d}\xi \int_{\mathbb{R}^3} \mathrm{d}\eta\, I(\varepsilon, r, \xi, \eta). \end{aligned} \tag{4.11}$$

Since $|a_+ - b_+| \leq |a - b|$ for real $a$ and $b$ (Lemma B.1) and since $|\varepsilon| \leq 1$ we get

$$|\sigma(\xi)| \left( [\tilde{\tau}(\eta) + |\sigma(\eta)| - r^2]_+ + [\tilde{\tau}(\eta) - r^2]_+ \right)$$

to be an integrable majorant of the integrand $I$ independent of $\varepsilon$. Indeed, we have

$$\begin{aligned} &\int_0^\infty \mathrm{d}r \int_{\mathbb{R}^3} \mathrm{d}\xi \int_{\mathbb{R}^3} \mathrm{d}\eta\, |\sigma(\xi)| [\tilde{\tau}(\eta) + |\sigma(\eta)| - r^2]_+ \\ &\qquad \leq \int_{\mathbb{R}^3} \mathrm{d}\xi\, |\sigma(\xi)| \int_0^\infty \mathrm{d}r \int_{\mathbb{R}^3} \mathrm{d}\eta\, [2\tilde{\tau}(\eta) - r^2]_+ \\ &\qquad\qquad = \int_{\mathbb{R}^3} \mathrm{d}\xi\, |\sigma(\xi)|\, \tfrac{2}{3} \int_{\mathbb{R}^3} \mathrm{d}\eta\, 2^{3/2}\, \tilde{\tau}(\eta)^{\frac{3}{2}} < \infty \end{aligned} \tag{4.12}$$

as $|\sigma| \leq \tilde{\tau}$. Now, to apply dominated convergence, we split the integral in two parts, namely the part where the pointwise limit of $I$ exists and the rest. Consider $\frac{[a+\varepsilon b]_+ - [a]_+}{\varepsilon}$ for $a, b \in \mathbb{R}$ in the limit where $\varepsilon$ tends to zero. In the case where $a = 0$, this limit does not exist. Whereas, if $a < 0$ then $\frac{[a+\varepsilon b]_+ - [a]_+}{\varepsilon} \to 0$, and if $a > 0$ then $\frac{[a+\varepsilon b]_+ - [a]_+}{\varepsilon} \to b$. In summary, $[a + \varepsilon b]_+ \to [a]_+$ as $\varepsilon \to 0$ for $a \neq 0$. This finally results in

$$\begin{aligned}\lim_{\varepsilon\to 0} T(\varepsilon) &= \lim_{\varepsilon\to 0} \int_0^\infty \mathrm{d}r \int_{\tilde{\tau}(\xi)=r^2} \mathrm{d}\xi \int_{\mathbb{R}^3} \mathrm{d}\eta\, I(\varepsilon, r, \xi, \eta) \\ &\qquad + \lim_{\varepsilon\to 0} \int_0^\infty \mathrm{d}r \int_{\tilde{\tau}(\xi)\neq r^2} \mathrm{d}\xi \int_{\mathbb{R}^3} \mathrm{d}\eta\, I(\varepsilon, r, \xi, \eta) \\ &= 2\int_0^\infty \mathrm{d}r \int_{\mathbb{R}^3} \mathrm{d}\xi \int_{\mathbb{R}^3} \mathrm{d}\eta\, \sigma(\xi)\theta(\tilde{\tau}(\xi) - r^2)[\tilde{\tau}(\eta) - r^2]_+. \end{aligned} \tag{4.13}$$

Indeed, the integration with respect to $r$ restricted to $\tilde{\tau}(\xi) = r^2$ yields zero.

In fact, this proves that $F$ is differentiable. Hence, integration with respect to $r$ yields

$$\begin{aligned}\int_{\mathbb{R}^3} \mathrm{d}\xi\, \sigma(\xi) \Big[ &\tfrac{3}{2}\xi^2 \tilde{\tau}(\xi)^{\frac{1}{2}} - \tfrac{3}{2}\gamma_{\mathrm{TF}}^{-1/2} Z \\ &+ \tfrac{3}{2}\cdot\tfrac{3}{4}\gamma_{\mathrm{TF}}^{-1/2} \int_{\mathbb{R}^3} \mathrm{d}\eta\, \big(2\,\tilde{\tau}(\eta)\tilde{\tau}_<(\xi,\eta)^{\frac{1}{2}} - \tfrac{2}{3}\,\tilde{\tau}_<(\xi,\eta)^{\frac{3}{2}}\big)\Big] = 0. \end{aligned} \tag{4.14}$$

Since $\sigma$ is arbitrary we arrive at the desired Euler equation (4.10) after substituting $\tilde{\tau}^{3/2} = \tau$. □

Since the integrand in (4.10) is nonnegative, the Euler equation implies the following pointwise bound on the minimizer:

$$\tau(\xi) \leq \gamma_{\mathrm{TF}}^{-3/2} \frac{Z^3}{|\xi|^6}. \tag{4.15}$$

In particular, this bound we got already from Lemma 4.4.

## 4.3. The Virial Theorem

**Theorem 4.7** (Virial Theorem)**.** *If $\tau$ minimizes $\mathcal{E}_{\mathrm{mTF}}$ on any $\mathcal{J}_N$, then*

$$2\mathcal{K}_m(\tau) = \mathcal{A}_m(\tau) - \mathcal{R}_m(\tau). \tag{4.16}$$

*Proof.* Suppose $\tau$ is the minimizer of $\mathcal{E}_{\mathrm{mTF}}$ on $\mathcal{J}_N$ and define $\tau_\lambda(\xi) := \lambda^{-3}\tau(\lambda^{-1}\xi)$ for some $\lambda > 0$. Note that $\tau_\lambda \in \mathcal{J}_N$ with $\|\tau_\lambda\|_1 = \|\tau\|_1$. Scaling yields

$$\mathcal{E}_{\mathrm{mTF}}(\tau_\lambda) = \lambda^2\mathcal{K}_m(\tau) - \lambda\mathcal{A}_m(\tau) + \lambda\mathcal{R}_m(\tau). \tag{4.17}$$

Consider $\mathcal{E}_{\mathrm{mTF}}(\tau_\lambda)$ as a function of $\lambda$. Then $\mathcal{E}_{\mathrm{mTF}}(\tau_\lambda)$ is differentiable for positive $\lambda$ and has its unique minimum at $\lambda = 1$. Thus,

$$0 = \left.\frac{\mathrm{d}\mathcal{E}_{\mathrm{mTF}}(\tau_\lambda)}{\mathrm{d}\lambda}\right|_{\lambda=1} = 2\mathcal{K}_m(\tau) - \mathcal{A}_m(\tau) + \mathcal{R}_m(\tau). \tag{4.18}$$

□

If $\tau$ is the minimizer of $\mathcal{E}_{\mathrm{mTF}}$ on $\mathcal{J}$ then another relation between $\mathcal{K}_m(\tau)$, $\mathcal{A}_m(\tau)$, and $\mathcal{R}_m(\tau)$ can be easily achieved via minimization, namely,

**Theorem 4.8.** *If $\tau$ minimizes $\mathcal{E}_{\mathrm{mTF}}$ on $\mathcal{J}$, then*

$$3\mathcal{K}_m(\tau) = 2\mathcal{A}_m(\tau) - 5\mathcal{R}_m(\tau). \tag{4.19}$$

*Proof.* Suppose $\tau$ is the minimizer of $\mathcal{E}_{\mathrm{mTF}}$ on $\mathcal{J}$ and define $\tau_\lambda(\xi) := \lambda\tau(\xi)$ for some $\lambda > 0$. Then the same reasoning as in the preceding proof gives

$$0 = \left.\frac{\mathrm{d}\mathcal{E}_{\mathrm{mTF}}(\tau_\lambda)}{\mathrm{d}\lambda}\right|_{\lambda=1} = \mathcal{K}_m(\tau) - \tfrac{2}{3}\mathcal{A}_m(\tau) + \tfrac{5}{3}\mathcal{R}_m(\tau). \tag{4.20}$$

□

**Corollary 4.9.** *If $\tau$ minimizes $\mathcal{E}_{\mathrm{mTF}}$ on $\mathcal{J}$, then the following ratio holds:*

$$\mathcal{K}_m(\tau) : \mathcal{A}_m(\tau) : \mathcal{R}_m(\tau) = 3 : 7 : 1.$$

*Proof.* The assertion follows from (4.16) and (4.19). □

*Remark.* The Virial Theorem can be also obtained using the operator $T$ and the Virial Theorem for $\mathcal{E}_{\mathrm{TF}}$ (Lieb and Simon [13, Theorem II.22]). The same applies to the corollary when using the corresponding relation between $\mathcal{K}(\rho)$, $\mathcal{A}(\rho)$, and $\mathcal{R}(\rho)$ for the atomic Thomas-Fermi density $\rho$ (Lieb and Simon [13, Corollary II.24]).

# 5. Asymptotic Exactness of Englert's Statistical Model of the Atom

In this chapter we show that the atomic momentum density converges on the scale $Z^{2/3}$ to the minimizer of the momentum energy functional $\mathcal{E}_{\mathrm{mTF}}$. Note that in the semiclassical regime this corresponds to the scale where $\hbar = Z^{-1/3}$ (cf. Eq. (3.5)).

As indicated already in the introduction this limit theorem for the density is essential to determine the linear response of atoms to perturbations that are local in momentum space. As a result of Theorem 4.1 from the previous chapter we already know that the ground state energy is asymptotic to the infimum of the momentum energy functional $\mathcal{E}_{\mathrm{mTF}}$ of the same order as the Thomas-Fermi energy is. Therefore,

$$\inf \sigma(H_N) = \inf_{\tau \in \mathcal{J}_N} \mathcal{E}_{\mathrm{mTF}}(\tau) + o(Z^{7/3})$$

if the ratio $N/Z$ is fixed. Now, we shall consider the Hamiltonian $H_N$ perturbed by some momentum dependent potential $\varphi_Z(\xi) := Z^{4/3}\varphi(Z^{-2/3}\xi)$, namely,

$$H_{N,\alpha} := H_N - \alpha \sum_{n=1}^{N} \varphi_Z(-\mathrm{i}\nabla_n) \tag{5.1}$$

with some $\alpha \in \mathbb{R}$. In fact, in the proposition of the limit theorem we will have some requirements on $\alpha$ and $\varphi$.

We shall consider the simultaneous limit $Z \to \infty$, $N \to \infty$ such that the ratio $N/Z$ is fixed. In order to simplify notation we avoid the introduction of a scaling parameter which incorporates the dependence of $N$ and $Z$. Moreover, the case where $N \neq Z$ requires the notion of an approximate ground state. So, we start with the introduction of some useful notations:

1. Let $\psi_N \in \bigwedge_{n=1}^N L^2(\mathbb{R}^3 : \mathbb{C}^q) =: \mathcal{H}$ be a sequence of normalized vectors such that
$$\frac{\inf \sigma(H_N) - \langle \psi_N, H_N \psi_N \rangle}{Z^{7/3}} \to 0$$
as $Z \to \infty$, $N \to \infty$ under the subsidiary condition that $N/Z$ is fixed. We call $\psi_N$ an approximate ground state of $H_N$.

2. The one-particle ground state density of any normalized vector $\psi \in \mathcal{H}$ is defined by
$$\rho_\psi(x) := N \sum_{\sigma_1=1}^{q} \cdots \sum_{\sigma_N=1}^{q} \int_{\mathbb{R}^{3(N-1)}} \mathrm{d}x_2 \cdots \mathrm{d}x_N \\ \times |\psi(x, \sigma_1; x_2, \sigma_2; \ldots; x_N, \sigma_N)|^2$$
in position space and
$$\tau_\psi(\xi) := N \sum_{\sigma_1=1}^{q} \cdots \sum_{\sigma_N=1}^{q} \int_{\mathbb{R}^{3(N-1)}} \mathrm{d}\xi_2 \cdots \mathrm{d}\xi_N \\ \times |\hat{\psi}(\xi, \sigma_1; \xi_2, \sigma_2; \ldots; \xi_N, \sigma_N)|^2$$
in momentum space where $\hat{\psi}$ denotes the Fourier transform of $\psi$ on $\bigwedge_{n=1}^N L^2(\mathbb{R}^3)$. The rescaled one-particle momentum density of $\psi$ is given by
$$\tilde{\tau}_\psi(\xi) := Z \tau_\psi(Z^{2/3}\xi).$$

3. We denote the set of all trace class operators on $L^2(\mathbb{R}^3 : \mathbb{C}^q)$ by $\mathfrak{S}^1(L^2(\mathbb{R}^3 : \mathbb{C}^q))$. Then
$$\mathcal{S} := \{\gamma \in \mathfrak{S}^1(L^2(\mathbb{R}^3 : \mathbb{C}^q)) \mid 0 \leq \gamma \leq 1\}$$
is called the set of fermionic one-particle density matrices.

4. The one-particle density matrix of a normalized $N$-particle state $\psi \in \mathcal{H}$ is denoted by $\gamma_\psi$ and it satisfies $\operatorname{tr} \gamma_\psi = N$.

5. Every $\gamma \in \mathcal{S}$ has a spectral decomposition into orthonormal eigenvectors $e_j \in L^2(\mathbb{R}^3 : \mathbb{C}^q)$ and the corresponding eigenvalues $0 \leq \lambda_j \leq 1$. We write

$$\tau_\gamma(\xi) := \sum_{\sigma=1}^{q} \sum_j \lambda_j |\hat{e}_j(\xi, \sigma)|^2$$

for the momentum density of $\gamma$. Here $\hat{e}_j$ denotes the Fourier transform of $e_j$ on $L^2(\mathbb{R}^3)$. The rescaled momentum density of $\gamma$ is given by

$$\tilde{\tau}_\gamma(\xi) := Z\tau_\gamma(Z^{2/3}\xi).$$

6. Let $\rho_N$ be the minimizer of the Thomas-Fermi functional $\mathcal{E}_{\mathrm{TF}}$ on $\mathcal{I}_N$ (see Theorem 3.3). Then $\rho_N$ obeys the Thomas-Fermi equation

$$\gamma_{\mathrm{TF}} \rho_N^{2/3} = [\phi_N - \mu]_+$$

where $\mu$ is some positive constant and $\phi_N$ denotes the Thomas-Fermi potential which is given by

$$\phi_N := Z/|\cdot| - \rho_N * |\cdot|^{-1}.$$

In particular, $\mu$ is uniquely determined by $\phi_N$. These quantities scale as

$$\begin{aligned} \phi_N(x) =: \phi(Z, N, x) &= Z^{4/3}\phi(1, N/Z, Z^{1/3}x), \\ \mu =: \mu(Z, N) &= Z^{4/3}\mu(1, N/Z). \end{aligned}$$

For references see, e. g., Lieb and Simon [12] or Lieb [10].

7. For $\alpha \in \mathbb{R}$, the effective one-particle Hamiltonian corresponding to the Thomas-Fermi potential is given by

$$h_{N,\alpha} := -\Delta - \phi_N - \alpha\, \varphi_Z(-\mathrm{i}\nabla)$$

and we write $h_{N,\alpha}(\xi, x)$ for its Hamilton function.

The following lemma provides a lower bound to the sum of the negative eigenvalues of the one-particle Hamiltonian $h_{N,\alpha}$.

**Lemma 5.1** (Neutral Case $N = Z$: Conta and Siedentop [27, Lemma 6])**.** *Let $\alpha \in \mathbb{R}$. Let $\mu \geq 0$ and $h_{N,\alpha}$ be given as in Notation 6 and 7 above. Assume $0 \leq (1 + |\cdot|^{-2})\varphi \in L^\infty(\mathbb{R}^3)$, $\varphi$ uniformly continuous, and $|\alpha| < v/2$ with $v := 1/(\||\cdot|^{-2}\varphi\|_\infty)$. Then, for every $\gamma \in \mathcal{S}$,*

$$\mathrm{tr}\,(h_{N,\alpha}\gamma) \geq \tfrac{q}{(2\pi)^3} \int_{h_{N,\alpha}(\xi,x)<-\mu} \mathrm{d}\xi \mathrm{d}x \, h_{N,\alpha}(\xi, x) - o(Z^{7/3}) \tag{5.2}$$

*uniformly in $\alpha$ for large $Z$ when the ratio $N/Z$ is fixed.*

*Remark.* The corresponding result for the unperturbed one-particle Hamiltonian $h_{N,0}$ can be found in the article of Lieb [10, Section V.A.2]. There he shows that, for all $\gamma \in \mathcal{S}$,

$$\mathrm{tr}\,(h_{N,0}\gamma) \geq \tfrac{q}{(2\pi)^3} \int_{h_{N,0}(\xi,x)<-\mu} \mathrm{d}\xi \mathrm{d}x \, h_{N,0}(\xi, x) - \mathrm{const}\, Z^{7/3-1/30}$$

if $N = O(Z)$. We will follow his proof modified by the momentum operator $\varphi_Z$.

*Proof of Lemma 5.1.* Note that due to the Thomas-Fermi equation and the requirements on $\alpha$ and $\varphi$ in the hypothesis of the lemma we have

$$\tfrac{q}{(2\pi)^3} \int_{h_{N,\alpha}(\xi,x)<-\mu} \mathrm{d}\xi \mathrm{d}x \leq \tfrac{q}{(2\pi)^3} \int_{\frac{1}{2}\xi^2-\phi_N(x)<-\mu} \mathrm{d}\xi \mathrm{d}x \leq \mathrm{const}\, N \tag{5.3}$$

and likewise

$$\tfrac{q}{(2\pi)^3} \int_{h_{N,\alpha}(\xi,x)<0} \mathrm{d}\xi \mathrm{d}x \, h_{N,\alpha}(\xi, x) \geq -\mathrm{const}\, Z^{\frac{7}{3}}$$

if $N = O(Z)$.

Next, we follow the lower bound of Lieb's asymptotic result (Lieb [10, Theorem 5.1]). To this end let $g \in C_0^\infty(\mathbb{R}^3)$ be a spherically symmetric positive function with $\mathrm{supp}(g)$ contained in the unit ball, $\int g^2 = 1$, and $g_R(x) := R^{3/2} g(Rx)$ its dilatation by $R$. Note that $\widehat{g_R} = \hat{g}_{R^{-1}}$ holds for the Fourier transform of $g_R$. Furthermore, let $f_{\xi,x}(r) := e^{\mathrm{i}\xi\cdot r} g_R(r - x)$ be the coherent states in $L^2(\mathbb{R}^3)$ and define the projection $\pi_{\xi,x} := |f_{\xi,x}\rangle\langle f_{\xi,x}| \otimes I_\sigma$ where $I_\sigma$ denotes the identity operator in spin space.

For any function $e_j \in L^2(\mathbb{R}^3 : \mathbb{C}^q)$ we have

$$\begin{aligned}\langle e_j, e_j\rangle &= \int \mathrm{d}\xi \mathrm{d}x \sum_{\sigma=1}^{q} |\mathcal{F}\big(g_R(\,\cdot\, - x)e_j(\,\cdot\,,\sigma)\big)(\xi)|^2 \\ &= \int \mathrm{d}\xi \mathrm{d}x \sum_{\sigma=1}^{q} \Big|\tfrac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} \mathrm{d}r\, e^{-\mathrm{i}\xi\cdot r}\, g_R(r-x)e_j(r,\sigma)\Big|^2 \\ &= \tfrac{1}{(2\pi)^3} \int \mathrm{d}\xi \mathrm{d}x\, \langle e_j, \pi_{\xi,x} e_j\rangle \end{aligned} \tag{5.4}$$

where $\mathcal{F}$ denotes the Fourier transform on $L^2(\mathbb{R}^3)$. We compute:

$$\begin{aligned}&\sum_{\sigma=1}^{q} \int_{\mathbb{R}^3} \mathrm{d}x\, (\phi_N * |g_R|^2)(x)|e_j(x,\sigma)|^2 \\ &\quad= \sum_{\sigma=1}^{q} \int \mathrm{d}\xi \mathrm{d}x\, \phi_N(x)|\mathcal{F}(g_R(\,\cdot\, - x)e_j(\,\cdot\,,\sigma)(\xi))|^2 \\ &\quad= \tfrac{1}{(2\pi)^3} \int \mathrm{d}\xi \mathrm{d}x\, \phi_N(x)\langle e_j, \pi_{\xi,x} e_j\rangle. \end{aligned} \tag{5.5}$$

Moreover,

$$\sum_{\sigma=1}^{q} \int_{\mathbb{R}^3} \mathrm{d}x\, (\varphi_Z * |\widehat{g_R}|^2)(-\mathrm{i}\nabla_x)|e_j(x,\sigma)|^2 \tag{5.6}$$

$$= \sum_{\sigma=1}^{q} \int_{\mathbb{R}^3} \mathrm{d}\xi\, (\varphi_Z * |\widehat{g_R}|^2)(\xi)|\hat{e}_j(\xi,\sigma)|^2 \tag{5.7}$$

$$= \sum_{\sigma=1}^{q} \int \mathrm{d}\xi \mathrm{d}x\, \varphi_Z(\xi)|\mathcal{F}(\widehat{g_R}(\xi - \,\cdot\,)\hat{e}_j(\,\cdot\,,\sigma))(x)|^2 \tag{5.8}$$

$$= \sum_{\sigma=1}^{q} \int \mathrm{d}\xi \mathrm{d}x\, \varphi_Z(\xi)\Big|\tfrac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} \mathrm{d}p\, e^{\mathrm{i}(\xi-p)\cdot x}\, \widehat{g_R}(\xi-p)\hat{e}_j(p,\sigma)\Big|^2 \tag{5.9}$$

$$= \sum_{\sigma=1}^{q} \int \mathrm{d}\xi \mathrm{d}x\, \varphi_Z(\xi)\Big|\tfrac{1}{(2\pi)^{3/2}}\big((e^{\mathrm{i}\,\cdot\,\cdot x}\,\widehat{g_R}) * \hat{e}_j(\,\cdot\,,\sigma)\big)(\xi)\Big|^2 \tag{5.10}$$

$$= \sum_{\sigma=1}^{q} \int \mathrm{d}\xi \mathrm{d}x\, \varphi_Z(\xi)|\mathcal{F}(g_R(\,\cdot\, - x)e_j(\,\cdot\,,\sigma))(\xi)|^2 \tag{5.11}$$

$$= \tfrac{1}{(2\pi)^3} \int \mathrm{d}\xi \mathrm{d}x\, \varphi_Z(\xi)\langle e_j, \pi_{\xi,x} e_j\rangle. \tag{5.12}$$

Thus, the identity

$$\sum_{\sigma=1}^{q} \int_{\mathbb{R}^3} \mathrm{d}x\, |\nabla_x e_j(x,\sigma)|^2 = \tfrac{1}{(2\pi)^3} \int \mathrm{d}\xi \mathrm{d}x\, \xi^2 \langle e_j, \pi_{\xi,x} e_j\rangle - \|e_j\|_2^2\, \|\nabla g_R\|_2^2 \tag{5.13}$$

can be easily verified by

$$\begin{aligned} \tfrac{1}{(2\pi)^3} \int \mathrm{d}\xi \mathrm{d}x\, \xi^2 \langle e_j, \pi_{\xi,x} e_j\rangle &= \sum_{\sigma=1}^{q} \int \mathrm{d}\xi \mathrm{d}p\, (\xi - p)^2\, |\widehat{g_R}(p)|^2 |\hat{e}_j(\xi,\sigma)|^2 \\ = \sum_{\sigma=1}^{q} \int \mathrm{d}\xi \mathrm{d}p\, \xi^2\, |\widehat{g_R}(p)|^2 |\hat{e}_j(\xi,\sigma)|^2 &+ \sum_{\sigma=1}^{q} \int \mathrm{d}\xi \mathrm{d}p\, p^2\, |\widehat{g_R}(p)|^2 |\hat{e}_j(\xi,\sigma)|^2 \\ &= \sum_{\sigma=1}^{q} \int_{\mathbb{R}^3} \mathrm{d}x\, |\nabla_x e_j(x,\sigma)|^2 + \|e_j\|_2^2\, \|\nabla g_R\|_2^2. \end{aligned} \tag{5.14}$$

Indeed, replacing $\varphi_Z$ by the square function in line (5.7) – line (5.12) yields the first equality. The second holds since $g$ is spherically symmetric. Eq. (5.4), (5.5), and (5.13) are also stated in the proof of Lieb [10, Theorem 5.1]. It follows that for any $\gamma \in \mathcal{S}$ written in the form $\gamma = \sum_j \lambda_j |e_j\rangle\langle e_j|$ (cf. Notation 5) we have

$$\begin{aligned} \mathrm{tr}\,(h_{N,\alpha}\gamma) = \tfrac{1}{(2\pi)^3} \int \mathrm{d}\xi \mathrm{d}x\, \big(h_{N,\alpha}(\xi,x) + \mu\, \mathbb{1}_h(\xi,x)\big) \sum_j \lambda_j \langle e_j, \pi_{\xi,x} e_j\rangle \\ - \mu\, \mathrm{tr}\, \mathbb{1}_h \gamma \\ - \mathrm{tr}\, \gamma R^2 \|\nabla g\|_2^2 - \mathrm{tr}\, [(\phi_N - \phi_N * |g_R|^2)\gamma] \\ - \alpha\, \mathrm{tr}\, \big[[(\varphi_Z - \varphi_Z * |\widehat{g_R}|^2)(-\mathrm{i}\nabla)]\gamma\big] \end{aligned} \tag{5.15}$$

where $\mathbb{1}_h$ is the projection to the negative spectral subspace of $h_{N,\alpha} + \mu$ and $\mathbb{1}_h(\xi, x)$ its symbol. Since we are interested in a lower bound we may assume $\mathrm{tr}\,\gamma \le \mathrm{const}\, Z$. Furthermore, $0 \le \sum_j \lambda_j \langle e_j, \pi_{\xi,x} e_j\rangle \le q$ hence

$$\begin{aligned} \mathrm{tr}\,(h_{N,\alpha}\gamma) \ge \tfrac{q}{(2\pi)^3} \int_{h_{N,\alpha}(\xi,x) < -\mu} \mathrm{d}\xi \mathrm{d}x\, (h_{N,\alpha}(\xi,x) + \mu) \\ - \mathrm{const}\, Z R^2 \|\nabla g\|_2^2 - \mathrm{tr}\, [(\phi_N - \phi_N * |g_R|^2)\gamma] \\ - \alpha\, \mathrm{tr}\, \big[[(\varphi_Z - \varphi_Z * |\widehat{g_R}|^2)(-\mathrm{i}\nabla)]\gamma\big]. \end{aligned} \tag{5.16}$$

The right hand side of the first line is the wanted main term added by an error term of order $O(Z)$. Indeed, sneaking in the constant $\mu$ generates an error term just of the same order as the phase space volume (Eq. (5.3)) which is uniformly in $\alpha$. This is negligible compared to the error of order $o(Z^{7/3})$ which the remaining terms bring up. Actually, if we choose $R = Z^{1/2}$ then the third line consists of error terms of order $O(Z^{7/3-1/30})$ (Lieb [10, Theorem 5.1]). The term in the last line is new and to see that it is a further error term we need an additional argument.

We have

$$\begin{aligned} &|\mathrm{tr}\,[(\varphi_Z(-\mathrm{i}\nabla) - (\varphi_Z * |\widehat{g_R}|^2)(-\mathrm{i}\nabla))\gamma]| \\ &\qquad \leq Z^{7/3} \int_{\mathbb{R}^3} \mathrm{d}\xi \int_{\mathbb{R}^3} \mathrm{d}p\, \tilde{\tau}_\gamma(\xi)|\varphi(\xi) - \varphi(\xi - p)||\hat{g}_{Z^{1/6}}(p)|^2. \end{aligned} \tag{5.17}$$

However, the integral of the right hand side converges to zero by uniform continuity of $\varphi$ and the fact that $\hat{g} \in \mathcal{S}(\mathbb{R}^3)$. To see this we show that $\|\varphi - \varphi * |\hat{g}_{Z^{1/6}}|^2\|_\infty$ is arbitrarily small for large $Z$: Let $\varepsilon > 0$. Since $\varphi$ is uniformly continuous, there exists $\delta > 0$ such that $|p| < \delta$ implies $|\varphi(\xi) - \varphi(\xi - p)| < \frac{\varepsilon}{2}$ for all $\xi, p \in \mathbb{R}^3$.

Note that $\hat{g}$ is a Schwartz function and hence there exists a constant $c > 0$ such that

$$|\hat{g}(p)|^2 < \frac{c}{|p|^4} \tag{5.18}$$

for all $p \in \mathbb{R}^3$. Moreover, for every $\varepsilon$, there is a $Z_0 > 0$ such that

$$2Z^{-1/6}c\,\|\varphi\|_\infty \int_{|p|>\delta} \mathrm{d}p\, |p|^{-4} < \tfrac{\varepsilon}{2}$$

for all $Z > Z_0$. With this choice, we estimate

$$\begin{aligned} &\int_{\mathbb{R}^3} \mathrm{d}p\, |\varphi(\xi) - \varphi(\xi - p)||\hat{g}_{Z^{1/6}}(p)|^2 \\ &\qquad = \int_{|p|<\delta} \mathrm{d}p\, |\varphi(\xi) - \varphi(\xi - p)||\hat{g}_{Z^{1/6}}(p)|^2 \\ &\qquad\quad + \int_{|p|>\delta} \mathrm{d}p\, |\varphi(\xi) - \varphi(\xi - p)||\hat{g}_{Z^{1/6}}(p)|^2 \\ &\qquad \leq \tfrac{\varepsilon}{2} + 2\|\varphi\|_\infty c \int_{|p|>\delta} \mathrm{d}p\, \frac{Z^{1/2}}{(Z^{1/6}|p|)^4} \leq \tfrac{\varepsilon}{2} + \tfrac{\varepsilon}{2}. \end{aligned} \tag{5.19}$$

Thus, $Z > Z_0$ implies

$$\int_{\mathbb{R}^3} \mathrm{d}\xi \int_{\mathbb{R}^3} \mathrm{d}p \, \tilde{\tau}_\gamma(\xi) |\varphi(\xi) - \varphi(\xi - p)| |\hat{g}_{Z^{1/6}}(p)|^2 \leq \varepsilon \int_{\mathbb{R}^3} \mathrm{d}\xi \, \tilde{\tau}_\gamma(\xi) = \mathrm{const}\, \varepsilon.$$

This proves that the last line of (5.16) is an error term of order $o(Z^{7/3})$ and that it is uniformly in $\alpha$. In fact, this finishes the proof. □

Now, the previous lemma allows us to prove the following asymptotic result for the density of the momentum functional $\mathcal{E}_{\mathrm{mTF}}$:

**Theorem 5.2** (Neutral Case $N = Z$: Conta and Siedentop [27, Theorem 3])**.** *Let $\psi_N$ be an approximate ground state of $H_N$ and $\tau_N$ the minimizer of $\mathcal{E}_{\mathrm{mTF}}$ on $\mathcal{J}_N$. Assume $(1 + |\cdot|^{-2})\varphi \in L^\infty(\mathbb{R}^3)$ and $\varphi$ uniformly continuous. Then, for $\lambda = N/Z$ fixed,*

$$\lim_{N\to\infty} \int_{\mathbb{R}^3} \mathrm{d}\xi \, \varphi(\xi) \tilde{\tau}_{\psi_N}(\xi) = \int_{\mathbb{R}^3} \mathrm{d}\xi \, \varphi(\xi) \tau_\lambda(\xi). \tag{5.20}$$

*Proof.* First we remark that it suffices to proof the theorem for positive $\varphi$ since we can split $\varphi$ into the part where it is strictly positive and strictly negative and do the proof separately for those cases.

The proof of Lieb's asymptotic result on the atomic energy [10, Theorem 5.1] implies

$$\begin{aligned} \langle \psi_N, H_{N,0} \psi_N \rangle &\leq \mathcal{E}_{\mathrm{TF}}(\rho_N) + \mathrm{const}\, Z^{11/5} \\ &= \tfrac{q}{(2\pi)^3} \int_{h_{N,0}(\xi,x) < -\mu} \mathrm{d}\xi \mathrm{d}x \, h_{N,0}(\xi, x) + \mathrm{const}\, Z^{11/5}. \end{aligned}$$

Moreover, using Lieb's correlation inequality [9] and $D[\rho_{\psi_N} - \rho_N] \geq 0$ we obtain

$$\begin{aligned} &\langle \psi_N, \sum_{1 \leq i < j \leq N} \frac{1}{|x_i - x_j|} \psi_N \rangle \\ &\qquad \geq D(\rho_\psi, \rho_N) + D[\rho_N] - \mathrm{const} \int_{\mathbb{R}^3} \mathrm{d}x \, \rho_{\psi_N}(x)^{\frac{4}{3}}. \end{aligned}$$

By the Cauchy-Schwarz inequality and the Lieb-Thirring inequality for the kinetic energy [16, 17] we have that for $N = O(Z)$

$$\int_{\mathbb{R}^3} \mathrm{d}x\, \rho_{\psi_N}(x)^{\frac{4}{3}} \leq \Big(N \int_{\mathbb{R}^3} \mathrm{d}x\, \rho_{\psi_N}(x)^{\frac{5}{3}}\Big)^{\frac{1}{2}}$$
$$\leq \mathrm{const}\, N^{\frac{1}{2}} \Big(\langle \psi_N, -\sum_{n=1}^{N} \Delta_n \psi_N\rangle\Big)^{\frac{1}{2}} \leq \mathrm{const}\, Z^{5/3}$$

since the kinetic energy $\langle \psi_N, -\sum_{n=1}^{N} \Delta_n \psi_N\rangle$ performs as $O(Z^{7/3})$.

Later, we will consider the limit when $\alpha \to 0$. Thus, let $\alpha \in \mathbb{R}$ be small enough, e. g., $|\alpha| < \frac{1}{2}\|\frac{\varphi}{|\cdot|^2}\|_\infty$ (cf. proposition of Lemma 5.1). Then

$$\alpha Z^{7/3} \int_{\mathbb{R}^3} \mathrm{d}\xi\, \varphi(\xi)\tilde{\tau}_{\psi_N}(\xi) = \langle \psi_N, H_{N,0}\psi_N\rangle - \langle \psi_N, H_{N,\alpha}\psi_N\rangle \tag{5.21}$$

$$\leq \mathcal{E}_{\mathrm{TF}}(\rho_N) + \mathrm{const}\, Z^{11/5} - \Big(\langle \psi_N, \sum_{n=1}^{N} h_{N,\alpha,n}\, \psi_N\rangle - D[\rho_N] - \mathrm{const} \int_{\mathbb{R}^3} \mathrm{d}x\, \rho_{\psi_N}(x)^{\frac{4}{3}}\Big) \tag{5.22}$$

$$= \tfrac{q}{(2\pi)^3} \int_{h_{N,0}(\xi,x)<-\mu} \mathrm{d}\xi \mathrm{d}x\, h_{N,0}(\xi,x) - \mathrm{tr}\,(h_{N,\alpha}\gamma_{\psi_N}) + \mathrm{const}\, Z^{11/5} \tag{5.23}$$

$$\leq \tfrac{q}{(2\pi)^3} \int_{h_{N,0}(\xi,x)<-\mu} \mathrm{d}\xi \mathrm{d}x\, h_{N,0}(\xi,x) - \tfrac{q}{(2\pi)^3} \int_{h_{N,\alpha}(\xi,x)<-\mu} \mathrm{d}\xi \mathrm{d}x\, h_{N,\alpha}(\xi,x) + o(Z^{7/3}) \tag{5.24}$$

$$= \alpha Z^{7/3} \int_{\mathbb{R}^3} \mathrm{d}\xi\, \varphi(\xi)\tau_\lambda(\xi) - \tfrac{q}{(2\pi)^3} \int_{\substack{h_{N,\alpha}(\xi,x)<-\mu \\ h_{N,0}(\xi,x)>-\mu}} \mathrm{d}\xi \mathrm{d}x\, h_{N,\alpha}(\xi,x) \tag{5.25}$$

$$+ \tfrac{q}{(2\pi)^3} \int_{\substack{h_{N,\alpha}(\xi,x)>-\mu \\ h_{N,0}(\xi,x)<-\mu}} \mathrm{d}\xi \mathrm{d}x\, h_{N,\alpha}(\xi,x) + o(Z^{7/3}) \tag{5.26}$$

where we used (5.2) in the second inequality.

Since

$$-\tfrac{q}{(2\pi)^3}\int_{\substack{h_{N,\alpha}(\xi,x)<-\mu\\ h_{N,0}(\xi,x)>-\mu}} \mathrm{d}\xi\mathrm{d}x\, h_{N,0}(\xi,x) \le \mu\,\tfrac{q}{(2\pi)^3}\int_{\substack{h_{N,\alpha}(\xi,x)<-\mu\\ h_{N,0}(\xi,x)>-\mu}} \mathrm{d}\xi\mathrm{d}x$$

the bound on $\alpha$ allows to estimate the phase space volume in the shell as $O(Z)$ independent of $\alpha$ (cf. Eq. (5.3)). In line (5.26) we dismiss a negative term. For the remaining phase integral in the energy shell in line (5.25) recall Notation 6. Then scaling yields

$$\alpha\,\tfrac{q}{(2\pi)^3}\int_{\substack{h_{N,\alpha}(\xi,x)<-\mu\\ h_{N,0}(\xi,x)>-\mu}} \mathrm{d}\xi\mathrm{d}x\,\varphi_Z(\xi) = \alpha\, Z^{7/3}\tfrac{q}{(2\pi)^3}\int_{\substack{\tilde h_{\lambda,\alpha}(\xi,x)<-\tilde\mu\\ \tilde h_{\lambda,0}(\xi,x)>-\tilde\mu}} \mathrm{d}\xi\mathrm{d}x\,\varphi(\xi) \tag{5.27}$$

where $\tilde\mu := \mu(1,\lambda)$ is uniquely related to $\phi(1,\lambda,x)$ via the Thomas-Fermi equation and

$$\tilde h_{\lambda,\alpha}(\xi,x) := \xi^2 - \phi(1,\lambda,x) - \alpha\,\varphi(\xi) = \xi^2 - \frac{1}{|x|} + (\rho_\lambda * |\cdot|^{-1})(x) - \alpha\,\varphi(\xi).$$

The integral on the right hand side of Eq. (5.27) depending only on $\lambda$ and $\alpha$ is of order $o(\alpha)$. Indeed, $\varphi(\xi)\chi_{\{(\xi,x)\in\mathbb{R}^6|\frac{1}{2}\xi^2-\phi(1,\lambda,x)<-\mu(1,\lambda)\}}(\xi,x)$ is an integrable majorant independent of $\alpha$. Thus, we get the announced asymptotics in $\alpha$ via dominated convergence. We proceed equivalently with $\alpha\,\frac{q}{(2\pi)^3}\int_{\substack{h_{N,\alpha}(\xi,x)>-\mu\\ h_{N,0}(\xi,x)<-\mu}} \mathrm{d}\xi\mathrm{d}x\,\varphi_Z(\xi)$, the remaining phase integral in the energy shell in line (5.26).

Eventually, we arrive at

$$\begin{aligned}
&\alpha\, Z^{7/3}\int_{\mathbb{R}^3}\mathrm{d}\xi\,\varphi(\xi)\tilde\tau_{\psi_N}(\xi)\\
&\quad\le \alpha\, Z^{7/3}\int_{\mathbb{R}^3}\mathrm{d}\xi\,\varphi(\xi)\tau_\lambda(\xi)\\
&\qquad - \tfrac{q}{(2\pi)^3}\int_{\substack{h_{N,\alpha}(\xi,x)<-\mu\\ h_{N,0}(\xi,x)>-\mu}} \mathrm{d}\xi\mathrm{d}x\, h_{N,\alpha}(\xi,x)\\
&\qquad + \tfrac{q}{(2\pi)^3}\int_{\substack{h_{N,\alpha}(\xi,x)>-\mu\\ h_{N,0}(\xi,x)<-\mu}} \mathrm{d}\xi\mathrm{d}x\, h_{N,\alpha}(\xi,x) + o(Z^{7/3})\\
&\quad = \alpha\, Z^{7/3}\int_{\mathbb{R}^3}\mathrm{d}\xi\,\varphi(\xi)\tau_\lambda(\xi) + Z^{7/3}o(\alpha) + o(Z^{7/3}).
\end{aligned}$$

Now, dividing first by $Z^{7/3}$ and sending $N$ to $\infty$ yields

$$\alpha \limsup_{N\to\infty} \int_{\mathbb{R}^3} \mathrm{d}\xi\, \varphi(\xi)\tilde{\tau}_{\psi_N}(\xi) \leq \alpha \int_{\mathbb{R}^3} \mathrm{d}\xi\, \varphi(\xi)\tau_\lambda(\xi) + o(\alpha). \tag{5.28}$$

For $\alpha \geq 0$, dividing by $\alpha$ and choosing $\alpha \downarrow 0$ yields the desired upper bound. If we reverse the sign of $\alpha$ then taking $\alpha \uparrow 0$ yields the reverse inequality for the limes inferior. Hence

$$\begin{aligned}\limsup_{N\to\infty} \int_{\mathbb{R}^3} \mathrm{d}\xi\, \varphi(\xi)\tilde{\tau}_{\psi_N}(\xi) &\leq \int \mathrm{d}\xi\, \varphi(\xi)\tau_\lambda(\xi) \\ &\leq \liminf_{N\to\infty} \int_{\mathbb{R}^3} \mathrm{d}\xi\, \varphi(\xi)\tilde{\tau}_{\psi_N}(\xi).\end{aligned}$$

In fact, this shows the wanted result. □

# Appendix

# A. Existence and Uniqueness of the Minimizer: An Alternative Proof

In the following we shall give another proof of the existence of the minimizer of $\mathcal{E}_{\mathrm{mTF}}$ which is not based on the known results in Thomas-Fermi theory.

Instead of studying $\mathcal{E}_{\mathrm{mTF}}$ we first turn to $\mathcal{E}_s$ given by (2.1). Besides the strict convexity (Lemma 2.2) $\mathcal{E}_s$ offers the advantage that we may apply Banach-Alaoglu (Theorem B.3) to extract weakly converging sequences in $\mathcal{J}_N^s$. From there we want to infer the existence of the minimizer via weak lower semicontinuity of $\mathcal{E}_s$. This idea has also been used by Lieb and Simon [13].

Before we go into detail we want to say a word about notation: In this chapter we will write $L^p$ for $L^p(\mathbb{R}^3, \mathrm{d}\xi)$ for all $1 \leq p \leq \infty$ as commonly used in literature and $L^p_{wt}$ for $L^p(\mathbb{R}^3, \xi^2\mathrm{d}\xi)$, the weighted $L^p$-space.

Now, we start with:

**Lemma A.1.** *Let* $\tilde{\tau} \in \mathcal{J}^s$ *and let* $(\tilde{\tau}_n)_{n\in\mathbb{N}}$ *be a sequence in* $\mathcal{J}^s$. *If* $0 \leq r < \frac{3}{2}$ *and* $\|\tilde{\tau}_n - \tilde{\tau}\|_{L^{3/2}(\mathbb{R}^3,|\xi|^r\mathrm{d}\xi)} + \|\tilde{\tau}_n - \tilde{\tau}\|_{L^{3/2}_{wt}} \to 0$ *as* $n \to \infty$, *then*

$$\lim_{n\to\infty} \mathcal{E}_s(\tilde{\tau}_n) = \mathcal{E}_s(\tilde{\tau}). \tag{A.1}$$

*Moreover, each term of* $\mathcal{E}_s(\tilde{\tau}_n)$ *converges to the corresponding term of* $\mathcal{E}_s(\tilde{\tau})$ *and, if* $\|\tilde{\tau}_n - \tilde{\tau}\|_{L^{3/2}} + \|\tilde{\tau}_n - \tilde{\tau}\|_{L^{3/2}_{wt}} \to 0$ *as* $n \to \infty$, *then* (A.1) *implies that* $\mathcal{E}_s$ *is norm continuous on* $\mathcal{J}^s$ *in the* $L^{3/2} \cap L^{3/2}_{wt}$ *topology.*

*Proof.* The kinetic energy is obviously continuous. For the external potential the continuity in the $L^{3/2}(\mathbb{R}^3, |\xi|^r\mathrm{d}\xi) \cap L^{3/2}_{wt}$ topology follows immediately from

$$\|\tilde\tau_n-\tilde\tau\|_1 \le \Big(\int_{|\xi|\le 1} \mathrm{d}\xi\, \tfrac{1}{|\xi|^{2r}}\Big)^{\frac13}\Big(\int_{\mathbb{R}^3}\mathrm{d}\xi\,|\xi|^r|\tilde\tau_n(\xi)-\tilde\tau(\xi)|^{\frac32}\Big)^{\frac23} + \Big(\int_{|\xi|>1} \mathrm{d}\xi\, \tfrac{1}{|\xi|^{4}}\Big)^{\frac13}\Big(\int_{\mathbb{R}^3}\mathrm{d}\xi\,|\xi|^2|\tilde\tau_n(\xi)-\tilde\tau(\xi)|^{\frac32}\Big)^{\frac23} \quad \text{(A.2)}$$

for all $0\le r<\frac32$.

We are left to prove continuity of $\mathcal{R}^s_m$. Recalling the integral representation of the interaction term (Definition 2.4) we consider the following estimate:

$$\Big|\int_0^\infty \mathrm{d}r\Big[\Big(\int_{\mathbb{R}^3}\mathrm{d}\xi\,[\tilde\tau_n(\xi)-r^2]_+\Big)^2-\Big(\int_{\mathbb{R}^3}\mathrm{d}\xi\,[\tilde\tau(\xi)-r^2]_+\Big)^2\Big]\Big| \quad \text{(A.3)}$$

$$\le \int_0^\infty \mathrm{d}r\int_{\mathbb{R}^3}\mathrm{d}\xi\int_{\mathbb{R}^3}\mathrm{d}\eta\,\big|[\tilde\tau_n(\xi)-r^2]_+-[\tilde\tau(\xi)-r^2]_+\big| \quad \text{(A.4)}$$

$$\times\big([\tilde\tau_n(\eta)-r^2]_+ + [\tilde\tau(\eta)-r^2]_+\big) \quad \text{(A.5)}$$

$$\le \int_{\mathbb{R}^3}\mathrm{d}\xi\,|\tilde\tau_n(\xi)-\tilde\tau(\xi)|\int_0^\infty\mathrm{d}r\int_{\mathbb{R}^3}\mathrm{d}\eta\,\big([\tilde\tau_n(\eta)-r^2]_+ + [\tilde\tau(\eta)-r^2]_+\big) \quad \text{(A.6)}$$

where we used $|a_+-b_+|\le|a-b|$ for $a,b\in\mathbb{R}$ (Lemma B.1) in the second inequality.

Let $\tilde\tau_n,\tilde\tau\in\mathcal{J}^s$ with properties as required in the proposition. Then, applying (A.2) the first integral in (A.6) vanishes as $n\to\infty$. To see that $|\mathcal{R}^s_m(\tilde\tau_n)-\mathcal{R}^s_m(\tilde\tau)|\to 0$, which will finish the proof, it suffices to show that the remaining integral expression in (A.6) is bounded. In fact,

$$\int_0^\infty\mathrm{d}r\int_{\mathbb{R}^3}\mathrm{d}\eta\,\big([\tilde\tau_n(\eta)-r^2]_+ + [\tilde\tau(\eta)-r^2]_+\big) = \tfrac23\int_{\mathbb{R}^3}\mathrm{d}\eta\,(\tilde\tau_n(\eta)^{\frac32}+\tilde\tau(\eta)^{\frac32}) \quad \text{(A.7)}$$

where the right hand side is obviously bounded. □

With the lemma just proven and the convexity of $\mathcal{E}_s$ (Lemma 2.2) we can now prove the weak lower semicontinuity of $\mathcal{E}_s$ in $L^{3/2}_{wt}$.

**Theorem A.2.** *For each $N < \infty$, let $\tilde\tau \in L^{3/2}_{wt}$ and let $(\tilde\tau_n)_{n\in\mathbb{N}}$ be a sequence in $\mathcal{J}^s_N$. If $\tilde\tau_n \rightharpoonup \tilde\tau$ in $L^{3/2}_{wt}$, then $\tilde\tau \in \mathcal{J}^s_N$ and*

$$\mathcal{E}_s(\tilde\tau) \le \liminf_{n\to\infty} \mathcal{E}_s(\tilde\tau_n). \tag{A.8}$$

*Moreover, if $\mathcal{E}_s(\tilde\tau) = \lim_{n\to\infty}\mathcal{E}_s(\tilde\tau_n)$, then each term in $\mathcal{E}_s(\tilde\tau_n)$ converges to the corresponding term in $\mathcal{E}_s(\tilde\tau)$ and $\|\tilde\tau_n - \tilde\tau\|_{L^{3/2}_{wt}} \to 0$.*

*Proof.* We have $\tilde\tau_n \rightharpoonup \tilde\tau$ in $L^{3/2}_{wt}$ with $\tilde\tau \in L^{3/2}_{wt}$. Since $\tilde\tau_n \in \mathcal{J}^s_N$ for all $n \in \mathbb{N}$ the sequence $(\tilde\tau_n)_{n\in\mathbb{N}}$ is bounded in $L^{3/2}$. Thus, we may apply Banach-Alaoglu (Theorem B.3) to come to a subsequence weakly converging in $L^{3/2}\cap L^{3/2}_{wt}$ with $\tilde\tau \in L^{3/2}\cap L^{3/2}_{wt}$. Indeed, $\tilde\tau \in \mathcal{J}^s_N$. To prove this, note that $\tilde\tau \ge 0$, $\tilde\tau^{1/2} \in L^3$, and $\int_{\mathbb{R}^3}\mathrm{d}\xi\,\tilde\tau_n(\xi)^{3/2} \le N$. Then, the weak convergence of $(\tilde\tau_n)_{n\in\mathbb{N}}$ in $L^{3/2}$ and Hölder's inequality yield

$$\begin{aligned}\int_{\mathbb{R}^3}\mathrm{d}\xi\,\tilde\tau(\xi)^{\frac32} &= \lim_{n\to\infty}\int_{\mathbb{R}^3}\mathrm{d}\xi\,\tilde\tau(\xi)^{\frac12}\tilde\tau_n(\xi)\\ &\le \lim_{n\to\infty}\Big(\int_{\mathbb{R}^3}\mathrm{d}\xi\,\tilde\tau(\xi)^{\frac32}\Big)^{\frac13}\Big(\int_{\mathbb{R}^3}\mathrm{d}\xi\,\tilde\tau_n(\xi)^{\frac32}\Big)^{\frac23} \le \Big(\int_{\mathbb{R}^3}\mathrm{d}\xi\,\tilde\tau(\xi)^{\frac32}\Big)^{\frac13}N^{2/3}.\end{aligned} \tag{A.9}$$

This certainly implies $\int_{\mathbb{R}^3}\mathrm{d}\xi\,\tilde\tau(\xi)^{\frac32} \le N$.

From Lemma A.1 and Lemma 2.2 we deduce that $\mathcal{E}_s$ is $L^{3/2}\cap L^{3/2}_{wt}$-norm continuous and convex on $\mathcal{J}^s_N$. Hence, $\mathcal{E}_s$ is weakly lower semicontinuous on $\mathcal{J}^s_N$ by Lemma B.2, which gives (A.8).

In particular, each term of $\mathcal{E}_s$ is norm continuous and convex on $\mathcal{J}^s_N$, thus each term is weakly lower semicontinuous. This in turn implies that, if $\mathcal{E}_s(\tilde\tau) = \lim_{n\to\infty}\mathcal{E}_s(\tilde\tau_n)$, then each term converges. In particular, $\|\tilde\tau\|_{L^{3/2}_{wt}} = \lim_{n\to\infty}\|\tilde\tau_n\|_{L^{3/2}_{wt}}$. Furthermore, $L^{3/2}_{wt}$ is uniformly convex. Then by Theorem B.4 weak convergence and convergence of the norms imply strong convergence. □

*Remark.* Alternatively, one could deduce $\tilde\tau \in \mathcal{J}^s_N$ from the weak convergence in $L^{3/2}_{wt}$ as well. Suppose $\int \mathrm{d}\xi\,\tilde\tau^{3/2} > N$. Then there exists some $R > 0$ such that $\int_{|\xi|>R}\mathrm{d}\xi\,\tilde\tau^{3/2} > N$, otherwise we would have $N < \int \mathrm{d}\xi\, \tilde\tau(\xi)^{3/2} = \lim_{R\to 0} \int_{|\xi|>R} \mathrm{d}\xi\, \tilde\tau(\xi)^{3/2} \le N$. Further, since $\int_{|\xi|>R} \mathrm{d}\mu \frac{\tilde\tau^{3/2}}{|\xi|^6} \le \frac{1}{R^6} \int \mathrm{d}\mu\, \tilde\tau(\xi)^{3/2}$, where $\mathrm{d}\mu$ denotes the measure $\xi^2 \mathrm{d}\xi$, we have that $|\cdot|^{-2} \chi_{\{\xi\in\mathbb{R}^3 | |\xi|>R\}} \tilde\tau^{1/2} \in L^3_{wt}$. Now, the weak convergence of $(\tilde\tau_n)_{n\in\mathbb{N}}$ in $L^{3/2}_{wt}$ and Hölder's inequality yield

$$\begin{aligned}\int_{|\xi|>R} \mathrm{d}\xi\, \tilde\tau(\xi)^{\frac32} &= \lim_{n\to\infty} \int_{\mathbb{R}^3} \mathrm{d}\mu\, \chi_{\{\xi\in\mathbb{R}^3 | |\xi|>R\}}(\xi) \frac{\tilde\tau(\xi)^{1/2}}{|\xi|^{2/3}} \frac{\tilde\tau_n(\xi)}{|\xi|^{4/3}} \\ &\le \lim_{n\to\infty} \Big(\int_{|\xi|>R} \mathrm{d}\xi\, \tilde\tau(\xi)^{\frac32}\Big)^{\frac13} \Big(\int_{\mathbb{R}^3} \mathrm{d}\xi\, \tilde\tau_n(\xi)^{\frac32}\Big)^{\frac23} \\ &\le \Big(\int_{|\xi|>R} \mathrm{d}\xi\, \tilde\tau(\xi)^{\frac32}\Big)^{\frac13} N^{\frac23} \qquad \text{(A.10)}\end{aligned}$$

and the claim follows by contradiction.

To prove the existence of a minimizer for $\mathcal{E}_s$ by means of the weak lower semicontinuity result we need a preliminary lemma. The uniqueness of the minimizer is then already guaranteed by Corollary 2.3.

**Lemma A.3.** *$\mathcal{E}_s$ is bounded from below on $\mathcal{J}^s_N$. Moreover, $\mathcal{E}_s$ is coercive in $L^{3/2}_{wt}$ on $\mathcal{J}^s$.*

*Proof.* Assume $\tilde\tau \in \mathcal{J}^s$. Let $X := \|\tilde\tau\|_{L^{3/2}}$ and $Y := \|\tilde\tau\|_{L^{3/2}_{wt}}$. For the external potential we have

$$\begin{aligned}\|\tilde\tau\|_1 \le \Big(\int_{|\xi|\le 1} \mathrm{d}\xi\Big)^{\frac13} \Big(\int_{\mathbb{R}^3} \mathrm{d}\xi\, \tilde\tau(\xi)^{\frac32}\Big)^{\frac23} \\ + \Big(\int_{|\xi|>1} \mathrm{d}\xi\, \frac{1}{\xi^4}\Big)^{\frac13} \Big(\int_{\mathbb{R}^3} \mathrm{d}\xi\, \xi^2 \tilde\tau(\xi)^{\frac32}\Big)^{\frac23} < \infty. \qquad \text{(A.11)}\end{aligned}$$

This together with the positivity of the electron-electron interaction term gives

$$\mathcal{E}_s(\tilde\tau) \ge Y^{3/2} - \tfrac32 \gamma_{\mathrm{TF}}^{1/2} Z \,\mathrm{const}\, X - \tfrac32 \gamma_{\mathrm{TF}}^{-1/2} Z \,\mathrm{const}\, Y. \qquad \text{(A.12)}$$

Obviously, $\mathcal{E}_s$ is coercive in the weighted $L^{3/2}$-norm and $X \le N^{2/3}$ if $\tilde\tau \in \mathcal{J}^s_N$. We conclude that $\mathcal{E}_s$ is bounded from below by an $N$-dependent constant and coercive in $Y$. □

**Theorem A.4.** *For each $N < \infty$, $\mathcal{E}_s$ has a unique minimizer on $\mathcal{J}^s_N$. Furthermore,*

$$\inf\{\mathcal{E}_s(\tilde{\tau}) \mid \tilde{\tau} \in \mathcal{J}^s_{\partial N}\} = \inf\{\mathcal{E}_s(\tilde{\tau}) \mid \tilde{\tau} \in \mathcal{J}^s_N\}.$$

*Proof.* $\mathcal{E}_s$ is bounded from below and coercive on $\mathcal{J}^s_N$ in $L^{3/2}_{wt}$ by the previous lemma. Consequently, there exists a minimizing sequence $(\tilde{\tau}_n)_{n\in\mathbb{N}}$ in $\mathcal{J}^s_N$ which is bounded in $L^{3/2}_{wt}$, i. e.,

$$\lim_{n\to\infty} \mathcal{E}_s(\tilde{\tau}_n) = \inf\{\mathcal{E}_s(\tilde{\tau}) \mid \tilde{\tau} \in \mathcal{J}^s_N\}$$

such that $\sup_{n\in\mathbb{N}} \|\tilde{\tau}_n\|_{L^{3/2}_{wt}} < \infty$. Applying Banach-Alaoglu (Theorem B.3) we get to a weakly converging subsequence in $L^{3/2}_{wt}$ which we denote by $(\tilde{\tau}_n)_{n\in\mathbb{N}}$ as well. Thus, we have $\tilde{\tau}_n \rightharpoonup \tilde{\tau}$ in $L^{3/2}_{wt}$ for some $\tilde{\tau} \in L^{3/2}_{wt}$, $\tilde{\tau} \geq 0$. By the weak lower semicontinuity of $\mathcal{E}_s$ (Theorem A.2) we get

$$\mathcal{E}_s(\tilde{\tau}) \leq \lim_{n\to\infty} \mathcal{E}_s(\tilde{\tau}_n) = \inf\{\mathcal{E}_s(\tilde{\tau}) \mid \tilde{\tau} \in \mathcal{J}^s_N\}$$

which proves the existence of a minimizer.

The uniqueness follows directly from the strict convexity of $\mathcal{E}_s$ (Lemma 2.2) as proven in Corollary 2.3.

It remains to show $\inf\{\mathcal{E}_s(\tilde{\tau}) \mid \tilde{\tau} \in \mathcal{J}^s_{\partial N}\} = \inf\{\mathcal{E}_s(\tilde{\tau}) \mid \tilde{\tau} \in \mathcal{J}^s_N\}$. Of course,

$$\inf\{\mathcal{E}_s(\tilde{\tau}) \mid \tilde{\tau} \in \mathcal{J}^s_{\partial N}\} \geq \inf\{\mathcal{E}_s(\tilde{\tau}) \mid \tilde{\tau} \in \mathcal{J}^s_N\}.$$

To obtain the reverse inequality let $\tilde{\tau}$ be the minimizer of $\mathcal{E}_s$ on $\mathcal{J}^s_N$, i. e., $\mathcal{E}_s(\tilde{\tau}) = \inf\{\mathcal{E}_s(\tilde{\tau}) \mid \tau \in \mathcal{J}^s_N\}$. Assume $\int_{\mathbb{R}^3} \mathrm{d}\xi\, \tilde{\tau}(\xi)^{3/2} = M < N$. Suppose that there exists a sequence $(\tilde{\tau}_n)_{n\in\mathbb{N}}$ in $\mathcal{J}^s_{\partial N}$ which satisfies $\|\tilde{\tau}_n - \tilde{\tau}\|_{L^{3/2}(\mathbb{R}^3, |\xi|^r \mathrm{d}\xi)} \to 0$ as $n \to \infty$ for some $0 < r \leq 3/2$, then the strong continuity of $\mathcal{E}_s$ (Lemma A.1) implies

$$\inf\{\mathcal{E}_s(\tilde{\tau}) \mid \tilde{\tau} \in \mathcal{J}^s_{\partial N}\} \leq \lim_{n\to 0} \mathcal{E}_s(\tilde{\tau}_n) = \inf_{\tilde{\tau}\in\mathcal{J}_N} \mathcal{E}_s(\tilde{\tau})$$

since $\inf\{\mathcal{E}_s(\tilde{\tau}) \mid \tilde{\tau} \in \mathcal{J}^s_{\partial N}\} \leq \mathcal{E}_s(\tilde{\tau}_n)$ and $\lim_{n\to 0} \mathcal{E}_s(\tilde{\tau}_n) = \mathcal{E}_s(\tilde{\tau}) = \inf\{\mathcal{E}_s(\tilde{\tau}) \mid \tilde{\tau} \in \mathcal{J}^s_N\}$.

The construction of the required sequence $(\tilde{\tau}_n)_{n\in\mathbb{N}}$ will finish the proof. Pick any $\tilde{\sigma} \in \mathcal{J}^s$ such that $\int_{\mathbb{R}^3} \mathrm{d}\xi\, \tilde{\sigma}(\xi)^{3/2} = N - M$ and define

$\tilde{\tau}_n(\xi)^{3/2} := \tilde{\tau}(\xi)^{3/2} + n^3\tilde{\sigma}(n\xi)^{3/2}$. Clearly, $\int_{\mathbb{R}^3} \tilde{\tau}_n(\xi)^{3/2} = N$. Note that $\tilde{\tau}_n \geq \tilde{\tau}$ as $\tilde{\sigma} \geq 0$. Applying $(a+b)^{2/3} \leq a^{2/3} + b^{2/3}$ for positive $a, b$ (Lemma B.1) we get

$$\begin{aligned} \|\tilde{\tau}_n - \tilde{\tau}\|^{3/2}_{L^{3/2}(\mathbb{R}^3, |\xi|^r \mathrm{d}\xi)} &= \int_{\mathbb{R}^3} \mathrm{d}\xi\, |\xi|^r (\tilde{\tau}_n(\xi) - \tilde{\tau}(\xi))^{\frac{3}{2}} \\ &\leq \int_{\mathbb{R}^3} \mathrm{d}\xi\, |\xi|^r n^3 \tilde{\sigma}(n\xi)^{\frac{3}{2}} = \tfrac{1}{n^r} \int_{\mathbb{R}^3} \mathrm{d}\xi\, |\xi|^r \tilde{\sigma}(\xi)^{\frac{3}{2}} \quad \text{(A.13)} \end{aligned}$$

for every $0 < r \leq 2$. □

**Definition A.5.** $E_{\mathrm{mTF}}(N, Z) \equiv \inf\{\mathcal{E}_{\mathrm{mTF}}(\tau) \mid \tau \in \mathcal{J}_{\partial N}\}$

Now, we can prove the following statement related to $\mathcal{E}_{\mathrm{mTF}}$:

**Theorem A.6.** *For each $N < \infty$, $\mathcal{E}_{\mathrm{mTF}}$ has a unique minimizer on $\mathcal{J}_N$. Furthermore,*

$$E_{\mathrm{mTF}}(N, Z) = \inf\{\mathcal{E}_{\mathrm{mTF}}(\tau) \mid \tau \in \mathcal{J}_N\} = \inf\{\mathcal{E}_s(\tau) \mid \tau \in \mathcal{J}^s_N\}.$$

*Proof.* Let $\tilde{\tau} \in \mathcal{J}^s_N$ be the minimizer of $\mathcal{E}_s$. Then $0 \leq \tilde{\tau}^{3/2} = \tau$ is the unique minimizer of $\mathcal{E}_{\mathrm{mTF}}$ on $\mathcal{J}_N$ since $\inf_{\tau \in \mathcal{J}_N} \mathcal{E}_{\mathrm{mTF}}(\tau) = \inf_{\tau \in \mathcal{J}^s_N} \mathcal{E}_s(\tau)$ (Eq. (2.2)). Likewise, $E_{\mathrm{mTF}}(N, Z) = \inf\{\mathcal{E}_s(\tilde{\tau}) \mid \tilde{\tau} \in \mathcal{J}^s_{\partial N}\}$ which completes the proof using Theorem A.4. □

**Corollary A.7.** *$E_{\mathrm{mTF}}(N, Z)$ is monotone nonincreasing in $N$.*

*Remark.* Actually, this follows immediately from Theorem A.6. But in the following proof we want to show that one can always add any unwanted piece of $\tau$ at the origin without increasing the energy.

*Proof of Corollary A.7.* Let $(\delta_n)_{n \in \mathbb{N}}$ be a Dirac sequence such that $\delta_n(\xi) := n^3\delta(n\xi)$ and $\delta_n \in \mathcal{J}$. Take, for example, $\delta(\xi) = \frac{3}{4\pi}$ if $0 \leq |\xi| \leq 1$ and $\delta(\xi) = 0$ otherwise.

We shall prove that

$$\mathcal{E}_{\mathrm{mTF}}(\tau + \delta_n) - \mathcal{E}_{\mathrm{mTF}}(\tau) < \mathrm{const}\, \tfrac{1}{n}. \quad \text{(A.14)}$$

In fact, this shows that if $N$ increases, we may add $\delta_n$ arbitrarily close to the origin by taking the limit $n \to \infty$. So, in order to prove (A.14), first note that

$$\mathcal{K}_m(\tau + \delta_n) = \mathcal{K}_m(\tau) + \tfrac{1}{n^2}\mathcal{K}_m(\delta). \quad \text{(A.15)}$$

Due to $(a+b)^{2/3} \leq a^{2/3} + b^{2/3}$ for positive $a, b$ (Lemma B.1) we get the following estimate for the attraction term:

$$\Big| \int_{\mathbb{R}^3} \mathrm{d}\xi \, (\tau(\xi) + \delta_n(\xi))^{\frac{2}{3}} - \tau(\xi)^{\frac{2}{3}} \Big| \leq \int_{\mathbb{R}^3} \mathrm{d}\xi \, \delta_n(\xi)^{\frac{2}{3}} = \tfrac{1}{n} \int_{\mathbb{R}^3} \mathrm{d}\xi \, \delta(\xi)^{\frac{2}{3}}. \tag{A.16}$$

Finally, the estimate for the electron-electron interaction of $\mathcal{E}_{\mathrm{mTF}}$, recalling $\mathcal{R}^s_m(\tilde{\tau}) = \mathrm{const} \int_0^\infty \mathrm{d}r \left( \int_{\mathbb{R}^3} \mathrm{d}\xi \, [\tilde{\tau}(\xi) - r^2]_+ \right)^2$ (Definition 2.4), reads:

$$\Big| \int_0^\infty \mathrm{d}r \Big[ \Big( \int_{\mathbb{R}^3} \mathrm{d}\xi \, [(\tau(\xi) + \delta_n(\xi))^{\frac{2}{3}} - r^2]_+ \Big)^2 \tag{A.17}$$

$$- \Big( \int_{\mathbb{R}^3} \mathrm{d}\xi \, [\tau(\xi)^{\frac{2}{3}} - r^2]_+ \Big)^2 \Big] \Big| \tag{A.18}$$

$$\leq \int_{\mathbb{R}^3} \mathrm{d}\xi \big( (\tau(\xi) + \delta_n(\xi))^{\frac{2}{3}} - \tau(\xi)^{\frac{2}{3}} \big) \tag{A.19}$$

$$\times \int_0^\infty \mathrm{d}r \int_{\mathbb{R}^3} \mathrm{d}\eta \, \big( [(\tau(\eta) + \delta_n(\eta))^{\frac{2}{3}} - r^2]_+ + [\tau(\eta)^{\frac{2}{3}} - r^2]_+ \big) \tag{A.20}$$

$$\leq \int_{\mathbb{R}^3} \mathrm{d}\xi \, \delta_n(\xi)^{\frac{2}{3}} \Big[ \tfrac{2}{3} \int_{\mathbb{R}^3} \mathrm{d}\eta \, (\tau(\eta) + \delta_n(\eta)) + \tfrac{2}{3} \int_{\mathbb{R}^3} \mathrm{d}\eta \, \tau(\eta) \Big] \tag{A.21}$$

$$= \tfrac{1}{n} \int_{\mathbb{R}^3} \mathrm{d}\xi \, \delta(\xi)^{\frac{2}{3}} \tfrac{2}{3} \int_{\mathbb{R}^3} \mathrm{d}\eta \, (2\tau(\eta) + \delta(\eta)) \, . \tag{A.22}$$

We get the first inequality equivalently to the inequalities (A.3) – (A.6) in the proof of Lemma A.1. Next, we apply $(a+b)^{2/3} \leq a^{2/3} + b^{2/3}$ for $a, b \geq 0$ (Lemma B.1) to the integral in (A.19) and evaluate the integration with respect to $r$. Eventually, this proves (A.14). □

# B. Supplemental Material

This chapter gathers two simple inequalities and well-known results in functional analysis which we refer to in this thesis. For details see, e. g., Brezis [1] if not stated otherwise.

**Lemma B.1.** *Let $a, b \in \mathbb{R}$. Then*

1. $|a_+ - b_+| \leq |a - b|$.
2. $|a + b|^{2/3} \leq |a|^{2/3} + |b|^{2/3}$.

*Proof.* The first claim follows for example by observing the different cases for $a$ and $b$, respectively. For the second claim, notice that any concave function $f : [0, \infty) \to [0, \infty)$ with $f(0) = 0$ is subadditive. Hence, we have $|a + b|^{2/3} \leq (|a| + |b|)^{2/3} \leq |a|^{2/3} + |b|^{2/3}$. □

**Lemma B.2.** *Let $X$ be a Banach space. Assume the map $F : X \to \mathbb{R}$ to be convex and norm continuous on $X$. Then $F$ is weakly lower semicontinuous on $X$.*

**Theorem B.3** (Banach-Alaoglu)**.** *Let $X$ be a Banach space and let $X^*$ denote its dual space. Then $B^* := \{\phi \in X^* \mid \|\phi\|_{X^*} \leq 1\}$ is compact in the weak-$*$-topology. If $X$ is reflexive, then every bounded sequence has a weakly convergent subsequence.*

**Theorem B.4.** *Let $X$ be a uniformly convex Banach space. Let $\tau_n, \tau \in L^p$ for $n \in \mathbb{N}$ such that $\tau_n \to \tau$ in the weak $L^p$ topology and $\limsup_n \|\tau_n\|_p \leq \|\tau\|_p$. Then $\tau_n \to \tau$ in the strong $L^p$ topology.*

**Theorem B.5** (Newton's Theorem [11, 18])**.** *Assume $x \in \mathbb{R}^3 \setminus \{0\}$ and $R \geq 0$. Then*

$$\int_{|y| \leq R} \mathrm{d}y \, \frac{1}{|x - y|} \leq \frac{1}{|x|} \int_{|y| \leq R} \mathrm{d}y.$$

*Equality holds if $|x| \geq R$.*

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## Eidesstattliche Versicherung

(Siehe Promotionsordnung vom 12.07.2011, §8, Abs. 2 Pkt. 5)

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

Verena von Conta

München, den 19.11.2014

Unterschrift Doktorand