**C**ommunications in **M**athematical **A**nalysis
*Special Volume in Honor of Prof. Peter Lax*
Volume 8, Number 2, pp. 92–102 (2010)
www.commun-math-anal.org
ISSN 1938-9787

# A Convex Minorant Problem Arising in Electron Density Theory

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Dedicated in great admiration to Peter Lax

(Communicated by Toka Diagana)

**Abstract**

We find the largest convex minorant of the function

$$F(x,y) = ax^2 + xy + by^2$$

where $a, b$ are positive constants and $x \geq 0,\ y \geq 0$. We explain how the problem is closely connected with finding the ground state Thomas-Fermi electron density for a spin polarized quantum mechanical system with the Fermi-Amaldi correction.

**AMS Subject Classification:** Primary: 52A41, 26B25; Secondary: 81Q99, 81V55, 92E10

**Keywords**: Convex minorant, Thomas-Fermi theory, Fermi-Amaldi correction, ground state electron density.

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# 1 THOMAS-FERMI THEORY

The Hamiltonian for an N electron system is

$$\begin{aligned} H &= T + V_{ee} + V_{ne} \\ &= -\frac{1}{2}\triangle + \frac{1}{2}\sum_{\substack{i,j=1 \\ i\neq j}}^{N} \frac{1}{|x_i - x_j|} + \sum_{j=1}^{N} V(x_j). \end{aligned} \tag{1.1}$$

The underlying Hilbert space is

$$\begin{aligned} \boldsymbol{\mathcal{H}} &= L^2_a\left(\mathbb{R}^{3N}\right) = \{u \in L^2(\mathbb{R}^{3N}, \mathbb{C}) : \\ u(x_{\pi_1}, ..., x_{\pi_N}) &= (sign\ \pi)\, u(x_1, ..., x_N) \text{ for all} \\ x &= (x_1, ..., x_N) \in \mathbb{R}^{3N} \text{ and all permutations } \pi \text{ of } \{1, ..., N\}. \end{aligned}$$

Here $x = (x_1, ..., x_N)$ with $x_j \in \mathbb{R}^3$ representing the position of the $j$th electron, sign $\pi$ is 1 or $-1$, according as the permutation $\pi$ is even or odd, and the antisymmetry is a mathematical expression of the Pauli exclusion principle for electrons. The kinetic energy operator is

$$T = -\frac{1}{2}\triangle = -\frac{1}{2}\sum_{i=1}^{N} \triangle_i \tag{1.2}$$

with $\triangle_i$ the Laplacian on $\mathbb{R}^3$ corresponding to the $i$th electron. The electron-electron (repulsive) potential energy operator is

$$V_{ee} = \frac{1}{2}\sum_{\substack{i,j=1 \\ i\neq j}}^{N} \frac{1}{|x_i - x_j|} \tag{1.3}$$

(Throughout this discussion, various constants have been normalized to be one.) The electron-nuclear (attractive) potential energy operator is

$$V_{ne} = \sum_{j=1}^{N} V(x_j) \tag{1.4}$$

where $V : \mathbb{R}^3 \to \mathbb{R}$ is a given potential. For a molecule with $M$ nuclei at fixed position $R_j,\ 1 \leq j \leq M,\ V$ is given by

$$V(y) = -\sum_{j=1}^{M} \frac{Z_j}{|y - R_j|}; \tag{1.5}$$

here $Z_j$ is the positive charge of the nucleus at $R_j$. But, for us, $V$ is allowed to vary in a large class of functions.

A basic problem in quantum chemistry is to find the ground state. That is, one wishes to find $E_{GS} \in \mathbb{R},\ \Psi_{GS} \in \boldsymbol{\mathcal{H}}$ such that $\|\Psi_{GS}\| = 1$ and $H\Psi_{GS} = E_{GS}\Psi_{GS}$ where

$$E_{GS} = \inf\{\langle H\varphi, \varphi\rangle : \varphi \in \boldsymbol{\mathcal{D}}(\boldsymbol{\mathcal{H}}),\ \ \|\varphi\| = 1\}.$$

For problems of bulk matter, with $N \simeq 10^{26}$ or so, this problem is extraordinarily difficult, both theoretically and numerically.

In 1927, L. Thomas [17] and E. Fermi [6] independently had the idea to replace this problem by one for the ground state density. If $\varphi$ is a wave function, i.e. a unit vector in $\boldsymbol{\mathcal{H}}$, then

$$\rho(x_1) = N \int\limits_{\mathbb{R}^{3(N-1)}} |\varphi(x_1, ..., x_N)|^2 \, dx_2 ... dx_N$$

is the corresponding position density. That is, $\int\limits_{\wedge} \rho(x_1)\, dx_1$ is the expected number of electrons in the Borel set $\wedge \in \mathbb{R}^3$ when $\varphi$ describes the state of the system.

Thomas and Fermi proposed to write the energy $\langle H\varphi, \varphi\rangle$ in the state $\varphi$ as a functional of $\rho$, $E(\rho)$, and to solve the minimization problem

$$E(\rho_{GS}) = \inf\{E(\rho) : \rho \geq 0, \int\limits_{\mathbb{R}^3} \rho(x)\, dx = N, \text{ and } \rho \in \boldsymbol{\mathcal{D}}(E)\}$$

for $\rho_{GS} \in \boldsymbol{\mathcal{D}}(E)$ with $\rho_{GS} \geq 0$, $\int\limits_{\mathbb{R}^3} \rho_{GS}(x)\, dx = N$. The problem with this approach is that the map $\varphi \to \rho$ is not injective. They proposed using an approximation

$$\widehat{E}(\rho) = \widehat{T}(\rho) + \widehat{V}_{ee}(\rho) + \widehat{V}_{ne}(\rho),$$

corresponding to

$$\langle H\varphi, \varphi\rangle = \langle T\varphi, \varphi\rangle + \langle V_{ee}\varphi, \varphi\rangle + \langle V_{ne}\varphi, \varphi\rangle$$

(see (1.1)-(1.4)). Specifically, they took

$$\widehat{E}(\rho) = \int\limits_{\mathbb{R}^3} c_o \rho(x)^{5/3}\, dx + \frac{c}{2} \int\limits_{\mathbb{R}^3}\int\limits_{\mathbb{R}^3} \frac{\rho(x)\,\rho(y)}{|x-y|} dxdy + \int\limits_{\mathbb{R}^3} V(x)\,\rho(x)\, dx. \tag{1.6}$$

The third term $\widehat{V}_{ne}(\rho) = \int\limits_{\mathbb{R}^3} V(x)\,\rho(x)\, dx$ equals $\langle V_{ne}\varphi, \varphi\rangle$. The second term, $\frac{c}{2}\int\limits_{\mathbb{R}^3}\int\limits_{\mathbb{R}^3} \frac{\rho(x)\rho(y)}{|x-y|} dxdy$, with $c = 1$, is the classical Coulomb electronic repulsion energy. It is a good approximation of $\langle V_{ne}\varphi, \varphi\rangle$, but it is not exact. For instance, when $N = 1$, we have $\langle V_{ee}\varphi, \varphi\rangle = 0$ since there is no electron electron repulsion with only one electron, while $\widehat{V}_{ee}(\rho) > 0$ for every $\rho$. The Fermi-Amaldi correction is to take $c = 1 - \frac{1}{N}$; this makes $\widehat{V}_{ee}(\rho) = 0$ when $N = 1$, but leaves $\widehat{V}_{ee}(\rho)$ relatively unchanged for large $N$.

The term $\widehat{T}(\rho) = c_o \int\limits_{\mathbb{R}^3} \rho(x)^{5/3}\, dx$ is the Thomas-Fermi kinetic energy, and the exponent 5/3 comes from scaling. More precisely, let $\varphi$ be a wave function, let

$\lambda > 0$, and let $\Psi_\lambda(x) = \lambda^{3N/2}\Psi(\lambda x)$ for $x \in \mathbb{R}^{3N}$. Then $U_\lambda \varphi = \varphi_\lambda$ defines a unitary mapping on $\boldsymbol{\mathcal{H}}$. Since $U_\lambda^{-1} = U_{1/\lambda}$, we easily see that

$$U_\lambda^{-1}(-\triangle)U_\lambda = \lambda^2(-\triangle),$$

so that "kinetic energy scales like $\lambda^2$". Suppose we consider an approximation for kinetic energy at the density level to be of the form $c_p \int\limits_{\mathbb{R}^3} \rho(x)^p\, dx$. The corresponding scaled electron density for the $N$ electron system is

$$\rho_\lambda(x) = \lambda^3 \rho(\lambda x)$$

for $\lambda > 0$ and $x \in \mathbb{R}^3$. An elementary calculation shows that

$$c_p \int\limits_{\mathbb{R}^3} \rho_\lambda(x)^p\, dx = \lambda^{3(p-1)} c_p \int\limits_{\mathbb{R}^3} \rho(y)\, dy.$$

Thus kinetic energy scales like $\lambda^{3(p-1)}$, which is $\lambda^2$ precisely when $p = 5/3$.

E. Lieb and B. Simon [13], [14] showed that for molecules and $c = 1$, the Thomas-Fermi problem

$$\{\text{minimize } \widehat{E}(\rho) \text{ (defined by (1.6), subject to } \rho \geq 0,\ \int\limits_{\mathbb{R}^3} \rho(x)\, dx = N,\ \rho \in \boldsymbol{\mathcal{D}}\left(\widehat{E}\right)\}$$

has a unique solution provided

$$0 < N \leq Z = \sum_{i=1}^{N} Z_i$$

(see (1.5)), and there is no solution for $N > Z$. Ph. Benilan and H. Brezis [1], [4], [5] extended this in many ways, replacing the kinetic energy density $\rho(x)^{5/3}$ by $J(\rho(x))$ for a large class of convex functions $J$, replacing $V$ defined by (1.5) by a very general class of potentials $V$, and in other ways as well. G. Goldstein (formerly G. Rieder) and J. Goldstein [16], [11] extended the $N_{\max} = Z$ result of Lieb-Simon to $N_{\max} = Z + 1$ when $c = 1 - \frac{1}{N}$.

Goldstein and Goldstein [10] extended the theory to spin polarized systems. Then Benilan, Goldstein and Goldstein [2], [3] studied the case of spin polarized Thomas-Fermi theory with the Fermi-Amaldi correction. Consider the energy functional

$$\boldsymbol{\mathcal{E}}(\rho_1, \rho_2) = \sum_{j=1}^{2} c_j \int\limits_{\mathbb{R}^3} \rho_j(x)^p + \int\limits_{\mathbb{R}^3} V(x)(\rho_1(x) + \rho_2(x))dx$$
$$+\frac{1}{2}\sum_{j=1}^{2}\left(1 - \frac{1}{N_j}\right)\int\limits_{\mathbb{R}^3}\int\limits_{\mathbb{R}^3} \frac{\rho_j(x)\,\rho_j(y)}{|x-y|}dxdy + \int\limits_{\mathbb{R}^3}\int\limits_{\mathbb{R}^3} \frac{\rho_1(x)\,\rho_2(y)}{|x-y|}dxdy \tag{1.7}$$

with domain

$$\boldsymbol{\mathcal{D}}(\boldsymbol{\mathcal{E}}) = \{(\rho_1, \rho_2) : \rho_i \geq 0,\ \int\limits_{\mathbb{R}^3} \rho_i(x)\, dx = N_i,\ \text{each integral in (1.7) is finite}\},$$

where $N_i > 1$ is given, $i = 1, 2$. Here $\rho_1$ [resp. $\rho_2$] is the position density of the spin up [resp. spin down] electrons. Let $V$ be given by (1.5). Then ( see [2], [12], [8]) the problem

$$\{\text{minimize } \boldsymbol{\mathcal{E}}(\rho_1, \rho_2) \text{ subject to } (\rho_1, \rho_2) \in \boldsymbol{\mathcal{D}}(\boldsymbol{\mathcal{E}})\}$$

has a solution for $p > 3/2$ and $N_1 + N_2 \leq Z + 1$. But uniqueness was not established.

In the previous problem discussed, the energy functional was strictly convex, but for the spin polarized case with the Fermi-Amaldi correction, the energy functional $\boldsymbol{\mathcal{E}}$ given by (1.7) (and $\boldsymbol{\mathcal{E}}_2$ also) is not convex. In the previous work, uniqueness followed from strict convexity.

Let $\widetilde{\boldsymbol{\mathcal{E}}}$ be the largest convex minorant of $\boldsymbol{\mathcal{E}}$, where $\boldsymbol{\mathcal{E}}$ is defined by (1.7). Then it is easy to see that $\widetilde{\boldsymbol{\mathcal{E}}}$ exists, $\min \boldsymbol{\mathcal{E}} = \min \widetilde{\boldsymbol{\mathcal{E}}}$, and $\widetilde{\boldsymbol{\mathcal{E}}}$ is convex. If one can show that $\widetilde{\boldsymbol{\mathcal{E}}}$ is strictly convex, then it follows that $\boldsymbol{\mathcal{E}}$ has a unique minimum (since each minimum for $\boldsymbol{\mathcal{E}}$ is also minimum of $\widetilde{\boldsymbol{\mathcal{E}}}$).

## 2 The 2-D Problem in the Calculus of Variations

Let $J : \boldsymbol{\mathcal{D}}(J) \subset X \to \mathbb{R}$ be a real functional defined on a convex subset of a Banach space $X$. Let $J_*$ be the *largest convex minorant* of $J$, i.e., $J_* = \boldsymbol{\mathcal{D}}(J) \to \mathbb{R}$, $J_*$ is convex on $\boldsymbol{\mathcal{D}}(J_*) = \boldsymbol{\mathcal{D}}(J)$, $J_*(u) \leq J(u)$ for all $u \in D(J)$; and if $K = \boldsymbol{\mathcal{D}}(J) \to \mathbb{R}$ satisfies all these conditions, then $K(u) \leq J_*(u)$ for all $u \in \boldsymbol{\mathcal{D}}(J)$.

We wish to find the largest convex minorant of the spin polarized Thomas-Fermi energy functional $\boldsymbol{\mathcal{E}}$ given by (1.7).

Write

$$\boldsymbol{\mathcal{E}} = \boldsymbol{\mathcal{E}}_1 + \boldsymbol{\mathcal{E}}_2$$

where

$$\boldsymbol{\mathcal{E}}_2 = \boldsymbol{\mathcal{E}}_{ee} = \sum_{i=1}^{2} \left(1 - \frac{1}{N_i}\right) \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{\rho_i(x)\,\rho_i(y)}{|x-y|} dxdy + \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{\rho_1(x)\,\rho_2(y)}{|x-y|} dxdy \quad (2.1)$$

and $\boldsymbol{\mathcal{E}}_1 = \boldsymbol{\mathcal{E}} - \boldsymbol{\mathcal{E}}_2$. Then $\boldsymbol{\mathcal{E}}_1$ is strictly convex but $\boldsymbol{\mathcal{E}}$ is not convex; in fact, $\boldsymbol{\mathcal{E}}$ (and $\boldsymbol{\mathcal{E}}_2$ also) is strictly concave on some subset of its domain when $N_1 \neq N_2$ which we assume (see [3]). Finding the greatest convex minorant of $\boldsymbol{\mathcal{E}}$ seems to be an extremely difficult problem, so we replaced it by an easier problem: Find the largest convex minorant of $\boldsymbol{\mathcal{E}}_2^*$ of $\boldsymbol{\mathcal{E}}_2$.

Solving this problem yields a convex minorant $\boldsymbol{\mathcal{E}}_1 + \boldsymbol{\mathcal{E}}_2^*$ for $\boldsymbol{\mathcal{E}}$. But this may not be the greatest convex minorant of $\boldsymbol{\mathcal{E}}$. Here is a simple one dimensional example to illustrate this. Let

$$J_1(x) = |x| - 1, \ x \in \mathbb{R},$$

$$J_2(x) = \begin{cases} 1 - |x| & \text{for } |x| \leq 1 \\ 0 & \text{for } |x| \geq 1 \end{cases}.$$

Thus $J_1$ is convex on $\mathbb{R}$ but $J_2$ is not. A straightforward calculation shows that the greatest convex minorant of $J_2$ is $J_2^* \equiv 0$. But $J_1 + J_2$ is convex, whence the convex minorant $J_1 + J_2^* = J_1$ is not the greatest convex minorant of $J_1 + J_2$.

A standard way to find the greatest convex minorant of a functional $B$ is to find its second Legendre dual $B^{**}$. For functions of two variables, this requires $B$ being defined on all of $\mathbb{R}^2$, rather than just the first quadrant. The Legendre dual $B^*$ of $B$ is defined to be

$$B^*(y) = \sup_{x\in\mathbb{R}^2} \{\langle x, y\rangle - B(x)\} \in [-\infty, \infty],$$

where $\langle ., .\rangle$ is the given inner product on $\mathbb{R}^2$.

We consider

$$B(x) = ax_1^2 + 2x_1x_2 + bx_2^2, \tag{2.2}$$
$$A(x) = ax_1^2 + 2|x_1x_2| + bx_2^2 \tag{2.3}$$

for $x = (x_1, x_2) \in \mathbb{R}^2,\ 0 < a, b < 1$. We have in mind $a = 1 - \frac{1}{N_1},\ b = 1 - \frac{1}{N_2}$ from the Thomas-Fermi analogue.

**Lemma 2.1.** *Define $B$, $A$ by (2.2), (2.3) where $0 < a, b < 1$.*

(i) *$B$ is not convex on $\mathbb{R}^2$.*

(ii) *$A$ is not convex on $\mathbb{R}^2$.*

(iii) *$B^*(y) = \infty$ for all $y \in \mathbb{R}^2$.*

*Proof.* Recall that $f : \mathbb{R}^2 \to \mathbb{R}$ is convex then for any two points P and Q in the plane, $f(M) \le (f(P) + f(Q))/2$, where $M = (P + Q)/2$ is the midpoint of the segment joining $P$ and $Q$.

$(i)$ Let $P = (1, 0)$ and $Q = (0, 1)$. Then $B(P) = a_1$ and $B(Q) = a_2$. Because $a_1 + a_2 < 2$, we have

$$B(M) = B\left(\frac{1}{2}, \frac{1}{2}\right) = \frac{a_1 + a_2}{4} + \frac{1}{2} > \frac{a_1 + a_2}{2} = \frac{B(P) + B(Q)}{2}.$$

It follows that $B$ is not convex.

$(ii)$ Because $A(x)$ and $B(x)$ agree on the first quadrant, the example given in (i) shows that $A$ is not convex.

$(iii)$ Let $x = (t, -t)$. Then $2 - a_1 - a_2 > 0$ implies that

$$\{\langle x, y\rangle - B(x)\} = t(y_1 - y_2) + (2 - a_1 - a_2)t^2 \to \infty \text{ as } t \to \infty.$$

Hence

$$B^*(y) := \sup_{x\in\mathbb{R}^2} \{\langle x, y\rangle - B(x)\} = \infty.$$

□

If we replace $B(x)$ by

$$B_1(x) = \max\{B(x),\ T\}$$

for some fixed $T \in \mathbb{R}$, then conclusions $(i)$, $(iii)$ hold for $B_1$ as well.

**Lemma 2.2.** *Let be $A$ be given by* (2.3)*. Then*

$$A^*(y) = \sup_{x\in\mathbb{R}^2}\{< x, y > -A(x)\} \in [0,\infty)$$

*for each* $y \in \mathbb{R}^2$.

*Proof.* First

$$A^*(y) \geq \{< 0, y > -A(0)\} = 0 \text{ for } y \in \mathbb{R}^2$$

Next, let

$$\begin{aligned} G_y(x) &:= < x, y > -A(x), \\ &= < x, y > -a_1x_1^2 - a_2x_2^2 - 2\left|x_1x_2\right|, \end{aligned}$$

$$G_y(x) \leq H_y(x) := < x, y > -a_1x_1^2 - a_2x_2^2. \tag{2.4}$$

The critical point $x$ for $H_y(x)$ is determined by

$$\frac{\partial H_y(x)}{\partial x_1} = 0 = y_1 - 2a_1x_1 \text{ , which implies that } x_1 = \frac{y_1}{2a_1},$$

$$\frac{\partial H_y(x)}{\partial x_2} = 0 = y_2 - 2a_2x_2 \text{ , which implies that } x_2 = \frac{y_2}{2a_2}.$$

This critical point is where $H_y(x)$ has its maximum. Plugging this critical point in (2.4), we get

$$\sup_z G_y(z) \leq \sup_z H_y(z) = H_y(x)$$

$$= < \left(\frac{y_1}{2a_1}, \frac{y_2}{2a_2}\right), (y_1, y_2) > -a_1\left(\frac{y_1}{2a_1}\right)^2 - a_2\left(\frac{y_2}{2a_2}\right)^2 < \infty.$$

□

**Theorem 2.3.** *Let* $A : \mathbb{R}^2 \to \mathbb{R}$ *be given by*

$$A(x) = a_1x_1^2 + a_2x_2^2 + 2\left|x_1x_2\right|,$$

*where* $0 < a_1, a_2 < 1$*. Then* $A^{**}$ *is convex and is given by*

$$A^{**}(x) = a_1x_1^2 + a_2x_2^2 + \sqrt{4a_1a_2}\left|x_1x_2\right|.$$

*Moreover,* $A^{**}(x)$ *is the largest convex minorant of* $A$*.*

*Proof.* Let $\mathrm{A}^*(y) := \sup_{x\in\mathbb{R}^2}\{< x, y > -A(x)\}$. To prove Theorem 1, we need two lemmas.

**Lemma 2.4.** $A^*(y) \geq \max\left\{\frac{y_1^2}{4a_1}, \frac{y_2^2}{4a_2}\right\}$ *for all* $y \in \mathbb{R}^2$.

*Proof.* First,

$$\begin{aligned} A^*(y) &\geq \sup_{x_1 \in \mathbb{R}} \left( \langle x, y \rangle - A(x) \right) \text{ for } x = (x_1, 0) \\ &= \sup_{x_1 \in \mathbb{R}} \left( x_1 y_1 - a_1 x_1^2 \right) =: Q. \end{aligned}$$

The critical point of $x_1 \to x_1 y_1 - a_1 x_1^2$ is $x_1 = \frac{y_1}{2a_1}$. At this critical point, the global maximum is attained. So

$$Q = \left( \frac{y_1}{2a_1} \right) y_1 - a_1 \left( \frac{y_1}{2a_1} \right)^2 = \frac{y_1^2}{4a_1}.$$

Similarly,

$$\begin{aligned} A^*(y) &\geq \sup_{x_1 \in \mathbb{R}} \left( \langle x, y \rangle - A(x) \right) \text{ for } x = (0, x_2) \\ &= \frac{y_2^2}{4a_2} \end{aligned}$$

by the same calculation. So

$$A^*(y) \geq \max \left\{ \frac{y_1^2}{4a_1}, \frac{y_2^2}{4a_2} \right\}.$$

□

**Lemma 2.5.** *If $A_1 \geq A_2$ on $\mathbb{R}^2$, then $A_1^* \leq A_2^*$ on $\mathbb{R}^2$.*

*Proof.* Obvious.

□

Let

$$A_1(y) = A^*(y), \ A_2(y) = \max\{ \frac{y_1^2}{4a_1}, \frac{y_2^2}{4a_2} \}.$$

By the previous Lemma, for all $z \in \mathbb{R}^2$,

$$A^{**}(z) = A_1^*(z) \leq A_2^*(z). \tag{2.5}$$

Now we compute $A_2^*(z)$. For $z \in \mathbb{R}^2$,

$$A_2^*(z) = \max_{i=1,2,3} \sup_{y \in R_i} \left( \langle z, y \rangle - A_2(y) \right),$$

where

$$\begin{aligned} R_1 &= \left\{ y \in \mathbb{R}^2 : \frac{y_1^2}{4a_1} < \frac{y_2^2}{4a_2} \right\}, \\ R_2 &= \left\{ y \in \mathbb{R}^2 : \frac{y_1^2}{4a_1} > \frac{y_2^2}{4a_2} \right\}, \\ R_3 &= \left\{ y \in \mathbb{R}^2 : \frac{y_1^2}{4a_1} = \frac{y_2^2}{4a_2} \right\}. \end{aligned}$$

Clearly $R_1,\ R_2,\ R_3$ are pairwise disjoint and $R_1 \cup R_2 \cup R_3 = \mathbb{R}^2$. Let us define

$$K(y) := \langle z, y\rangle - A_2(y)$$

where $y \in R_1$ with $y_1$ fixed, and $z$ is fixed with $z_2 \neq 0$. Then

$$K(y) = \langle z, y\rangle - A_2(y) = z_1 y_1 + z_2 y_2 - \frac{y_2^2}{4a_2}.$$

Next we calculate $\sup\limits_{y\in R_1} K(y)$. Now $K(y)$ is maximized as a function of $y_2$ for fixed $y_1$ when $z_2 - \frac{y_2}{2a_2} = 0$ or $y_2 = 2a_2 z_2$. So, after substituting $y_2 = 2a_2 z_2$ in $R_1$, we get

$$\frac{y_1^2}{4a_1} < \frac{y_2^2}{4a_2} = a_2 z_2^2.$$

Now we see the fixed value of $y_1$ gives $y_1^2 < 4a_1 a_2 z_2^2$. Then

$$\begin{aligned} K(y) &= \langle z, y\rangle - A_2(y) = z_1 y_1 + z_2(2a_2 z_2) - \frac{(2a_2 z_2)^2}{4a_2} \\ &= z_1 y_1 + a_2 z_2^2. \end{aligned}$$

After maximizing over $y_1$, we get $\sqrt{4a_1 a_2}\,|z_1 z_2| + a_2 z_2^2$ as the maximum of $K(y)$ over $\overline{R}_1$. Now we can interchange $R_1$ and $R_2$, and using continuity we get

$$\begin{aligned} A_2^*(z) &\leq \max\left\{a_1 z_1^2,\ a_2 z_2^2\right\} + \sqrt{4a_1 a_2}\,|z_1 z_2| \\ &\leq a_1 z_1^2 + a_2 z_2^2 + \sqrt{4a_1 a_2}\,|z_1 z_2| =: G(z). \end{aligned}$$

Using (2.5) we see that

$$A^{**}(z) \leq a_1 z_1^2 + a_2 z_2^2 + \sqrt{4a_1 a_2}\,|z_1 z_2| = G(z).$$

Here $G(z)$ is convex on $\mathbb{R}^2$, and $G \leq A$. Since $A^{**}$ is the largest convex minorant of $A$ on $R^2$, thus $A^{**} = G$.

So to get the largest convex minorant of $A$, we replace the coefficient 2 of $|x_1 x_2|$ in $A$ (see (2.3)) by $\sqrt{4a_1 a_2}$ with $a_i = \left(1 - \frac{1}{N_i}\right)$ for $i = 1, 2$.

# 3 THE SPIN POLARIZED THOMAS-FERMI PROBLEM

It follows from Theorem 2.3 and some additional analysis that the largest convex minorant of $\boldsymbol{\mathcal{E}}_2$ defined by (2.1) is $\boldsymbol{\mathcal{E}}_2^*$ given by

$$\boldsymbol{\mathcal{E}}_2^*(\rho_1, \rho_2) = \sum_{i=1}^{2} \left(1 - \frac{1}{N_i}\right) \int\limits_{\mathbb{R}^3}\int\limits_{\mathbb{R}^3} \frac{\rho_i(x)\,\rho_i(y)}{|x-y|} dxdy$$

$$+2\left\{\left(1 - \frac{1}{N_1}\right)\left(1 - \frac{1}{N_2}\right)\right\}^{1/2} \int\limits_{\mathbb{R}^3}\int\limits_{\mathbb{R}^3} \frac{\rho_1(x)\,\rho_2(y)}{|x-y|} dxdy$$

for $(\rho_1, \rho_2) \in \boldsymbol{\mathcal{D}}(\boldsymbol{\mathcal{E}})$.

The Thomas-Fermi problem with $\boldsymbol{\mathcal{E}}^* = \boldsymbol{\mathcal{E}}_1 + \boldsymbol{\mathcal{E}}_2^*$ can be solved by adopting the methods of [2] used to solve the Thomas-Fermi problem for $\boldsymbol{\mathcal{E}} = \boldsymbol{\mathcal{E}}_1 + \boldsymbol{\mathcal{E}}_2$. More accurately, one adapts those methods, but additional nontrivial complications arise in the proof, especially in the topological degree theory portion of the argument. This was done in the thesis [15] and a paper in preparation [9]. Besides existence, we get uniqueness for the minimum of $\boldsymbol{\mathcal{E}}^*$, since $\boldsymbol{\mathcal{E}}^*$ is strictly convex. But this does not imply uniqueness for the minimum of $\boldsymbol{\mathcal{E}}$, because the convex minorant of $\boldsymbol{\mathcal{E}}^*$ of $\boldsymbol{\mathcal{E}}$ may not be the maximal. The problem of uniqueness for minimum of $\boldsymbol{\mathcal{E}}$ remains open.

More precisely, what is proved in [9], [15] is that the (Thomas-Fermi) minimization problem for $\boldsymbol{\mathcal{E}}^*$ has a unique solution for $(N_1,\ N_2)$, such that $N_1 > 1,\ N_2 > 1,\ N_1 + N_2 \leq Z + 1 = \left(\sum_{i=1}^{M} Z_i\right) + 1$ and $|N_1 - N_2| \leq \varepsilon$ for a suitable $\varepsilon > 0$. This last condition says that the number of spin up electrons cannot differ too much from the number of spin down electrons.

### Acknowledgments

We thank Cecil Rousseau for simplifying our original proof of Lemma 2.1.

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