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Stability of Relativistic Matter via Thomas–Fermi Theory

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This article is dedicated to our colleagues, teachers, and coauthors Klaus Hepp and Walter Hunziker on the occasion of their sexagesimal birthdays. Their enthusiasm for quantum mechanics as an unending source of interesting physics and mathematics has influenced many.

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Abstract A Thomas-Fermi-Weizsäcker type theory is constructed, by means of which we are able to give a relatively simple proof of the stability of relativistic matter. Our procedure has the advantage over previous ones in that the lower bound on the critical value of the fine structure constant, α , is raised from 0.016 to 0.77 (the critical value is known to be less than 2.72). When $\alpha = 1/137$, the largest nuclear charge is 59 (compared to the known optimum value 87). Apart from this, our method is simple, for it parallels the original Lieb-Thirring proof of stability of nonrelativistic matter, and it adds another perspective on the subject.

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1. Introduction

The ‘stability of relativistic matter’ concerns the N -body Hamiltonian (in units of $\hbar c$)

$$H = \sum_{i=1}^N |p_i| + \alpha V_c , \quad (1.1)$$

where V_c is the Coulomb potential of K fixed nuclei with nuclear charge Ze , with locations R_j in $\mathbf{R}^3$, and with N electrons. The Coulomb potential is

$$V_c = -V + R + U , \quad (1.2)$$

where

$$V := Z \sum_{i=1}^N \sum_{j=1}^K |x_i - R_j|^{-1} , \quad (1.3)$$

$$R := \sum_{1 \leq i < j \leq N} |x_i - x_j|^{-1} , \quad (1.4)$$

$$U := Z^2 \sum_{1 \leq i < j \leq K} |R_i - R_j|^{-1} . \quad (1.5)$$

As usual $p = -i\nabla$ and $|p| = \sqrt{-\Delta}$, and the x_j are the electron coordinates. The electrons are assumed to have q spin states each, $q = 2$ being the physical value. This means that the Hilbert space for the N -electron functions is the N -fold antisymmetric tensor product of $L^2(\mathbf{R}^3; \mathbf{C}^q)$. The constant $\alpha = e^2/\hbar c$ is called the fine structure constant.

We can easily include a magnetic field, which means replacing $|p_i|$ by $|p_i + A(x_i)|$. The vector field, A , is the vector potential (in suitable units) of a magnetic field, $A = \text{curl} B$, and can be arbitrary, as far as the present work is concerned. A mass can be included as well, i.e., $|p_i + A(x_i)|$ can be replaced by $\sqrt{|p_i + A(x_i)|^2 + m^2} - m$. The inclusion of a mass or magnetic field, while it changes the energy, does not affect stability. The reason for this and the requisite changes will be pointed out in the final section. It is for simplicity and clarity that we set $m = 0$ and $A = 0$.

‘Stability of matter’ means that the operator, H , is bounded below by a universal constant times $N + K$, independent of the R_j and A . In our case, because everything scales as an inverse length, the lower bound for H is either $-\infty$ or 0. Thus, we have to find the conditions under which H is a positive operator.

Many people worked on various aspects of this problem, including J. Conlon (who gave the first proof [C84]), I. Daubechies, C. Fefferman, I. Herbst, T. Kato, E. Lieb, R. de la Llave, R. Weder, and H-T. Yau. A careful, and still current, review of the history is contained in the introduction to [LY88], to which we refer the reader. For present purposes it suffices to note the current state of affairs concerning the best available constants needed for stability, as derived in [LY88]. We can list these in a sequence of remarks as follows:

1. Stability for any given values, α_* and Z_* , implies stability for all $0 \leq \alpha < \alpha_*$ and $Z < Z_*$. In fact, we can allow the nuclei to have different charges Z_i , $1 \leq i \leq K$, provided $Z_i \leq Z_*$ for all i . This follows from some simple concavity considerations and has nothing to do with the nature of the proof leading to α_* and Z_* .
2. Theorem 2 of [LY88] has the strongest results, but it is limited to the case of zero magnetic field, $A = 0$. The result is that stability occurs if

$$q\alpha \leq 1/47 \quad \text{and} \quad Z\alpha \leq 2/\pi . \quad (1.6)$$

It is not clear to us how to incorporate a magnetic field in the proof of Theorem 2, and we leave this as an open problem.

3. Theorem 1 of [LY88] has weaker results, but a simpler proof. That proof generalizes easily to the $A \neq 0$ case, as pointed out in [LLS95]. The result is complicated to state in full generality, but a representative example is that stability holds if

$$q\alpha \leq 0.032 \quad \text{and} \quad Z\alpha \leq 1/\pi . \quad (1.7)$$

It is possible to let $Z\alpha \rightarrow 2/\pi$ at the expense of $q\alpha \rightarrow 0$.

4. Instability definitely occurs if $Z\alpha > 2/\pi$, or if $Z_i\alpha > 2/\pi$ for any i . It also occurs if

$$\alpha > 128/(15\pi) \approx 2.72 \quad (1.8)$$

for *any* positive value of Z and any value of q . In other words, if $\alpha > 128/(15\pi)$ and if $Z > 0$ then one can produce collapse with only one electron, $N = 1$, by utilizing sufficiently many nuclei, i.e., by choosing K sufficiently large.

5. Instability also definitely occurs if ([LY88], Theorem 4)

$$\alpha > 36q^{-1/3}Z^{-2/3} , \quad (1.9)$$

which implies that bosonic matter (which can always be thought of as fermionic matter with $q = N$) is *always* unstable. (Note: there is a typographical error in Theorem 4 of [LY88].)

2. Main Results

The proof of the stability of *nonrelativistic* matter in [LT75] uses a series of inequalities to relate the ground state energy of the Hamiltonian to the Thomas-Fermi energy of the electron density, $\rho(x)$. The chief point is the kinetic energy inequality for an N -electron state Ψ , namely

$$\langle \Psi | \sum_{i=1}^N |p_i|^2 | \Psi \rangle > \text{const.} \int \rho^{5/3} .$$

The same approach will not work in the relativistic case because the corresponding inequality [D83] is, for dimensional reasons,

$$\langle \Psi | \sum_{i=1}^N |p_i| | \Psi \rangle > \text{const.} \int \rho^{4/3} .$$

While $\int \rho^{5/3}$ can control the Coulomb attraction $-Z\alpha \int \rho(x)/|x|$, unfortunately $\int \rho^{4/3}$ cannot do so. For this reason no attempt seems to have been made to imitate the proof in [LT75] of stability in the relativistic case.

However, the Coulomb singularity *can* be controlled by a Weizsäcker type term, namely $(\sqrt{\rho}, |p| \sqrt{\rho})$. The relativistic kinetic energy can, in turn, be bounded below by a term of this type plus a term of the $\int \rho^{4/3}$ type. This and other essential inequalities will be explained more fully below. With the ‘Coulomb tooth’ now gone, TF theory with $\int \rho^{4/3}$ can deal adequately with the rest of the Coulomb energy (with the aid of the exchange-correlation energy inequality [LO81], whose remainder term also has the form $\int \rho^{4/3}$).

Before going into details, let us state our main results. First, we define Thomas-Fermi-Weizsäcker (TFW) theory as follows: The class of functions (‘densities’) to be considered, denoted by $\mathcal{C}$, consists of those nonnegative functions $\rho : \mathbf{R}^3 \rightarrow \mathbf{R}^+$ such that $\sqrt{\rho}$ and $\sqrt{|p|\rho}$ have finite $L^2(\mathbf{R}^3)$ norms, i.e.,

$$\mathcal{C} = \left\{ \rho : \rho(x) \geq 0 \text{ and } \int_{\mathbf{R}^3} (1 + |p|) |\widehat{\sqrt{\rho}}(p)|^2 dp < \infty \right\} , \quad (2.1)$$

where $\widehat{\sqrt{\rho}}(p) := (2\pi)^{-3/2} \int_{\mathbf{R}^3} \exp[-ip \cdot x] \sqrt{\rho}(x) dx$ denotes the Fourier transform of the function $\sqrt{\rho}(x)$.

Next, we define the functional

$$T(\rho) := \int_{\mathbf{R}^3} |p| |\widehat{\sqrt{\rho}}(p)|^2 dp \equiv (\sqrt{\rho}, |p| \sqrt{\rho}) . \quad (2.2)$$

The TFW functional, with arbitrarily given positive constants β and γ , is then

$$\mathcal{E}(\rho) := \beta T(\rho) + \frac{3}{4} \gamma \int_{\mathbf{R}^3} \rho^{4/3}(x) dx - \alpha \int_{\mathbf{R}^3} V(x) \rho(x) dx + \alpha D(\rho, \rho) + \alpha U \quad (2.3)$$

with

$$D(\rho, \rho) := (1/2) \int_{\mathbf{R}^3} \int_{\mathbf{R}^3} \rho(x) \rho(y) |x - y|^{-1} dx dy .$$

The quantity of principal interest is the energy

$$E^{TFW} := \inf \{ \mathcal{E}(\rho) : \rho \in \mathcal{C} \} . \quad (2.4)$$

This quantity depends on the parameters α, β and γ and on the nuclear coordinates, R_j . If, however, we try to minimize E over all choices of the nuclear coordinates then the result is either 0 or $-\infty$, as can be easily seen from the fact that all the terms in $\mathcal{E}$ scale, under dilation, as an inverse length.

THEOREM 1. (Stability of TFW theory). *The TFW energy, E^{TFW} , in (2.4) is nonnegative if*

$$\beta \geq \frac{\pi}{2} Z\alpha, \quad \text{and} \quad \gamma \geq 4.8158 Z^{2/3} \alpha \quad (2.5)$$

On the other hand, if $\beta < (\pi/2)Z\alpha$ then $E = -\infty$ for every choice of the nuclear coordinates.

For the next theorem we have to define the density corresponding to an N -body wave function. If Ψ is an antisymmetric function of N space-spin coordinates, normalized to unity in the usual way, we define

$$\rho_\Psi(x) := N \sum_{1 \leq \sigma_1, \dots, \sigma_N \leq q} \int_{\mathbf{R}^{3(N-1)}} |\Psi(x, \sigma_1; x_2, \sigma_2; \dots; x_N, \sigma_N)|^2 dx_2 \cdots dx_N. \quad (2.6)$$

THEOREM 2. (TFW theory bounds quantum mechanics). *Let Ψ be any normalized antisymmetric function, with ρ_Ψ defined in (2.6). Choose*

$$\beta = \frac{\pi}{2} Z\alpha \quad \text{and} \quad \gamma = \frac{4}{3} \left[1.63q^{-1/3} \left(1 - \frac{\pi}{2} Z\alpha \right) - 1.68 \alpha \right]. \quad (2.7)$$

Assume that γ is positive. Then, with this definition of the TFW functional (2.3),

$$\langle \Psi | H | \Psi \rangle \geq \mathcal{E}(\rho_\Psi). \quad (2.8)$$

A corollary of these two theorems is that *our Hamiltonian, H , in (1.1) is stable if*

$$\left(\frac{\pi}{2}\right)Z + 2.2159 q^{1/3} Z^{2/3} + 1.0307 q^{1/3} \leq 1/\alpha. \quad (2.9)$$

(Cf. (1.9)) In particular, *with $q = 2$ for electrons, relativistic matter is stable if $\alpha < 0.77$ and if Z is not too large. When $\alpha = 1/137$ the allowed Z is 59, which compares favorably with the best possible value $87 \approx 137(2/\pi)$.*

We leave it as a challenge to improve our method so as to achieve the value $137(2/\pi)$ (with a magnetic field present). As noted above, this value has been achieved in [LY88], but without a magnetic field. The most noteworthy point is the large value of the critical fine structure constant: $\alpha_{critical} \geq 0.77$ when $q = 2$.

The bound in (2.9) is, in some respects, similar to Theorem 1 in [LY88], but it is far simpler, clearer and gives the correct q -dependence of α (note that (1.9) gives a similar

bound in the other direction). The chief methodological difference is that Theorem 6 is used in [LY88], which bounds the Coulomb potential below by a one-body potential. Here, we use the exchange-correlation inequality (3.9) instead. We repeat that the results above also hold with a magnetic field.

It is to be emphasized that our stability result is really contained in Theorem 2. Theorem 1 only gives a condition for which $\mathcal{E}(\rho) \geq 0$. A better estimate on the TFW functional will, via Theorem 2, yield a better stability bound.

3. Some Essential Inequalities

There are five known inequalities about Coulomb systems that will be needed in our proof of our main theorems. We begin by recalling them.

KINETIC ENERGY LOCALIZATION, [LY88] pp. 186 and 188.

Denote by Γ_j the Voronoi cell in $\mathbf{R}^3$ that contains R_j , i.e., the set

$$\Gamma_j := \{x \in \mathbf{R}^3 : |x - R_j| \leq |x - R_k| \text{ for all } k\} , \quad (3.1)$$

and let D_j be half the distance of the j -th nucleus to its nearest neighbor. These Γ_j are disjoint, except for their boundaries and, being the intersection of half-spaces they are convex sets. The ball centered at R_j with radius D_j is denoted by B_j . Obviously, $B_j \subset \Gamma_j$.

For any function $f \in L^2(\mathbf{R}^3)$ there is the inequality

$$(f, |p| f) \geq \sum_{j=1}^K \int_{B_j} |f(x)|^2 \left\{ \frac{2}{\pi} |x - R_j|^{-1} - \frac{1}{D_j} Y \left(\frac{|x - R_j|}{D_j} \right) \right\} dx . \quad (3.2)$$

The function Y is given, for $0 < r < 1$, by

$$Y(r) = \frac{2}{\pi(1+r)} + \frac{1+3r^2}{\pi r(1+r^2)} \ln(1+r) - \frac{1-r^2}{\pi r(1+r^2)} \ln(1-r) - \frac{4r}{\pi(1+r^2)} \ln r . \quad (3.3)$$

Numerically it is found that [LY88] (2.27)

$$4\pi \int_0^1 Y(r)^4 r^2 dr < 7.6245 . \quad (3.4)$$

RELATIVISTIC KINETIC ENERGY BOUND FOR FERMIONS, [D83].

Let Ψ and ρ_Ψ be as in (2.6). Then

$$\langle \Psi | \sum_{i=1}^N |p_i| | \Psi \rangle \geq 1.63q^{-1/3} \int_{\mathbf{R}^3} \rho_\Psi^{4/3}(x) dx . \quad (3.5)$$

A generalization of this, of importance if we wish to include a mass, is

$$\langle \Psi | \sum_{i=1}^N [\sqrt{p_i^2 + m^2} - m] | \Psi \rangle \geq \frac{3}{8} m^4 C \int_{\mathbf{R}^3} g \left((\rho_{\Psi}(x)/C)^{1/3} m^{-1} \right) dx, \quad (3.6)$$

with $C = 0.163q$ (*sic*) and with

$$g(t) := t(1+t^2)^{1/2}(1+2t^2) - \frac{8}{3}t^3 - \ln \left[t + (1+t^2)^{1/2} \right]. \quad (3.7)$$

GENERAL KINETIC ENERGY BOUND, [C84], p.454, (and [HO77] for the nonrelativistic case). The following bound follows from a judicious application of Schwarz's inequality.

$$\langle \Psi | \sum_{i=1}^N |p_i| | \Psi \rangle \geq (\sqrt{\rho_{\Psi}}, |p| \sqrt{\rho_{\Psi}}). \quad (3.8)$$

This bound holds irrespective of the symmetry type of the wave function.

EXCHANGE AND CORRELATION INEQUALITY, [LO81]. If Ψ is a normalized N -particle wave function there is a lower bound on the interparticle Coulomb repulsion in terms of its density:

$$\langle \Psi | \sum_{1 \leq i < j \leq N} |x_i - x_j|^{-1} | \Psi \rangle \geq D(\rho_{\Psi}, \rho_{\Psi}) - 1.68 \int_{\mathbf{R}^3} \rho_{\Psi}^{4/3}(x) dx. \quad (3.9)$$

(Once again, the antisymmetry of Ψ plays no role in this inequality.)

ELECTROSTATIC INEQUALITY, [LY88], p.196. First, we define a function, Φ on $\mathbf{R}^3$ with the aid of the Voronoi cells mentioned above. In the cell Γ_j , Φ equals the electrostatic potential generated by all the nuclei *except* for the nucleus situated in Γ_j itself, i.e., for x in Γ_j

$$\Phi(x) := Z \sum_{\substack{i=1 \\ i \neq j}}^K |x - R_i|^{-1}. \quad (3.10)$$

If ν is any bounded Borel measure on $\mathbf{R}^3$ (not necessarily positive) then

$$\frac{1}{2} \int_{\mathbf{R}^3} \int_{\mathbf{R}^3} |x - y|^{-1} d\nu(x) d\nu(y) - \int_{\mathbf{R}^3} \Phi(x) d\nu(x) + U \geq \frac{1}{8} Z^2 \sum_{j=1}^K D_j^{-1}. \quad (3.11)$$

4. Proofs of Theorems 1 and 2

To prove Theorem 1 we take $\beta = \pi Z\alpha/2$ (if $\beta > \pi Z\alpha/2$ we simply throw away the excess positive quantity). Using (3.2) with f replaced by $\sqrt{\rho}$, we have that

$$\mathcal{E}(\rho) \geq \mathcal{E}_1(\rho) + \alpha \mathcal{E}_2(\rho) , \quad (4.1)$$

where, by adding and subtracting a term $\int \Phi \rho$, with $\Phi(x)$ as in (3.10),

$$\mathcal{E}_1(\rho) := \frac{3}{4} \gamma \int_{\mathbf{R}^3} \rho^{4/3}(x) dx - \alpha \int_{\mathbf{R}^3} W(x) \rho(x) dx + \alpha \int_{\mathbf{R}^3} \Phi(x) \rho(x) dx \quad (4.2)$$

and

$$\mathcal{E}_2(\rho) := D(\rho, \rho) - \int_{\mathbf{R}^3} \Phi(x) \rho(x) dx + U . \quad (4.3)$$

The function $W(x)$ is defined as follows: In the Voronoi cell Γ_j it is given by

$$W(x) := \Phi(x) + \begin{cases} Z|x - R_j|^{-1}, & \text{if } |x - R_j| > D_j \\ (\pi Z/2) D_j^{-1} Y(|x - R_j|/D_j), & \text{if } |x - R_j| \leq D_j . \end{cases} \quad (4.4)$$

Note that while the terms $\pm \int \Phi \rho$ that appear in (4.2), (4.3) are merely 'strategic', the presence of the term $\Phi(x)$ in (4.4) is properly part of the potential energy of the electron and is not arbitrary. Actually, this strategic decomposition of $\mathcal{E}(\rho)$ is the one used in the easy part of Fenchel's duality theorem (see [R70], p. 327). This duality principle was used in connection with Thomas-Fermi theory by Firsov [F57] (see also [L81]); the full blown duality theory is not needed for our purposes, so we omit it.

We can now seek lower bounds for $\mathcal{E}_1(\rho)$ and $\mathcal{E}_2(\rho)$ separately. Using Hölder's inequality, for example, one easily concludes that the absolute minimum of $\mathcal{E}_1(\rho)$ is

$$\begin{aligned} \mathcal{E}_1(\rho) &\geq -\frac{\alpha^4}{4\gamma^3} \int_{\mathbf{R}^3} [W(x) - \Phi(x)]_+^4 dx \\ &= -\frac{(\alpha Z)^4}{4\gamma^3} \sum_{j=1}^K \left(\frac{\pi}{2}\right)^4 \int_{B_j} D_j^{-4} Y(|x - R_j|/D_j)^4 dx + \int_{\Gamma_j \setminus B_j} |x - R_j|^{-4} dx \end{aligned} \quad (4.5)$$

$$\geq -\frac{(\alpha Z)^4}{4\gamma^3} \left\{ \left(\frac{\pi}{2}\right)^4 (4\pi) \int_0^1 Y(r)^4 r^2 dr + 3\pi \right\} \sum_{j=1}^K D_j^{-1} \quad (4.6)$$

$$> -\frac{(\alpha Z)^4}{4\gamma^3} \left\{ 7.6245 \left(\frac{\pi}{2}\right)^4 + 3\pi \right\} \sum_{j=1}^K D_j^{-1} . \quad (4.7)$$

The last formula uses (3.4). The second integral in (4.5) is evaluated in (4.6) as $3\pi/D_j$, and the explanation is the following: If we integrate $|x - R_j|^{-4}$ over the exterior of B_j we would obtain $4\pi/D_j$ as the result. However, we know that the Voronoi cell Γ_j lies on

one side of the mid-plane defined by the nearest neighbor nucleus. This means that the integral over $\Gamma_j \setminus B_j$ is bounded above by the integral

$$D_j^{-1} \int_1^\infty dz \int_0^\infty (2\pi r dr) [r^2 + z^2]^{-2} = 3\pi/D_j .$$

The $\mathcal{E}_2$ term can be bounded using (3.11) with $d\nu(x) = \rho(x)dx$. Thus,

$$\mathcal{E}_2(\rho) \geq \frac{Z^2}{8} \sum_{j=1}^K D_j^{-1} . \quad (4.8)$$

Combining (4.1), (4.7) and (4.8) we have proved Theorem 1. ■

Theorem 2 is proved by splitting the relativistic kinetic energy $|p|$ into $\beta|p|$ and $(1 - \beta)|p|$, with the choice $\beta = \pi Z\alpha/2$. The inequalities (3.5), (3.8) and (3.9) immediately give us Theorem 2. ■

5. Inclusion of Mass and Magnetic Fields

INCLUSION OF MASS. We replace $|p|$ by $\sqrt{p^2 + m^2} - m$ and, in the corresponding TFW theory, we replace the right side of (3.5) by the right side of (3.6). It is not easy to carry out the rest of the program in closed form with this more complicated function, however. Moreover, it unfortunately gives a slightly worse constant than before, even when we set $m = 0$; instead of $1.63q^{-1/3}$ in (3.5) we now have $C^{-1/3} \approx 1.37q^{-1/3}$. The new energy will not be positive in the stability regime, as we had before. Instead, it will be a negative constant times N . This new value for the energy is in accord with stability of matter and represents the binding energy of the electron-nuclear system.

Another way to deal with the mass is to observe, simply, that $\sqrt{p^2 + m^2} - m > |p| - m$, the effect of which is to add a term $-Nm$ to the energy estimate. This term satisfies the criterion for stability, but it has the defect that is huge in real-world terms, for it equals the rest energy of the electron.

INCLUSION OF MAGNETIC FIELD. Theorem 2, with a magnetic field included, is a consequence of the following two inequalities (proved below) which replace (3.6) and (3.8):

$$\langle \Psi | \sum_{i=1}^N [\sqrt{(p_i + A(x_i))^2 + m^2} - m] | \Psi \rangle \geq \frac{3}{8} m^4 C \int_{\mathbb{R}^3} g \left((\rho_\Psi(x)/C)^{1/3} m^{-1} \right) dx , \quad (5.1)$$

and

$$\langle \Psi | \sum_{i=1}^N |p_i + A(x_i)| | \Psi \rangle \geq (\sqrt{\rho_\Psi} , |p| \sqrt{\rho_\Psi}) . \quad (5.2)$$

As in (3.8), inequality (5.2) holds irrespective of the symmetry type of Ψ .

To define $\sqrt{|p + A|^2 + m^2}$, note that if $A \in L^2_{loc}(\mathbf{R}^3; \mathbf{R}^3)$, then $f \mapsto \|(p + A)f\|_2^2$ is a closed quadratic form with $C_0^\infty(\mathbf{R}^3)$ being a form core [K78], [S79-1], [LS81]. Thus it defines a selfadjoint operator and it is then possible to define $\sqrt{|p + A|^2 + m^2}$ via the spectral calculus.

The *diamagnetic inequality for the heat kernel* [S79-2] is the pointwise inequality

$$\left| \exp \left[-t(p + A)^2 \right] f(x) \right| \leq \exp \left[-tp^2 \right] |f|(x) . \quad (5.3)$$

Using the formula

$$e^{-|a|} = \frac{1}{\sqrt{\pi}} \int_0^\infty e^{-a^2/4t} \frac{dt}{\sqrt{t}} , \quad (5.4)$$

which holds for any real number a (and hence for any selfadjoint operator), we obtain the diamagnetic inequality for the 'relativistic heat kernel'

$$\left| \exp \left[-t\sqrt{(p + A)^2 + m^2} \right] f(x) \right| \leq \exp \left[-t\sqrt{p^2 + m^2} \right] |f|(x) . \quad (5.5)$$

By using (5.5), and following the proof of (3.6) in [D83] step by step, we obtain (5.1). Likewise, (5.5) and the formula

$$(f, \sqrt{(p + A)^2 + m^2} f) = \lim_{t \rightarrow 0} \frac{1}{t} \left\{ (f, f) - (f, \exp \left[-t\sqrt{(p + A)^2 + m^2} \right] f) \right\} , \quad (5.6)$$

yields

$$(f, |p + A| f) \geq (|f|, |p| |f|) . \quad (5.7)$$

To prove (5.2) we apply (5.7) to the function $|\Psi|$ and then use (3.8).

References

- [C84] Conlon, J.G., *The ground state energy of a classical gas*, Commun. Math. Phys. **94**, 439-458 (1984).
- [D83] Daubechies, I., *An uncertainty principle for fermions with generalized kinetic energy*, Commun. Math. Phys. **90**, 511-520 (1983).
- [F57] Firsov, O.B., *Calculation of the interaction potential of atoms for small nuclear separations*, Sov. Phys. JETP **5**, 1192-1196 (1957).
- [HO77] Hoffmann-Ostenhof, M. and Hoffman-Ostenhof, T., *Schrödinger inequalities and asymptotic behavior of the electronic density of atoms and molecules*, Phys. Rev. A **16**, 1782-1785 (1977).

- [K78] Kato, T., *Remarks on Schrödinger operators with vector potentials*, Int. Eq. Operator Theory **1**, 103-113 (1978).
- [LS81] Leinfelder, H., Simader, C., *Schrödinger operators with singular magnetic vector potentials*, Math. Z. **176**, 1-19 (1981).
- [L81] Lieb, E.H. *Thomas-Fermi and related theories of atoms and molecules*, Rev. Mod. Phys. **53** 603-641 (1981). Errata, *ibid* **54**, 311 (1982).
- [LLS95] Lieb, E.H., Loss, M. and Solovej, J.P., *Stability of Matter in Magnetic Fields*, Phys. Rev. Lett. **75**, 985-989 (1995).
- [LO81] Lieb, E.H. and Oxford, S., *Improved lower bound on the indirect Coulomb energy*, Int. J. Quant. Chem. **19**, 427-439 (1981).
- [LY88] Lieb, E.H. and Yau, H-T., *The stability and instability of relativistic matter*, Commun. Math. Phys. **118**, 177-213 (1988).
- [LT75] Lieb, E.H., and Thirring, W.E., *Bound for the kinetic energy of fermions which proves the stability of matter*, Phys. Rev. Lett. **35**, 687-689 (1975). Erratum, *ibid*, 1116.
- [R70] Rockafellar, R.T., *Convex Analysis*, Princeton University Press (1970).
- [S79-1] Simon, B., *Maximal and minimal Schrödinger forms*, J. Opt. Theory **1**, 37-47 (1979).
- [S79-2] Simon, B., *Kato's inequality and the comparison of semigroups*, J. Funct. Anal. **32**, 97-101 (1979).