

## RELATIVISTIC STRONG SCOTT CONJECTURE: A SHORT PROOF

RUPERT L. FRANK, KONSTANTIN MERZ, AND HEINZ SIEDENTOP

ABSTRACT. We consider heavy neutral atoms of atomic number  $Z$  modeled with kinetic energy  $(c^2 p^2 + c^4)^{1/2} - c^2$  used already by Chandrasekhar. We study the behavior of the one-particle ground state density on the length scale  $Z^{-1}$  in the limit  $Z, c \rightarrow \infty$  keeping  $Z/c$  fixed. We give a short proof of a recent result by the authors and Barry Simon showing the convergence of the density to the relativistic hydrogenic density on this scale.

### 1. INTRODUCTION

A simple description exhibiting some qualitative features of atoms of large atomic number  $Z$  with  $N$  electrons and with  $q$  spin states each is offered by the Chandrasekhar operator

$$(1) \quad \sum_{\nu=1}^N \left( \sqrt{-c^2 \Delta_{\nu} + c^4} - c^2 - \frac{Z}{|x_{\nu}|} \right) + \sum_{1 \leq \nu < \mu \leq N} \frac{1}{|x_{\nu} - x_{\mu}|} \quad \text{in} \quad \bigwedge_{\nu=1}^N L^2(\mathbb{R}^3 : \mathbb{C}^q)$$

where  $c$  denotes the velocity of light. It is defined as the Friedrichs extension of the corresponding quadratic form with form domain  $\bigwedge_{\nu=1}^N C_0^{\infty}(\mathbb{R}^3 : \mathbb{C}^q)$ . By Kato's inequality [7, Chapter 5, Equation (5.33)], it follows that the form is bounded from below if and only if  $Z/c \leq 2/\pi$  (see also Herbst [5, Theorem 2.5] and Weder [14]). For  $Z/c < 2/\pi$  its form domain is  $H^{1/2}(\mathbb{R}^{3N} : \mathbb{C}^{q^N}) \cap \bigwedge_{\nu=1}^N L^2(\mathbb{R}^3 : \mathbb{C}^q)$ . Since there is no interaction involving the electron's spin present, we set  $q = 1$  for notational simplicity. Moreover, we are restricting ourselves to neutral atoms  $N = Z$  and fix  $\gamma = Z/c \in (0, 2/\pi)$ . We denote the resulting Hamiltonian by  $C_Z$ .

In the following, we are interested in properties of ground states of this system. Lewis et al [8] proved that the ground state energy is an eigenvalue of  $C_Z$  belonging to the discrete spectrum of  $C_Z$ . Given any orthonormal base of the ground state space  $\psi_1, \dots, \psi_M$  any ground state of  $C_Z$  can be written as

$$\sum_{\mu=1}^M w_{\mu} |\psi_{\mu}\rangle \langle \psi_{\mu}|$$

where  $w_{\mu} \geq 0$  are weights such that  $\sum_{\mu=1}^M w_{\mu} = 1$ . In the following, we would not even need a ground state. States which approximate the ground state energy sufficiently well would be enough. However, we refrain from such generalizations and simply pick the state that occurs according to Lüders [11] when measuring the ground state energy, namely the one with equal weights  $w_1 = \dots = w_M = M^{-1}$ .

We write  $d_Z$  for this state. Its one-particle ground state density is

$$\rho_Z(x) := N \sum_{\mu=1}^M w_\mu \int_{\mathbb{R}^{3(N-1)}} |\psi_\mu(x, x_2, \dots, x_N)|^2 dx_2 \cdots dx_N.$$

For  $\ell \in \mathbb{N}_0$  we denote by  $Y_{\ell,m}$ ,  $m = -\ell, \dots, \ell$ , a basis of spherical harmonics of degree  $\ell$ , normalized in  $L^2(\mathbb{S}^2)$  [12, Formula (B.93)] and by

$$(2) \quad \Pi_\ell = \sum_{m=-\ell}^{\ell} |Y_{\ell,m}\rangle \langle Y_{\ell,m}|$$

the projection onto the angular momentum channel  $\ell$ . The electron density  $\rho_{\ell,Z}$  of the Lüders state in the  $\ell$ -th angular momentum channel is

$$(3) \quad \rho_{\ell,Z}(x) := \frac{N}{4\pi} \sum_{\mu=1}^M w_\mu \sum_{m=-\ell}^{\ell} \int_{\mathbb{R}^{3(N-1)}} \left| \int_{\mathbb{S}^2} \overline{Y_{\ell,m}(\omega)} \psi_\mu(|x|\omega, x_2, \dots, x_N) d\omega \right|^2 dx_2 \cdots dx_N.$$

We note the relation

$$(4) \quad \rho_Z = \sum_{\ell=0}^{\infty} \rho_{\ell,Z}.$$

Our main result concerns these densities on distances of order  $Z^{-1}$  from the nucleus. We recall that electrons on these length scales are responsible for the Scott correction in the asymptotic expansion of the ground state energy [13, 3] and are described by the Chandrasekhar hydrogen Hamiltonian  $\sqrt{-\Delta + 1} - 1 - \gamma|x|^{-1}$  in  $L^2(\mathbb{R}^3)$ . Spherical symmetry leads to the radial operators

$$(5) \quad C_{\ell,\gamma} := \sqrt{-\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{r^2} + 1} - 1 - \frac{\gamma}{r}$$

in  $L^2(\mathbb{R}_+) := L^2(\mathbb{R}_+, dr)$ . We write  $\psi_{n,\ell}^H$ ,  $n \in \mathbb{N}_0$ , for a set orthonormal eigenfunctions of  $C_{\ell,\gamma}$  spanning its pure point spectral space. The hydrogenic density in channel  $\ell$  is

$$(6) \quad \rho_\ell^H(x) := (2\ell + 1) \sum_{n=0}^{\infty} |\psi_{n,\ell}^H(|x|)|^2 / (4\pi|x|^2), \quad x \in \mathbb{R}^3,$$

and the total hydrogenic density is then given by

$$(7) \quad \rho^H := \sum_{\ell=0}^{\infty} \rho_\ell^H.$$

The generalization of Lieb's strong Scott conjecture [9, Equation (5.37)] to the present situation asserts the convergence of the rescaled ground state densities  $\rho_Z$  and  $\rho_{\ell,Z}$  to the corresponding relativistic hydrogenic densities  $\rho^H$  and  $\rho_\ell^H$ . Whereas the non-relativistic conjecture was proven by Iantchenko et al [6], it was shown in the present context in [2], including the convergence of the sums defining the limiting objects  $\rho_\ell^H$  and  $\rho^H$ . Here, we will take the existence of the limiting densities for granted. The purpose of this note is to offer a simpler proof of the core of the above convergence of the quantum densities. It is a simple virial type argument which allows us to obtain the central estimate on the difference of perturbed and

unperturbed one-particle Chandrasekhar eigenvalues in an easy way. In addition we will refrain from using the elaborate classes of test functions of [2].

**Theorem 1** (Convergence for fixed angular momentum). *Pick  $\gamma \in (0, \frac{2}{\pi})$ ,  $\ell_0 \in \mathbb{N}_0$ , assume  $Z/c = \gamma$  fixed and  $U : \mathbb{R}_+ \rightarrow \mathbb{R}$  with  $C_{\ell, -\gamma}^{-1/2} \circ U \circ C_{\ell, -\gamma}^{-1/2} \in \mathfrak{B}(L^2(\mathbb{R}_+))$ . Then*

$$(8) \quad \lim_{Z \rightarrow \infty} \int_{\mathbb{R}^3} c^{-3} \rho_{\ell_0, Z}(c^{-1}x) U(|x|) dx = \int_{\mathbb{R}^3} \rho_{\ell_0}^H(x) U(|x|) dx.$$

We would like to add three remarks:

1. Our hypothesis allows for Coulomb tails of  $U$  in contrast to [2, Theorem 1.1] where the test functions were assumed to decay like  $O(r^{-1-\varepsilon})$ .

2. Since  $C_{\ell, 0} \geq C_{0, 0}$  the Sobolev inequality shows that  $U$  such that  $U \circ |\cdot| \in L^3(\mathbb{R}^3) \cap L^{3/2}(\mathbb{R}^3)$  is allowed.

3. Picking a suitable class of test functions  $U$ , we may – by an application of Weierstraß’ criterion – sum (8) and interchange the limit  $Z \rightarrow \infty$  with the sum over  $\ell_0$ . This yields for  $\gamma \in (0, 2/\pi)$  and  $Z/c = \gamma$  fixed the convergence of the total density

$$(9) \quad \lim_{Z \rightarrow \infty} \int_{\mathbb{R}^3} c^{-3} \rho_Z(c^{-1}x) U(|x|) dx = \int_{\mathbb{R}^3} \rho^H(x) U(|x|) dx.$$

We refer to [2] for details.

## 2. PROOF OF THE CONVERGENCE

The general strategy of the proof of Theorem 1 is a linear response argument which was already used by Baumgartner [1] and Lieb and Simon [10] for the convergence of the density on the Thomas-Fermi scale and by Iantchenko et al [6] and [2] in the context of the strong Scott conjecture. The rescaled density integrated against a test function  $U$  is written by the Hellmann-Feynman theorem as a derivative of the energy with respect to perturbing one-particle potential  $-\lambda U$  and taking the limit  $Z \rightarrow \infty$  as the representation

$$(10) \quad \int_{\mathbb{R}^3} \frac{1}{c^3} \rho_{\ell, Z}(x/c) U(|x|) dx = \frac{1}{\lambda c^2} \text{Tr}\{[C_Z - (C_Z - \lambda \sum_{\nu=1}^Z (U_c \otimes \Pi_\ell)_\nu)] d_Z\}$$

where  $U_c(r) := c^2 U(cr)$ . Of course, it is enough to prove (9) for positive  $U$ , since we can simply prove the result for the positive and negative part separately and take the difference. By standard estimates following [2] (which in turn are patterned by Iantchenko et al [6]) one obtains

**Proposition 1.** *Fix  $\gamma := Z/c \in (0, 2/\pi)$ ,  $\ell \in \mathbb{N}_0$ , and assume that  $U \geq 0$  is a measurable function on  $(0, \infty)$  that is form bounded with respect to  $C_{\ell, \gamma}$ , and assume that  $|\lambda|$  is sufficiently small. Then*

$$(11) \quad (2\ell + 1) \sum_n \frac{e_{n, \ell}(0) - e_{n, \ell}(\lambda)}{\lambda} \begin{cases} \geq \limsup_{Z \rightarrow \infty} \int_{\mathbb{R}^3} \rho_{\ell, Z}(c^{-1}x) U(|x|) dx & \text{if } \lambda > 0 \\ \leq \liminf_{Z \rightarrow \infty} \int_{\mathbb{R}^3} \rho_{\ell, Z}(c^{-1}x) U(|x|) dx & \text{if } \lambda < 0 \end{cases},$$

where  $e_{n, \ell}(\lambda)$  is the  $n$ -th eigenvalue of  $C_{\ell, \gamma} - \lambda U$ .

Thus the limit (8) exists, if the derivative of the sum of the eigenvalues with respect to  $\lambda$  exists at 0, i.e.,

$$(12) \quad \frac{d}{d\lambda} \sum_n e_{n,\ell}(\lambda) \Big|_{\lambda=0}$$

exists and – when multiplied by  $-(2\ell + 1)$  – is equal to the right of (8). Put differently: the wanted limit exists, if the Hellmann–Feynman theorem does not only hold for a single eigenvalue  $e_{n,\ell}(\lambda)$  of  $C_{\ell,\gamma} - \lambda U$  but for the sum of all eigenvalues. However, the differentiability would follow immediately, if we were allowed to interchange the differentiation and the sum in (12), since the Hellmann–Feynman theorem is valid for each individual nondegenerate eigenvalue and yields the wanted contribution to the derivative. In turn, the validity of the interchange of these two limiting processes would follow by the Weierstraß criterion for absolute and uniform convergence, if we had in a neighborhood of zero a  $\lambda$ -independent summable majorant of the moduli of the summands on the left side of (11). This, in turn is exactly the content of Lemma 1 enabling to interchange the limit  $\lambda \rightarrow 0$  with the sum over  $n$  and concluding the proof of Theorem 1.

Before ending the section we comment on the difference to previous work: Already Iantchenko et al [6, Lemma 2] proved a bound similar to (18) in the non-relativistic setting where – in contrast to the Chandrasekhar case – the hydrogenic eigenvalues are explicitly known. However, this was initially not accessible in the present context. Instead, the differentiability of the sum was shown in [2, Theorems 3.1 and 3.2] by an abstract argument for certain self-adjoint operators whose negative part is trace class. To prove the analogue majorant for the Chandrasekhar hydrogen operator is the new contribution of the present work yielding a substantial simplification.

### 3. THE MAJORANT

Before giving the missing majorant, we introduce some useful notations. Set

$$(13) \quad A := 2 + \frac{2^{3/2}}{\pi(\sqrt{2} - 1)}.$$

For  $\gamma \in (0, 2/\pi)$  and  $t \in [0, 1)$  we set

$$(14) \quad F_\gamma(t) := (1-t) \left( \frac{1+t}{1-t} \right)^{1+A} \left( \frac{\frac{2}{\pi} - \gamma}{\frac{2}{\pi} - \frac{1+t}{1-t}\gamma} \right)^A = \frac{(1+t)^{1+A}}{\left(1 - \frac{\frac{2}{\pi} + \gamma}{\frac{2}{\pi} - \gamma} t\right)^A}.$$

Obviously  $F_\gamma \in C^1([-t_0, t_0])$  with  $t_0 := (\frac{1}{\pi} - \frac{\gamma}{2}) / (\gamma + \frac{2}{\pi})$ . We set

$$(15) \quad \tilde{M}_\gamma := \max F'_\gamma([-t_0, t_0]).$$

Furthermore, we write  $C_\gamma$  for the optimal constant in the following inequality [4, Theorem 2.2] bounding all hydrogenic Chandrasekhar eigenvalues from below by the corresponding hydrogenic Schrödinger eigenvalues, i.e.,

$$(16) \quad C_\gamma e_n(p^2/2 - \gamma/|x|) \leq e_n(\sqrt{p^2 + 1} - 1 - \gamma/|x|).$$

(Here, and sometimes also later, it is convenient to use a slightly more general notation for eigenvalues of self-adjoint operators  $A$  which are bounded from below:

we write  $e_0(A) \leq e_1(A) \leq \dots$  for its eigenvalues below the essential spectrum counting their multiplicity.)

Finally, we set

$$(17) \quad M_\gamma := C_\gamma \tilde{M}_\gamma$$

This allows us to formulate our central Lemma which allows to interchange the derivative in (12) and proves Theorem 1. We recall that we write  $e_{n,\ell}(\lambda)$  for the eigenvalues of  $C_{\ell,\gamma} - \lambda U$  (see Proposition 1).

**Lemma 1.** *Assume  $\gamma \in (0, 2/\pi)$  and  $U : \mathbb{R}_+ \rightarrow \mathbb{R}_+$  such that the operator norm  $b := \|C_{\ell,-\gamma}^{-\frac{1}{2}} U C_{\ell,-\gamma}^{-\frac{1}{2}}\|$  is finite. Then for all  $\lambda \in [-t_0/b, t_0/b]$  and all  $\ell, n \in \mathbb{N}_0$*

$$(18) \quad |e_{n,\ell}(\lambda) - e_{n,\ell}(0)| \leq M_\gamma b |\lambda| \frac{\gamma^2}{(n + \ell + 1)^2}.$$

For the proof, we need some preparatory results. We begin with a bound on the change of Coulomb eigenvalues with the coupling constant which is the core of our argument.

**Proposition 2.** *For all  $\gamma, \gamma' \in (0, 2/\pi)$  with  $\gamma \leq \gamma'$  and all  $n \in \mathbb{N}_0$*

$$(19) \quad e_n(\sqrt{p^2 + 1} - 1 - \gamma'|x|^{-1}) \geq e_n(\sqrt{p^2 + 1} - 1 - \gamma|x|^{-1}) \left(\frac{\gamma'}{\gamma}\right)^{1+A} \left(\frac{\frac{2}{\pi} - \gamma}{\frac{2}{\pi} - \gamma'}\right)^A.$$

For the proof we will quantify the fact that eigenfunctions live essentially in a bounded region of momentum space.

**Lemma 2.** *For all  $\gamma \in (0, 2/\pi)$  and all eigenfunctions  $\psi$  of  $\sqrt{p^2 + 1} - 1 - \gamma/|x|$*

$$(20) \quad \left\langle \psi, \left(\sqrt{p^2 + 1} - 1\right) \psi \right\rangle \leq \frac{\frac{2}{\pi} A}{\frac{2}{\pi} - \gamma} \left\langle \psi, \left(1 - (p^2 + 1)^{-1/2}\right) \psi \right\rangle.$$

*Proof.* Let  $\psi_> = \mathbb{1}_{\{|p|>1\}} \psi$  and  $\psi_< = \mathbb{1}_{\{|p|\leq 1\}} \psi$ . Then

$$\left\langle \psi, \left(\sqrt{p^2 + 1} - 1\right) \psi \right\rangle = \left\langle \psi_<, \left(\sqrt{p^2 + 1} - 1\right) \psi_< \right\rangle + \left\langle \psi_>, \left(\sqrt{p^2 + 1} - 1\right) \psi_> \right\rangle$$

and

$$\left\langle \psi, \left(1 - (p^2 + 1)^{-1/2}\right) \psi \right\rangle = \left\langle \psi_<, \left(1 - (p^2 + 1)^{-1/2}\right) \psi_< \right\rangle + \left\langle \psi_>, \left(1 - (p^2 + 1)^{-1/2}\right) \psi_> \right\rangle.$$

We have

$$\left\langle \psi_<, \left(\sqrt{p^2 + 1} - 1\right) \psi_< \right\rangle \leq \sqrt{2} \left\langle \psi_<, \left(1 - (p^2 + 1)^{-1/2}\right) \psi_< \right\rangle,$$

since  $\sup_{0 \leq e \leq 1} (\sqrt{e+1} - 1)(1 - 1/\sqrt{e+1})^{-1} = \sup_{0 \leq e \leq 1} \sqrt{e+1} = \sqrt{2}$ .

Moreover, by Kato's inequality,

$$\left\langle \psi_>, \left(\sqrt{p^2 + 1} - 1\right) \psi_> \right\rangle \leq \langle \psi_>, |p| \psi_> \rangle \leq \frac{2/\pi}{2/\pi - \gamma} \langle \psi_>, (|p| - \gamma|x|^{-1}) \psi_> \rangle.$$

Now using the eigenvalue equation for  $\psi$  we obtain

$$\begin{aligned} \left\langle \psi_>, (|p| - \gamma|x|^{-1}) \psi_> \right\rangle &= \left\langle \psi_>, (|p| - \gamma|x|^{-1}) \psi \right\rangle + \gamma \left\langle \psi_>, |x|^{-1} \psi_< \right\rangle \\ &= \left\langle \psi_>, \left(E + |p| - \sqrt{p^2 + 1} + 1\right) \psi \right\rangle + \gamma \left\langle \psi_>, |x|^{-1} \psi_< \right\rangle \\ &= \left\langle \psi_>, \left(E + |p| - \sqrt{p^2 + 1} + 1\right) \psi_> \right\rangle + \gamma \left\langle \psi_>, |x|^{-1} \psi_< \right\rangle \\ &\leq 2 \left\langle \psi_>, \left(1 - (p^2 + 1)^{-1/2}\right) \psi_> \right\rangle + \gamma \left\langle \psi_>, |x|^{-1} \psi_< \right\rangle. \end{aligned}$$

In the last inequality we used  $E \leq 0$  (which was shown by Herbst [5, Theorem 2.2]) and  $\sup_{e \geq 1} (\sqrt{e} - \sqrt{e+1} + 1)(1 - 1/\sqrt{e+1})^{-1} = 2$ .

Moreover, by Hardy's inequality

$$\langle \psi_>, |x|^{-1} \psi_< \rangle \leq \|\psi_>\| \| |x|^{-1} \psi_< \| \leq 2 \|\psi_>\| \| |p| \psi_< \| \leq \|\psi_>\|^2 + \| |p| \psi_< \|^2.$$

Since

$$\|\psi_>\|^2 \leq \frac{1}{1 - 1/\sqrt{2}} \langle \psi_>, (1 - (p^2 + 1)^{-1/2}) \psi_> \rangle$$

and

$$\| |p| \psi_< \|^2 \leq \frac{1}{1 - 1/\sqrt{2}} \langle \psi_<, (1 - (p^2 + 1)^{-1/2}) \psi_< \rangle,$$

we can now collect terms and get

$$\begin{aligned} \langle \psi, (\sqrt{p^2 + 1} - 1) \psi \rangle &\leq \left( \sqrt{2} + \frac{\sqrt{2} \frac{2}{\pi} \gamma}{(\sqrt{2} - 1)(\frac{2}{\pi} - \gamma)} \right) \langle \psi_<, (1 - (p^2 + 1)^{-1/2}) \psi_< \rangle \\ (21) \quad &+ \frac{\frac{2}{\pi}}{\frac{2}{\pi} - \gamma} \left( 2 + \frac{\sqrt{2} \gamma}{\sqrt{2} - 1} \right) \langle \psi_>, (1 - (p^2 + 1)^{-1/2}) \psi_> \rangle \\ &\leq \frac{\frac{2}{\pi}}{\frac{2}{\pi} - \gamma} \left( 2 + \frac{\sqrt{2} \gamma}{\sqrt{2} - 1} \right) \langle \psi, (1 - (p^2 + 1)^{-1/2}) \psi \rangle \end{aligned}$$

which gives the desired bound, since  $\gamma < 2/\pi$ .  $\square$

**Corollary 1.** *Let  $\gamma \in (0, 2/\pi)$  and  $A$  be the constant of the previous lemma. Then, for any normalized eigenfunction  $\psi$  of  $\sqrt{p^2 + 1} - 1 - \gamma/|x|$  with eigenvalue  $E$*

$$(22) \quad \langle \psi, \frac{\gamma}{|x|} \psi \rangle \leq \left( \frac{\frac{2}{\pi} A}{\frac{2}{\pi} - \gamma} + 1 \right) |E|.$$

*Proof.* With the abbreviation  $D := \frac{2}{\pi} A (\frac{2}{\pi} - \gamma)^{-1}$  we write the inequality in the previous lemma in the form

$$(23) \quad \left\langle \psi, \frac{p^2}{\sqrt{p^2 + 1}} \psi \right\rangle \geq (1 + D^{-1}) \langle \psi, (\sqrt{p^2 + 1} - 1) \psi \rangle.$$

By the virial theorem (Herbst [5, Theorem 2.4]) the left sides of (22) and (23) are equal. Thus,

$$\begin{aligned} \langle \psi, \gamma |x|^{-1} \psi \rangle &= (D + 1) \langle \psi, \gamma |x|^{-1} \psi \rangle - D \left\langle \psi, \frac{p^2}{\sqrt{p^2 + 1}} \psi \right\rangle \\ &\leq (D + 1) \langle \psi, \gamma |x|^{-1} \psi \rangle - D(1 + D^{-1}) \langle \psi, (\sqrt{p^2 + 1} - 1) \psi \rangle \\ &= - (D + 1) \langle \psi, (\sqrt{p^2 + 1} - 1 - \gamma |x|^{-1}) \psi \rangle = - (D + 1) E \end{aligned}$$

as claimed.  $\square$

We are now in position to give the

*Proof of Proposition 2.* By the variational principle, for any  $n \in \mathbb{N}_0$  the function  $\kappa \mapsto e_n(\sqrt{p^2 + 1} - 1 - \kappa|x|^{-1})$  is Lipschitz and therefore differentiable almost everywhere. By perturbation theory, at every point where its derivative exists, it is given by

$$\frac{d}{d\kappa} e_n(\sqrt{p^2 + 1} - 1 - \kappa|x|^{-1}) = -\langle \psi_\kappa, |x|^{-1} \psi_\kappa \rangle,$$

where  $\psi_\kappa$  is a normalized eigenfunction of  $\sqrt{p^2 + 1} - 1 - \kappa|x|^{-1}$  corresponding to the eigenvalue  $e_n(\sqrt{p^2 + 1} - 1 - \kappa|x|^{-1})$ . Thus, by Corollary 1, we have for all  $\kappa \in (0, \gamma']$

$$\frac{d}{d\kappa} e_n(\sqrt{p^2 + 1} - 1 - \kappa|x|^{-1}) \geq \left( \frac{\frac{2}{\pi}A}{\frac{2}{\pi} - \kappa} + 1 \right) \kappa^{-1} e_n(\sqrt{p^2 + 1} - 1 - \kappa|x|^{-1}).$$

Thus,

$$(24) \quad \frac{d}{d\kappa} \log |e_n(\sqrt{p^2 + 1} - 1 - \kappa|x|^{-1})| \leq \frac{A+1}{\kappa} + \frac{A}{\frac{2}{\pi} - \kappa}.$$

Integrating this bound we find for  $\gamma \leq \gamma'$  that

$$\log \frac{|e_n(\sqrt{p^2 + 1} - 1 - \gamma'|x|^{-1})|}{|e_n(\sqrt{p^2 + 1} - 1 - \gamma|x|^{-1})|} \leq (A+1) \log \frac{\gamma'}{\gamma} - A \log \frac{\frac{2}{\pi} - \gamma'}{\frac{2}{\pi} - \gamma},$$

i.e.,

$$e_n(\sqrt{p^2 + 1} - 1 - \gamma'|x|^{-1}) \geq e_n(\sqrt{p^2 + 1} - 1 - \gamma|x|^{-1}) \left( \frac{\gamma'}{\gamma} \right)^{A+1} \left( \frac{\frac{2}{\pi} - \gamma}{\frac{2}{\pi} - \gamma'} \right)^A$$

quod erat demonstrandum.  $\square$

Eventually we can address the

*Proof of Lemma 1.* First let  $0 < \lambda \leq t_0/b$ . Then

$$\sqrt{p_\ell^2 + 1} - 1 - \frac{\gamma}{r} - \lambda U \geq (1 - b\lambda) \left( \sqrt{p_\ell^2 + 1} - 1 - \frac{1 + b\lambda}{1 - b\lambda} \cdot \frac{\gamma}{r} \right)$$

and therefore for all  $n \in \mathbb{N}_0$ ,

$$e_n \left( \sqrt{p_\ell^2 + 1} - 1 - \frac{\gamma}{r} - \lambda U \right) \geq (1 - b\lambda) e_n \left( \sqrt{p_\ell^2 + 1} - 1 - \frac{1 + b\lambda}{1 - b\lambda} \cdot \frac{\gamma}{r} \right).$$

By Proposition 2 with  $\gamma' = \gamma(1 + b\lambda)/(1 - b\lambda)$  (which fulfills  $\gamma < \gamma' \leq \frac{1}{\pi} + \frac{\gamma}{2} < \frac{2}{\pi}$  under our assumptions)

$$\begin{aligned} & e_n \left( \sqrt{p_\ell^2 + 1} - 1 - \frac{1 + b\lambda}{1 - b\lambda} \cdot \frac{\gamma}{r} \right) \\ & \geq e_n \left( \sqrt{p_\ell^2 + 1} - 1 - \frac{\gamma}{r} \right) \cdot \left( \frac{1 + b\lambda}{1 - b\lambda} \right)^{1+A} \left( \frac{\frac{2}{\pi} - \gamma}{\frac{2}{\pi} - \frac{1+b\lambda}{1-b\lambda}\gamma} \right)^A. \end{aligned}$$

Combining the previous two inequalities shows that

$$e_{n,\ell}(\lambda) \geq F_\gamma(\lambda b) e_{n,\ell}(0)$$

and therefore, if  $\lambda \leq t_0/b$ ,

$$\begin{aligned} e_{n,\ell}(\lambda) - e_{n,\ell}(0) &\geq (F_\gamma(\lambda b) - F_\gamma(0)) e_{n,\ell}(0) = \int_0^{\lambda b} F'_\gamma(t) dt e_{n,\ell}(0) \\ &\geq \tilde{M}_\gamma \cdot b \cdot \lambda \cdot e_{n,\ell}(0) \geq -M_\gamma \cdot b \cdot \lambda \cdot \frac{\gamma^2}{(n + \ell + 1)^2}. \end{aligned}$$

In the last inequality we used the lower bound (15).

The case of negative  $\lambda$  is similar.  $\square$

#### ACKNOWLEDGMENTS

The authors warmly thank Barry Simon for his initial contributions and continuing support and interest in the relativistic strong Scott conjecture. They also acknowledge partial support by the U.S. National Science Foundation through grants DMS-1363432 and DMS-1954995 (R.L.F.), by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) through grant SI 348/15-1 (H.S.) and through Germany's Excellence Strategy EXC-2111 390814868 (R.L.F., H.S.). One of us (K.M.) would like to thank the organizers of the program *Density Functionals for Many-Particle Systems: Mathematical Theory and Physical Applications of Effective Equations*, which took place at the Institute for Mathematical Sciences (IMS) at the National University of Singapore (NUS), for their invitation to speak, their kind hospitality, as well as for generous financial support by the Julian Schwinger foundation that made his stay possible.

#### REFERENCES

- [1] Bernhard Baumgartner. The Thomas-Fermi-theory as result of a strong-coupling-limit. *Comm. Math. Phys.*, 47(3):215–219, 1976.
- [2] Rupert L. Frank, Konstantin Merz, Heinz Siedentop, and Barry Simon. Proof of the strong Scott conjecture for Chandrasekhar atoms. *Pure and Applied Functional Analysis*, preprint *arXiv:1907.04894*, In press, 2019.
- [3] Rupert L. Frank, Heinz Siedentop, and Simone Warzel. The ground state energy of heavy atoms: Relativistic lowering of the leading energy correction. *Comm. Math. Phys.*, 278(2):549–566, 2008.
- [4] Rupert L. Frank, Heinz Siedentop, and Simone Warzel. The energy of heavy atoms according to Brown and Ravenhall: the Scott correction. *Doc. Math.*, 14:463–516, 2009.
- [5] Ira W. Herbst. Spectral theory of the operator  $(p^2 + m^2)^{1/2} - Ze^2/r$ . *Comm. Math. Phys.*, 53:285–294, 1977.
- [6] Alexei Iantchenko, Elliott H. Lieb, and Heinz Siedentop. Proof of a conjecture about atomic and molecular cores related to Scott's correction. *J. reine angew. Math.*, 472:177–195, March 1996.
- [7] Tosio Kato. *Perturbation Theory for Linear Operators*, volume 132 of *Grundlehren der mathematischen Wissenschaften*. Springer-Verlag, Berlin, 1 edition, 1966.
- [8] Roger T. Lewis, Heinz Siedentop, and Simeon Vugalter. The essential spectrum of relativistic multi-particle operators. *Annales de l'Institut Henri Poincaré*, 67(1):1–28, 1997.
- [9] Elliott H. Lieb. Thomas-Fermi and related theories of atoms and molecules. *Rev. Mod. Phys.*, 53(4):603–641, October 1981.
- [10] Elliott H. Lieb and Barry Simon. The Thomas-Fermi theory of atoms, molecules and solids. *Advances in Math.*, 23(1):22–116, 1977.
- [11] Gerhart Lüders. Über die Zustandsänderung durch den Meßprozeß. *Ann. Physik (6)*, 8:322–328, 1951.
- [12] Albert Messiah. *Mécanique Quantique*, volume 1. Dunod, Paris, 2 edition, 1969.
- [13] Jan Philip Solovej, Thomas Østergaard Sørensen, and Wolfgang L. Spitzer. The relativistic Scott correction for atoms and molecules. *Commun. Pure Appl. Math.*, 63:39–118, January 2010.



- [14] R. A. Weder. Spectral properties of one-body relativistic spin-zero Hamiltonians. *Ann. Inst. H. Poincaré Sect. A (N.S.)*, 20:211–220, 1974.

MATHEMATISCHES INSTITUT, LUDWIG-MAXIMILANS UNIVERSITÄT MÜNCHEN, THERESIENSTR. 39, 80333 MÜNCHEN, GERMANY, AND MUNICH CENTER FOR QUANTUM SCIENCE AND TECHNOLOGY (MCQST), SCHELLINGSTR. 4, 80799 MÜNCHEN, GERMANY, AND MATHEMATICS 253-37, CALTECH, PASADENA, CA 91125, USA

*E-mail address:* `rlfrank@caltech.edu`

INSTITUT FÜR ANALYSIS UND ALGEBRA, CAROLO-WILHELMINA, UNIVERSITÄTSPLATZ 2, 38106 BRAUNSCHWEIG

*E-mail address:* `k.merz@tu-bs.de`

MATHEMATISCHES INSTITUT, LUDWIG-MAXIMILANS UNIVERSITÄT MÜNCHEN, THERESIENSTR. 39, 80333 MÜNCHEN, GERMANY, AND MUNICH CENTER FOR QUANTUM SCIENCE AND TECHNOLOGY (MCQST), SCHELLINGSTR. 4, 80799 MÜNCHEN, GERMANY

*E-mail address:* `h.s@lmu.de`