Stability of the Relativistic Electron-Positron Field of Atoms in Hartree-Fock Approximation: Heavy Elements [1]

Raymond Brummelhuis, Norbert Röhrl, Heinz Siedentop

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Abstract. We show that the modulus of the Coulomb Dirac operator with a sufficiently small coupling constant bounds the modulus of the free Dirac operator from above up to a multiplicative constant depending on the product of the nuclear charge and the electronic charge. This bound sharpens a result of Bach et al [2] and allows to prove the positivity of the relativistic electron-positron field of an atom in Hartree-Fock approximation for all elements occurring in nature.

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1. Introduction

A complete formulation of quantum electrodynamics has been an elusive topic to this very day. In the absence of a mathematically and physically complete model various approximate models have been studied. A particular model which is of interest in atomic physics and quantum chemistry is the the electron-positron field (see, e.g., Chaix et al [4, 5]). The Hamiltonian of the electron-positron field in the Furry picture is given by

$$\mathbb{H} := \int d^3x : \Psi^*(x) D_{g,m} \Psi(x) : + \frac{\alpha}{2} \int d^3x \int d^3y \frac{: \Psi^*(x)\Psi(y)^*\Psi(y)\Psi(x) :}{|\mathbf{x}-\mathbf{y}|},$$

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where the normal ordering and the definition of the meaning of electrons and positrons is given by the splitting of $L^2(\mathbb{R}^2)\otimes\mathbb{C}^4$ into the positive and negative spectral subspaces of the atomic Dirac operator

$$D_{g,m} = \frac{1}{i}\boldsymbol{\alpha}\cdot\nabla + m\beta - \frac{g}{|\mathbf{x}|}.$$

This model agrees up to the complete normal ordering of the interaction energy and the omission of all magnetic field terms with the standard Hamiltonian as found, e.g., in the textbook of Bjorken and Drell [3, (15.28)]. (Note that we freely use the notation of Thaller [8], Helffer and Siedentop [6], and Bach et al [2].)
From a mathematical point of view the model has been studied in a series of papers [2, 1, 7]. The first paper is of most interest to us. There it is shown that the energy $\mathcal{E}(\rho) := \rho(\mathbb{H})$ is nonnegative, if ρ is a generalized Hartree-Fock state provided that the fine structure constant $\alpha := e^2$ is taken to be its physical value $1/137$ and the atomic number Z does not exceed 68 (see Bach et al [2, Theorem 2]). This pioneering result is not quite satisfying from a physical point of view, since it does not allow for all occurring elements in nature, in particular not for the heavy elements for which relativistic mechanics ought to be most important. The main result of the present paper is

Theorem 1. *The energy $\mathcal{E}(\rho)$ is nonnegative in Hartree-Fock states ρ, if $\alpha \leq (4/\pi)(1-g^2)^{1/2}(\sqrt{4g^2+9}-4g)/3$.*

We use g instead of the nuclear number $Z = g/\alpha$ as the parameter for the strength of the Coulomb potential because this is the mathematically more natural choice. For the physical value of $\alpha \approx 1/137$ the latter condition is satisfied, if the atomic number Z does not exceed 117.
Our main technical result to prove Theorem 1 is

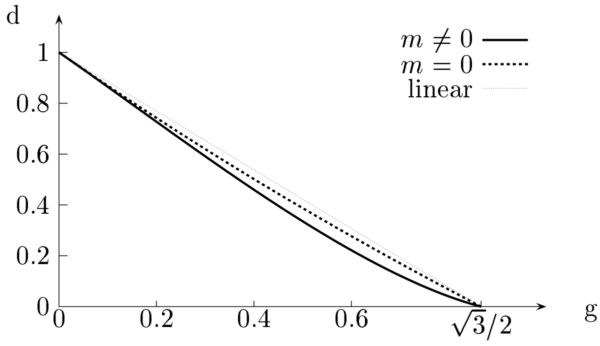
Lemma 1. *Let $g \in [0, \sqrt{3}/2]$ and*

$$d = \begin{cases} \frac{1}{3}(\sqrt{4g^2+9}-4g) & m = 0 \\ \sqrt{1-g^2}\,\frac{1}{3}(\sqrt{4g^2+9}-4g) & m > 0 \end{cases}.$$

Then we have for $m \geq 0$

$$|D_{g,m}| \geq d|D_{0,0}|. \tag{1}$$

The following graph gives an overview of the dependence of d on the coupling constant g



Our paper is organized as follows: in Section 2 we show how Lemma 1 proves our stability result. Section 3 contains the technical heart of our result. Among other things we will prove Theorem 1 in that section. Eventually, Section 4 contains some additional remarks on the optimality of our result.

2. Positivity of the Energy

As mentioned in the introduction, a first – but non-satisfactory result as far as it concerns heavy elements – is due to Bach et al [2]. Their proof consists basically of three steps:
(i) They show that positivity of the energy $\mathcal{E}(\rho)$ in generalized Hartree-Fock states ρ is equivalent to showing positivity of the Hartree-Fock functional

$$\mathcal{E}^{HF} : X \to \mathbb{R},$$
$$\mathcal{E}^{HF}(\gamma) = \mathrm{tr}(D_{g,m}\gamma) + \alpha D(\rho_\gamma, \rho_\gamma) - \frac{\alpha}{2}\int dxdy \frac{|\gamma(x,y)|^2}{|\mathbf{x}-\mathbf{y}|}$$

where $D(f,g) := (1/2)\int_{\mathbb{R}^6} d\mathbf{x}d\mathbf{y}\overline{f(\mathbf{x})}g(\mathbf{y})|\mathbf{x}-\mathbf{y}|^{-1}$ is the Coulomb scalar product, X is the set of trace class operators γ for which $|D_{0,m}|\gamma$ is also trace class and which fulfills $-P_- \leq \gamma \leq P_+$, and $\rho_\gamma(\mathbf{x}) := \sum_{\sigma=1}^4 \gamma(x,x)$. (See [2], Section 3.)
(ii) They show, that the positivity of $\mathcal{E}^{HF}$ follows from the inequality

$$|D_{g,m}| \geq d|D_{g,0}|$$

(Inequality (1)), if $\alpha \leq 4d/\pi$ (see [2], Theorem 2).
(iii) They show this inequality for $d = 1 - 2g$ implying then the positivity of $\mathcal{E}(\rho)$ in Hartree-Fock states ρ, if $\alpha \approx 1/137$ and $Z \leq 68$.
From the first two steps, the proof of Theorem 1 follows using Lemma 1. – Step (iii) indicates that it is essential to improve (1) which we shall accomplish in the next section.

3. Inequality Between Moduli of Dirac Operators

We now start with the main technical task, namely the proof of the key Lemma 1. We will first prove Inequality (1) in the massless case. Then we will roll back the "massive" case to the massless one.
Because there is no easy known way of writing down $|D_{g,0}|$ explicitly, we prove the stronger inequality

$$D_{g,0}^2 \geq d^2 D_{0,0}^2 \tag{2}$$

again following Bach et al [2]. However, those authors proceeded just using the triangular inequality. In fact this a severe step. Instead we shall show (2) with the sharp constant $d^2 = (\sqrt{4g^2+9} - 4g)^2/9$ in the massless case. Since the Coulomb Dirac operator is essentially selfadjoint on $\mathcal{D} := C_0^\infty(\mathbb{R}^3 \setminus \{0\}) \otimes \mathbb{C}^4$ for $g \leq \sqrt{3}/2$, (2) is equivalent to showing

$$\|D_{g,0}f\|_2^2 - d^2\|D_{0,0}f\|_2^2 \geq 0$$

for all $f \in \mathcal{D}$.
Since the Coulomb Dirac operator – and thus also its square – commutes with the total angular momentum operator, we use a partial wave decomposition. The Dirac operator $D_{g,m}$ in channel κ equals to

$$h_{g,m,\kappa} := \begin{pmatrix} m - \frac{g}{r} & -\frac{d}{dr} + \frac{\kappa}{r} \\ \frac{d}{dr} + \frac{\kappa}{r} & -m - \frac{g}{r} \end{pmatrix}.$$

It suffices to show (2) for the squares of $h_{g,0,\kappa}$ and $h_{0,0,\kappa}$ for $\kappa = \pm 1, \pm 2, \ldots$.
Notice that $h_{g,0,\kappa}$ is homogeneous of degree -1 under dilations. Therefore it becomes – up to a shift – a multiplication operator under (unitary) Mellin transform. The unitary Mellin transform $\mathcal{M} : L^2(0,\infty) \to L^2(\mathbb{R}), f \mapsto f^\#$ used here is given by

$$f^\#(s) = \frac{1}{\sqrt{2\pi}} \int_0^\infty r^{-1/2-is} f(r) dr.$$

Unitarity can be seen by considering the isometry

$$\begin{array}{cccc} \iota : & L^2(0,\infty) & \longrightarrow & L^2(-\infty,\infty) \\ & f : r \mapsto f(r) & \mapsto & h : z \mapsto \mathrm{e}^{z/2} f(\mathrm{e}^z) \end{array}.$$

The Mellin transform is just the composition of the Fourier transform and ι. We recall the following two rules for $f^\# = \mathcal{M}(f)$ on smooth functions of compact support in $(0,\infty)$.

$$(r^\alpha f)^\# (s) = f^\#(s + i\alpha)$$

$$\left(\frac{d}{dr} f\right)^\# (s) = (is + \frac{1}{2}) f^\#(s - i)$$

These two rules give

$$\mathcal{M} h_{g,0,\kappa} \begin{pmatrix} f^+ \\ f^- \end{pmatrix} = \begin{pmatrix} -g & -is - \frac{1}{2} + \kappa \\ +is + \frac{1}{2} + \kappa & -g \end{pmatrix} \begin{pmatrix} \mathcal{M}f^+(s - \mathrm{i}) \\ \mathcal{M}f^-(s - \mathrm{i}) \end{pmatrix}.$$

If we denote above matrix by $h^{\mathcal{M}}_{g,0,\kappa}$, we see that (2) is equivalent to

$$(3)\quad (h^{\mathcal{M}}_{g,0,\kappa})^* h^{\mathcal{M}}_{g,0,\kappa} - d^2 (h^{\mathcal{M}}_{0,0,\kappa})^* h^{\mathcal{M}}_{0,0,\kappa} = \begin{pmatrix} g^2 + (1-d^2)(s^2 + (\kappa + \frac{1}{2})^2) & -2(\kappa - is)g \\ -2(\kappa + is)g & g^2 + (1-d^2)(s^2 + (\kappa - \frac{1}{2})^2) \end{pmatrix} \geq 0,$$

where $\kappa = \pm 1, \pm 2, \dots$. This is true if and only if the eigenvalues of the matrix on the left hand side of (3) are nonnegative for all $s \in \mathbb{R}$ and $\kappa = \pm 1, \pm 2, \dots$. The eigenvalues are the solutions of the quadratic polynomial

$$\lambda^2 - 2\lambda\big(g^2 + (1-d^2)(s^2+\kappa^2+\frac{1}{4})\big) + \big(g^2 + (1-d^2)(s^2+\kappa^2+\frac{1}{4})\big)^2 - (1-d^2)^2\kappa^2 - 4g^2(s^2+\kappa^2).$$

Hence the smaller one equals

$$\lambda_1 = g^2 + (1-d^2)(s^2+\kappa^2+\frac{1}{4}) - \sqrt{(1-d^2)^2\kappa^2 + 4g^2(s^2+\kappa^2)}.$$

Here we can already see that d may not exceed 1, and that $d = 1$ is only possible for $g = 0$. It the following we therefore restrict d to the interval $[0, 1)$. At first we look at the necessary condition $\lambda_1(s = 0) \geq 0$. Now,

$$\lambda_1(s=0) = g^2 + (1-d^2)(\kappa^2 + \frac{1}{4}) - |\kappa|\sqrt{(1-d^2)^2 + 4g^2}$$

is positive, if $|\kappa|$ not in between the two numbers

$$\frac{\sqrt{(1-d^2)^2+4g^2} \pm \sqrt{(1-d^2)^2 + 4g^2 - 4(1-d^2)(g^2 + (1-d^2)/4)}}{2(1-d^2)} = \frac{\sqrt{(1-d^2)^2+4g^2} \pm 2gd}{2(1-d^2)}.$$

But since we are only interested in integer $|\kappa| \geq 1$, we want to get the critical interval below 1 (to get the interval above 1 would require $g > \sqrt{3}/2$), i.e.,

$$\frac{\sqrt{(1-d^2)^2+4g^2} + 2gd}{2(1-d^2)} \leq 1,$$

or – equivalently –

$$\sqrt{(1-d^2)^2+4g^2} \leq 2(1-d^2) - 2gd.$$

Since by definition of d we have $g \leq (1-d^2)/d$, the right hand side of above inequality is non-negative. Hence, the above line is equivalent to

$$(4)\qquad 4g^2 + 8dg - 3(1-d^2) \leq 0.$$

Solving (4) for d yields

$$(5)\qquad d \leq 1/6\big(-8g + \sqrt{16g^2+36}\big) = 1/3\left(\sqrt{4g^2+9} - 4g\right).$$

We also need the solution for g:

$$g \leq \frac{1}{2}(\sqrt{3+d^2} - 2d) = \frac{3}{2}\frac{1-d^2}{\sqrt{3+d^2}+2d}. \tag{6}$$

We now compute the derivative

$$\frac{\partial \lambda_1}{\partial s} = 2s[1 - d^2 - 2g^2\big((1-d^2)^2\kappa^2 + 4g^2(s^2+\kappa^2)\big)^{-1/2}].$$

The possible extrema are $s = 0$ and the zeros of $[\dots]$. We will show below that under condition (5) only $s = 0$ is an extremum. It is necessarily a minimum, since $\lambda(s = \pm\infty) = \infty$, which concludes the proof. Now we show $[\dots] > 0$. The expression obviously reaches the smallest value if we choose $\kappa^2 = 1$ and $s = 0$. In this case we get the inequality

$$4g^4 - (1-d^2)^2((1-d^2)^2 + 4g^2) < 0,$$

which implies

$$g^2 < \frac{1+\sqrt{2}}{2}(1-d^2)^2. \tag{7}$$

By the necessary condition (6) we get a sufficient condition for (7) to hold

$$\frac{3}{2}\frac{1-d^2}{\sqrt{3+d^2}+2d} < \sqrt{\frac{1+\sqrt{2}}{2}}(1-d^2).$$

Because $d < 1$ this is equivalent to

$$3 < \sqrt{2}\sqrt{1+\sqrt{2}}(\sqrt{3+d^2}+2d)$$

and the right hand side is bigger than 3 for all d.

Before we proceed to the massive case, we note that we did not loose anything in the above computation, i.e., our value of d^2 is sharp for Inequality (2).

Next, we reduce the massive inequality to the already proven massless one. We have the following relation between the squares of the massive and massless Dirac operator

$$D_{g,m}^2 = D_{g,0}^2 + m^2 - 2m\beta g/|x|.$$

The above operator is obviously positive, but we will show in the following that we only need a fraction of the massless Dirac to control the mass terms.

To implement this idea, we show

$$\epsilon D_{g,0}^2 + m^2 - 2m\beta g/|x| \geq 0, \tag{8}$$

if and only if $\epsilon \geq g^2$.

To show (8), we note that from the known value of the least positive eigenvalue of the Coulomb Dirac operator (see, e.g., Thaller [8]) we have $D_{g,m}^2 \geq m^2(1-g^2)$. Scaling the mass with $1/\epsilon$ and multiplying the equation by ϵ yields

$$\epsilon\frac{m^2(1-g^2)}{\epsilon^2} \leq \epsilon D_{g,m/\epsilon}^2 = \epsilon D_{g,0}^2 + \frac{1}{\epsilon}m^2 - 2m\beta g/|x|.$$

It follows that

$$\epsilon D_{g,0}^2 + m^2 - 2m\beta g/|x| \geq \left(1 - 1/\epsilon + \frac{1-g^2}{\epsilon}\right) m^2 = \left(1 - \frac{g^2}{\epsilon}\right) m^2,$$

showing (8), if $\epsilon \geq g^2$. This is also necessary, since all inequalities in the proof are sharp for f equal to the ground state eigenfunction.
With (8) the massive inequality follows in a single line:

$$D_{g,m}^2 = (1-g^2)D_{g,0}^2 + g^2 D_{g,0}^2 + m^2 - 2m\beta g/|x| \geq (1-g^2)d^2 D_{0,0}^2.$$

4. Supplementary Remarks on the Necessity of the Hypothesis $g < \sqrt{3}/2$

We wish to shed some additional light, on why g in our lemma does not exceed $\sqrt{3}/2$. In this section we will show again that for the "squared" inequality

$$D_{g,m}^2 \geq d^2 D_{0,m}^2 \tag{9}$$

we inevitably get $d^2 \leq 0$ for $g = \sqrt{3}/2$. This is because there are elements of the domain of $D_{\sqrt{3}/2,m}$ whose derivatives are not square integrable. One example is the eigenfunction of the lowest eigenvalue.
For general $g \in [0, \sqrt{3}/2]$ this function is given in channel $\kappa = -1$ as

$$n_g \begin{pmatrix} -g \\ 1-s \end{pmatrix} r^s \mathrm{e}^{-gmr},$$

where $s = \sqrt{1-g^2}$ and n_g is the normalization constant for the L^2-norm. Its derivative is square integrable, if and only if $s > 1/2$ or equivalently $g < \sqrt{3}/2$. To make the argument precise, we compute the L^2-norm of $h_{\sqrt{3}/2,m,-1}\Psi_\beta$ and $h_{0,m,-1}\Psi_\beta$ with $\beta \in (1,2]$, $g = \sqrt{3/2}$, $s = 1/2$, $m' > 0$, and

$$\Psi_\beta := n_\beta \begin{pmatrix} -g \\ -(s-1) \end{pmatrix} r^{\beta s} \mathrm{e}^{-gm'r}$$

with the normalization constant n_β. We will see that as $\beta \to 1$, the first one stays finite and the second one tends to infinity. This only leaves $d^2 \leq 0$ for $g = \sqrt{3}/2$ in (9). The value of m' is not relevant; it is just necessary to take $m \neq m'$ if $m = 0$ to keep Ψ_β square integrable. Now,

$$\begin{aligned} h_{g,m,-1}\Psi_\beta &= n_\beta \begin{pmatrix} -gm + g^2/r + (s-1)\frac{d}{dr} + (s-1)/r \\ -g\frac{d}{dr} + g/r + (s-1)m + (s-1)g/r \end{pmatrix} r^{\beta s} \mathrm{e}^{-gm'r} \\ &= n_\beta \begin{pmatrix} g^2 + (\beta s + 1)(s-1) + r(-gm - (s-1)gm') \\ -g\beta s + g + (s-1)g + r(g^2 m' + (s-1)m) \end{pmatrix} r^{\beta s - 1} \mathrm{e}^{-gm'r}. \end{aligned}$$

Writing the above function as

$$n_\beta \begin{pmatrix} f_1(\beta) + r \cdot h_1 \\ f_2(\beta) + r \cdot h_2 \end{pmatrix} r^{\beta/2 - 1} \mathrm{e}^{-gm'r},$$

we get the following expression for its norm

$$n_\beta^2 \int_0^\infty ((f_1(\beta) + r \cdot h_1)^2 + (f_2(\beta) + r \cdot h_2)^2) r^{\beta-2} \mathrm{e}^{-2gm'r} dr.$$

The potentially unbounded terms are those involving f_i^2. Now, $f_1(\beta) = (1 - \beta)/4$, $f_2(\beta) = (1-\beta)\sqrt{3}/2$, and for $a \in (-1, 0), b > 0$ we have the straight forward inequality

$$\int_0^\infty r^a \mathrm{e}^{-br} dr \le \frac{1}{a+1} + \frac{\mathrm{e}^{-b}}{b}.$$

Hence

$$(1-\beta)^2 \int_0^\infty r^{\beta-2} e^{-2gm'r}\ dr \to 0 \text{ for } \beta \to 1.$$

Proceeding as before we get in the free case

$$\begin{aligned} h_{0,m,-1}\Psi_\beta &= n_\beta \begin{pmatrix} -gm + (s-1)\frac{d}{dr} + (s-1)/r \\ -g\frac{d}{dr} + g/r + (s-1)m \end{pmatrix} r^{\beta s} \mathrm{e}^{-gm'r} \\ &= n_\beta \begin{pmatrix} (\beta s + 1)(s-1) + r(-gm - (s-1)gm') \\ -g\beta s + g + r(g^2 m' + (s-1)m) \end{pmatrix} r^{\beta s - 1} \mathrm{e}^{-gm'r}. \end{aligned}$$

But now the terms that depend on r like $r^{\beta s-1}$ do not vanish for $\beta \to 1$. Therefore the L^2-norm is unbounded.

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Raymond Brummelhuis
Department of Mathematics
Université de Reims
51687 Reims
France
raymond.brummelhuis@univ-reims.fr

Norbert Röhrl
Mathematik, LMU
Theresienstraße 39
80333 München
Germany
ngr@rz.mathematik.uni-muenchen.de

Heinz Siedentop
Mathematik, LMU
Theresienstraße 39
80333 München
Germany
hkh@rz.mathematik.uni-muenchen.de