The Ground State Energy of Relativistic One-Electron Atoms According to Jansen and Hess

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Abstract. Jansen and Heß – correcting an earlier paper of Douglas and Kroll – have derived a (pseudo-)relativistic energy expression which is very successful in describing heavy atoms. It is an approximate no-pair Hamiltonian in the Furry picture. We show that their energy in the one-particle Coulomb case, and thus the resulting self-adjoint Hamiltonian and its spectrum, is bounded from below for $\alpha Z \leq 1.006$.

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1 Introduction

The energy of relativistic electrons in the electric field of a nucleus of charge Ze is described by the Dirac Operator

$$D_\gamma = c\boldsymbol{\alpha} \cdot \frac{\hbar}{i}\nabla + mc^2\beta - \frac{\gamma}{|\mathfrak{x}|} \tag{1}$$

with $\gamma = Ze^2$ and α, β the four Dirac matrices. The constant m is the mass of the electron, c is the velocity of light, and $\hbar$ is the rationalized Planck constant which we both take equal to one by a suitable choice of units. This operator describes both electrons and positrons. In low energy processes as, e.g., in quantum chemistry, there occur, however, only electrons. Brown and Ravenhall [2] proposed to project the positrons out and to use the electronic degrees of freedom only. They originally took the electrons and positrons given by the free Dirac operator D_0. Later it was observed that it might be suitable to define electrons directly by their external field (Furry picture). (See Sucher [17] for a review.) This strategy, however, meets immediate difficulties, since the projection $\chi_{(0,\infty)}(D_\gamma)$ is much harder to find for positive γ than for $\gamma = 0$. To handle this problem Douglas and Kroll [4] used an approximate Foldy-Wouthuysen transform to decouple the positive and negative spectral subspaces of D_γ. Their approximation is perturbative of second order in the coupling constant γ. Jansen and Heß [11] — correcting a sign mistake in [4] — wrote down pseudo-relativistic one- and multi-particle operators to describe the energy which were successfully used to describe heavy relativistic atoms (see, e.g., [12]).

This derivation yields the operator (see [11], Equation (17))

$$H_D^{\mathrm{ext}} = \beta e + E + \frac{1}{2}\left[W, O\right], \tag{2}$$

where

$$\begin{aligned} e(p) &:= \sqrt{\mathfrak{p}^2 + m^2}, && (3)\\ E &:= A(V + RVR)A, && (4)\\ O &:= \beta A[R, V]A, && (5)\\ A(\mathfrak{p}) &:= \left(\frac{e(p)+m}{2e(p)}\right)^{\frac{1}{2}}, && (6)\\ R(\mathfrak{p}) &:= \frac{\alpha\cdot\mathfrak{p}}{e(p)+m}, && (7)\\ W(\mathfrak{p},\mathfrak{p}') &= \beta\frac{O(\mathfrak{p},\mathfrak{p}')}{e(p)+e(p')}. && (8) \end{aligned}$$

(Note that we write p for $|\mathfrak{p}|$.) Here V is the external potential which in the case at hand is the Coulomb potential, and in configuration space it is multiplication by $-\gamma/|\mathfrak{x}|$.

This operator – which acts on four spinors – is then sandwiched by the projection onto the first two components, namely $(1+\beta)/2$. The resulting upper left corner matrix operator $J_\gamma : C_0^\infty(\mathbb{R}^3)\otimes\mathbb{C}^2 \to L^2(\mathbb{R}^3)\otimes\mathbb{C}^2$ is

$$J_\gamma := B_\gamma + \gamma^2\tilde{K} = e - (\gamma/(2\pi^2))K + \gamma^2\tilde{K}. \tag{9}$$

with

$$K(\mathfrak{p},\mathfrak{p}') = \frac{(e(p)+m)(e(p')+m) + (\mathfrak{p}\cdot\boldsymbol{\sigma})(\mathfrak{p}'\cdot\boldsymbol{\sigma})}{n(p)|\mathfrak{p}-\mathfrak{p}'|^2 n(p')} \tag{10}$$

where $n(p) := (2e(p)(e(p)+m))^{1/2}$, i.e., B_γ is the Brown-Ravenhall operator [2]. (See also Bethe and Salpeter[1] and Evans et al. [5]).

The last summand in (9) is given by the kernel

$$\tilde{K}(\mathfrak{p},\mathfrak{p}') = -\frac{1}{2}\int d\mathfrak{p}''[W(\mathfrak{p},\mathfrak{p}'')P(\mathfrak{p}'',\mathfrak{p}') + P(\mathfrak{p},\mathfrak{p}'')W(\mathfrak{p}'',\mathfrak{p}')] \tag{11}$$

with

$$P(\mathfrak{p},\mathfrak{p}') = \frac{\boldsymbol{\sigma}\cdot\mathfrak{p}(e(p')+m) - (e(p)+m)\boldsymbol{\sigma}\cdot\ gp'}{2\pi^2 n(p)|\mathfrak{p}-\mathfrak{p}'|^2 n(p')} \tag{12}$$

and

$$W(\mathfrak{p},\mathfrak{p}') = \frac{P(\mathfrak{p},\mathfrak{p}')}{e(p)+e(p')}. \tag{13}$$

Introducing $b(p) := p/n(p)$ and $a(p) := ((e(p)+m)/2e(p))^{1/2}$ we get more explicitly

$$\begin{aligned}
&\tilde{K}(\mathfrak{p},\mathfrak{p}') \\
&\quad = \frac{1}{2(2\pi^2)^2}\int d\mathfrak{p}'' \frac{1}{|\mathfrak{p}-\mathfrak{p}''|^2|\mathfrak{p}''-\mathfrak{p}'|^2}\left(\frac{1}{e(p)+e(p'')}+\frac{1}{e(p'')+e(p')}\right) \\
&\quad \big[\,(\omega_{\mathfrak{p}}\cdot\boldsymbol{\sigma})\,(\omega_{\mathfrak{p}'}\cdot\boldsymbol{\sigma})\,b(p)a(p'')^2 b(p') - (\omega_{\mathfrak{p}}\cdot\boldsymbol{\sigma})\,(\omega_{\mathfrak{p}''}\cdot\boldsymbol{\sigma})\,b(p)b(p'')a(p'')a(p') \\
&\qquad + a(p)b(p'')^2 a(p') - (\omega_{\mathfrak{p}''}\cdot\boldsymbol{\sigma})\,(\omega_{\mathfrak{p}'}\cdot\boldsymbol{\sigma})\,a(p)b(p'')a(p'')b(p')\big].
\end{aligned} \tag{14}$$

(For later use we name the expression in the first line of the integrand in (14) C and the four terms in the square bracket $T_1, ..., T_4$.)
The corresponding energy in a state $u \in C_0^\infty(\mathbb{R}^3)\otimes\mathbb{C}^2$ is

$$\mathcal{J}(u) := (u, J_\gamma u) = \mathcal{B}(u) + \gamma^2(u, \tilde{K}u) \tag{15}$$

with

$$\mathcal{B}(u) = \int_{\mathbb{R}^3} d\mathfrak{p}\, e(p)|u(\mathfrak{p})|^2 - \frac{\gamma}{2\pi^2}\int_{\mathbb{R}^3} d\mathfrak{p}\int_{\mathbb{R}^3} d\mathfrak{p}' u(\mathfrak{p})^* K(\mathfrak{p},\mathfrak{p}')u(\mathfrak{p}') \tag{16}$$

It is the quadratic form $\mathcal{J}$ which is our prime interest.
Throughout the paper we will use the following constants $\gamma_c := 4\pi(\pi^2+4-\sqrt{-\pi^4+24\pi^2-16})/(\pi^2-4)^2)$, $\gamma_c^B := 2/(\pi/2+2/\pi)$, and $d_\gamma := 1-\gamma-4\sqrt{2}(3+\sqrt{2})\gamma^2$. Our goal is to show

Theorem 1. *For all nonnegative masses m the following holds:*

1. *If $\gamma \in [0,\gamma_c]$ then $\mathcal{J}$ is bounded from bellow, i.e., there exist a constant $c \in \mathbb{R}$ such that for all $u \in C_0^\infty(\mathbb{R}^3)\otimes\mathbb{C}^2$*

$$\mathcal{J}(u) \geq -cm\|u\|^2.$$

2. *If $\gamma > \gamma_c$, then $\mathcal{J}(u)$ is unbounded from below.*
3. *If $\gamma \in [0,\gamma_c^B]$ then*

$$\mathcal{J}(u) \geq d_\gamma m\|u\|^2.$$

Note that $\gamma_c \approx 1.006077340$. Because $\gamma = \alpha Z$ where α is the Sommerfeld fine structure constant which has the physical value of about $1/137$ and Z is the atomic number, this allows for the treatment of all known elements.

It also means that the method is applicable for all αZ where the Coulomb-Dirac operator can be defined in a natural way through form methods (Nenciu [15]). — Note, in particular, that the energy is bounded from below, even if $\gamma_c > \gamma > 1$ although the perturbative derivation of the symmetric operator $H_D^{\rm ext}$ is questionable in this case.
We would like to remark that the lower bound can most likely be improved for positive masses. In fact, we conjecture that the energy is positive for all sub-critical γ. However, this is outside the scope of this work.
According to Friedrichs our theorem has the following immediate consequence:

Corollary 1. *The symmetric operator J_γ has a unique self-adjoint extension whose form domain contains $C_0^\infty(\mathbb{R}^3)\otimes\mathbb{C}^2$ for $\gamma\in[0,\gamma_c]$.*

In fact for $\gamma < \gamma_c$, since the potential turns out to be form bounded with relative bound less than one, the self-adjoint operator defined has form domain $H^{1/2}(\mathbb{R}^3)\otimes\mathbb{C}^2$.
The structure of the paper is as follow: in Section 2 using spherical symmetry we decompose the operator in angular momentum channels. In Section 3 we prove the positivity of the massless operators. Since these operators are homogeneous under dilation an obvious tool to use is the Mellin transform, a method that previously has been used with success to obtain tight estimates on critical coupling constant (see, e.g., [3]). In Section 4 we find that the difference between the massless and the massive operator is bounded. Finally, some useful identities are given in the Appendix.

2 Partial Wave Analysis of the Energy

To obtain a sharp estimate for the potential energy we decompose the operator as direct sum on invariant subspaces. Because of the rotational symmetry of the problem one might suspect that the angular momenta are conserved quantities. Indeed, as a somewhat lengthy calculation shows, the total angular momentum $\mathfrak{J}=\frac{1}{2}(\mathfrak{x}\times\mathfrak{p}+\boldsymbol{\sigma})$ commutes with $H^{\rm ext}$. In fact we can largely follow a strategy carried out by Hardekopf and Sucher [9] and Evans et al. [5] in somewhat simpler contexts.
We begin by observing that those of the spherical spinors

$$\Omega_{l,m,s}(\omega) := \begin{cases} \begin{pmatrix} \sqrt{\frac{l+s+m}{2(l+s)}}Y_{l,m-\frac{1}{2}}(\omega)\\ \sqrt{\frac{l+s-m}{2(l+s)}}Y_{l,m+\frac{1}{2}}(\omega)\end{pmatrix} & s=\frac{1}{2}\\ \begin{pmatrix} -\sqrt{\frac{l+s-m+1}{2(l+s)+2}}Y_{l,m-\frac{1}{2}}(\omega)\\ \sqrt{\frac{l+s+m+1}{2(l+s)+2}}Y_{l,m+\frac{1}{2}}(\omega)\end{pmatrix} & s=-\frac{1}{2}\end{cases} \tag{17}$$

with $l=0,1,2,...$ and $m=-l-\frac{1}{2},...,l+\frac{1}{2}$, that do not vanish, form an orthonormal basis of $L^2(S^2)\otimes\mathbb{C}^2$. Here $Y_{l,k}$ are normalized spherical harmonics on the unit sphere S^2 (see, e.g., [14], p. 421) with the convention that $Y_{l,k} = 0$, if $|k| > l$. We denote the corresponding index set by I, i.e., $I := \{(l,m,s) | l \in \mathbb{N}_0, m = -l - \frac{1}{2}, ..., l + \frac{1}{2}, s = \pm\frac{1}{2}, \Omega_{l,m,s} \neq 0\}$. Thus any $u \in L^2(\mathbb{R}^3) \otimes \mathbb{C}^2$ can be written as

$$u(\mathfrak{p}) = \sum_{(l,m,s)\in I} p^{-1} f_{l,m,s}(p) \Omega_{l,m,s}(\omega_{\mathfrak{p}}) \tag{18}$$

where $p = |\mathfrak{p}|$, $\omega_{\mathfrak{p}} = \mathfrak{p}/p$, and

$$\sum_{(l,m,s)\in I} \int_0^\infty |f_{l,m,s}(p)|^2 dp = \int_{\mathbb{R}^3} |u(\mathfrak{p})|^2 d\mathfrak{p}.$$

We now remind the reader that the expansion of the Coulomb potential in spherical harmonics is given by

$$\frac{1}{|\mathfrak{p} - \mathfrak{p}'|^2} = \frac{2\pi}{pp'} \sum_{l=0}^{\infty} \sum_{m=-l}^{l} q_l(p/p') Y_{l,m}(\omega_{\mathfrak{p}}) \overline{Y}_{l,m}(\omega_{\mathfrak{p}'}) \tag{19}$$

where $q_l(x) := Q_l((x + 1/x)/2)$; Q_l are Legendre functions of the second kind, i.e.,

$$Q_l(z) = \tfrac{1}{2} \int_{-1}^{1} \tfrac{P_l(t)}{z-t} dt \tag{20}$$

where the P_l are Legendre polynomials. [See Stegun [16] for the notation and some properties of these special functions.]
Inserting the expansion (18) and (19) into (15) yields

$$\mathcal{J}(u) = \sum_{(l,m,s)\in I} \mathcal{J}_{l,s}(f_{l,m,s})$$

with

$$\begin{aligned}\mathcal{J}_{l,s}(f) := \int_0^\infty e(p)|f(p)|^2 dp - \frac{\gamma}{\pi} \int_0^\infty \int_0^\infty \overline{f(p)} k_{l,s}(p,p') f(p) dp dp' \\ + \gamma^2 \int_0^\infty dp \int_0^\infty dp' \overline{f(p)} \tilde{k}_{l,s}(p,p') f(p')\end{aligned} \tag{21}$$

and

$$k_{l,s}(p',p) = \frac{(e(p') + m) q_l(\frac{p'}{p})(e(p) + m) + p' q_{l+2s}(\frac{p'}{p}) p}{n(p') n(p)} \tag{22}$$

and

$$\begin{aligned}\tilde{k}_{l,s}(p,p') = \frac{1}{2\pi^2} \int_0^\infty dp'' \left(\frac{1}{e(p) + e(p'')} + \frac{1}{e(p'') + e(p')} \right) \\ \Big[q_{l+2s}(\frac{p}{p''}) q_{l+2s}(\frac{p'}{p''}) b(p) a(p'')^2 b(p') - q_{l+2s}(\frac{p}{p''}) q_l(\frac{p''}{p'}) b(p) b(p'') a(p'') a(p') \\ + q_l(\frac{p}{p''}) q_l(\frac{p'}{p''}) a(p) b(p'')^2 a(p') - q_l(\frac{p}{p''}) q_{l+2s}(\frac{p''}{p'}) a(p) b(p'') a(p'') b(p') \Big].\end{aligned} \tag{23}$$

The Legendre functions of the second kind appear here for exactly the same reasons as in the treatment of the Schrödinger equation for the hydrogen atom in momentum space (Flügge [6], Problem 77).] To obtain (21), we also use that $(\omega_\mathfrak{p}\cdot\boldsymbol{\sigma})\Omega_{l,m,s}(\omega_\mathfrak{p}) = -\Omega_{l+2s,m,-s}(\omega_\mathfrak{p})$ (see, e.g., Greiner [8], p. 171, (12)). The operators $h_{l,s}$ defined by the sesquilinear form (21) via the equation $(f, h_{l,s}f) = \mathcal{J}_{l,s}(f)$ are reducing the operator H^{ext} on the corresponding angular momentum subspaces.

3 The Massless Operators and Their Positivity

To proceed, we will first consider the massless operators. The lower bound in the massive case will be a corollary of the positivity of the massless one. The energy in angular momentum channel (l,m,s) in the massless case can be read of from (14) and is given by

$$\mathcal{J}_{l,s}(f) := \mathcal{B}_{l,s}(f) + \gamma^2 \int_0^\infty dp \int_0^\infty dp' \overline{f(p)} \tilde{k}_{l,s}(p,p') f(p') \tag{24}$$

with

$$\begin{aligned}&\mathcal{B}_{l,s}(f)\\ &= \int_0^\infty p|f(p)|^2 dp - \frac{\gamma}{2\pi}\int_0^\infty dp \int_0^\infty dp' \overline{f(p)} \left(q_l(\frac{p}{p'}) + q_{l+2s}(\frac{p}{p'})\right) f(p')\end{aligned} \tag{25}$$

and

$$\begin{aligned}\tilde{k}_{l,s}(p,p') = \frac{1}{8\pi^2}\int_0^\infty dp'' &\left(\frac{1}{p+p''} + \frac{1}{p''+p'}\right)\\ &\Big[q_{l+2s}(\frac{p}{p''}) q_{l+2s}(\frac{p''}{p'}) - q_{l+2s}(\frac{p}{p''}) q_l(\frac{p''}{p'})\\ &\quad + q_l(\frac{p}{p''}) q_l(\frac{p''}{p'}) - q_l(\frac{p}{p''}) q_{l+2s}(\frac{p''}{p'})\Big].\end{aligned} \tag{26}$$

Using the simplifications of Appendix A, Formulae (57) and (59) we get

$$\begin{aligned}\tilde{k}_{l,s}(p,p') = \frac{1}{8\pi^2}\int_0^\infty \frac{dp''}{p''} &\Big(q_l(\frac{p}{p''}) q_l(\frac{p''}{p'}) - q_{l+2s}(\frac{p}{p''}) q_l(\frac{p''}{p'})\\ &- q_l(\frac{p}{p''}) q_{l+2s}(\frac{p''}{p'}) + q_{l+2s}(\frac{p}{p''}) q_{l+2s}(\frac{p''}{p'})\Big).\end{aligned} \tag{27}$$

Since the operator in question is homogeneous of degree minus one we Mellin transform (see Appendix B) the quadratic form $\varepsilon_{l,s}$. If we write this form as a functional $\mathcal{J}^{\#}_{l,s}$ of the Mellin transformed radial functions $f^{\#}$, we get

$$\mathcal{J}^{\#}_{l,s}\left(f^{\#}\right) = \mathcal{B}^{\#}_{l,s}\left(f^{\#}\right) + \frac{1}{2}\left(\frac{\gamma}{2\pi}\right)^2 \int_{-\infty}^{\infty} dt \left| f^{\#}\left(t + i/2\right)\right|^2 F^{\#}(t) \tag{28}$$

where $\mathcal{B}^{\#}_{l,s}$ is the Brown-Ravenhall energy in angular momentum channel (l,s) in Mellin space, i.e.,

$$\mathcal{B}^{\#}_{l,s}(g) := \int_{-\infty}^{\infty} dt\, |g\,(t+i/2)|^2 \left[1 - \frac{\gamma}{2}(V_l(t) + V_{l+2s}(t))\right] \tag{29}$$

with

$$V_l(t) = \sqrt{\frac{2}{\pi}} q_l^{\#}\,(t - i/2) = \frac{1}{2}\left|\frac{\Gamma\left(\frac{l+1-it}{2}\right)}{\Gamma\left(\frac{l+2-it}{2}\right)}\right|^2 \tag{30}$$

(see Tix [19] [note also the factor $\sqrt{2/\pi}$ which is different from Tix's original formula]) and

$$F^{\#}(t) = \sqrt{2\pi}\left(q_l^{\#}(t-i/2) - q_{l+2s}^{\#}(t-i/2)\right)^2. \tag{31}$$

Formulae (29), (30), and (31) are obtained from (24), (25), and (27) using the fact that the occurring integrals can be read as a Mellin convolution which is turned by the Mellin transform into a product (see Appendix B, Formulae (61) and (63)).
Note that V_l is the Coulomb potential after Fourier transform, partial wave analysis, and Mellin transform.

3.1 Positivity of the Brown-Ravenhall Energy

To warm up for the minimization of $\mathcal{J}^{\#}_{l,s}$ we start with $\mathcal{B}^{\#}_{l,s}$ only. To this end we first note

Lemma 1. *We have*

$$V_{l+1}(t) \leq V_{l+1}(0) \leq V_l(0). \tag{32}$$

Note, that this is similar to Lemma 2 in [5].

Proof. First note that $q_0 \geq q_1 \geq q_2 ...$ which follows from the integral representation in [21], Chapter XV, Section 32, p. 334. This implies

$$\begin{aligned} \left|q_{l+1}^{\#}(t-i/2)\right| =& \frac{1}{\sqrt{2\pi}}\left|\int_0^\infty q_{l+1}(p)p^{-it}\frac{dp}{p}\right| \leq \frac{1}{\sqrt{2\pi}}\int_0^\infty q_{l+1}(p)\frac{dp}{p} \\ \leq& \frac{1}{\sqrt{2\pi}}\int_0^\infty q_l(p)\frac{dp}{p}, \end{aligned} \tag{33}$$

which implies the lemma. □

Theorem 2. *For all $u \in C_0^\infty(\mathbb{R}^3) \otimes \mathbb{C}^2$ and $m = 0$ we have $\mathcal{B} \geq 0$ if and only if $\gamma \leq \gamma_c^B$.*

Proof. Note that

$$V_l(t) + V_{l+2s}(t) \le V_0(0) + V_1(0) = \frac{\pi}{2} + \frac{2}{\pi}. \tag{34}$$

Thus

$$\mathcal{B}^{\#}_{l,s}(g) \ge \int_{-\infty}^{\infty} dt\, |g\,(t+i/2)|^2 \left(1 - \frac{\gamma}{2}\left(\frac{\pi}{2} + \frac{2}{\pi}\right)\right) \tag{35}$$

which implies that the energy is nonnegative if $\gamma \le 2/(\pi/2 + 2/\pi)$. □

We remark that Theorem 2 was proved by Evans et al. [5]. However, since g can be localized at $t = 0$, our method shows that Inequality (35) is sharp, i.e., the present proof shows also the sharpness of γ_c^B, a result of Hundertmark et al. [10] obtained by different means.
Since — according to Tix [19] — the difference of the massive and massless Brown-Ravenhall operators is bounded, Theorem 2 shows also that the energy in the massive case is bounded from below under the same condition on γ as in the massless case.

3.2 The Jansen-Hess Energy

We now wish to treat the full relativistic energy according to Jansen and Heß as given in (28) through (31). From these equations it is obvious that the energy is positive, if the coupling constant γ does not exceed γ_c^B, since the additional energy term is non-negative. However, as can be expected, the critical coupling constant is in fact bigger, i.e. we want to prove Theorem 1 in the massless case.

Lemma 2. *For all $u \in C_0^\infty(\mathbb{R}^3) \otimes \mathbb{C}^2$, $m = 0$, and $\gamma \le \gamma_c$ we have $(u, \mathcal{J}u) \ge 0$. Moreover, if $\gamma > \gamma_c$, then $\mathcal{J}$ is not bounded from bellow.*

Proof. We write the energy density in Mellin space as given in Equations (28) through (31) as

$$j_{l,s}(t) := 1 - \frac{\gamma}{2}(V_l(t) + V_{l+2s}(t)) + \frac{\gamma^2}{8}(V_l(t) - V_{l+2s}(t))^2. \tag{36}$$

As in the case of the Brown-Ravenhall energy we want to show that $j_{l,s}$ attains its minimum for $l = 0$ and $t = 0$.
First we note, that $j_{l,s}(t) = j_{l+2s,-s}(t)$ which means that we can restrict the following to $s = 1/2$, i.e., to $j_{l,1/2}$.
Next we show that it is monotone decreasing in l. For $\gamma \le 4/\pi$ we have

$$\begin{aligned} 0 &\le 1 - \frac{\gamma}{2}V_0(0) \le 1 - \frac{\gamma}{2}V_l(t) \le 1 - \frac{\gamma}{4}V_l(t) - \frac{\gamma}{4}V_{l+2}(t) \\ &\le 1 + \frac{\gamma}{2}V_{l+1}(t) - \frac{\gamma}{4}V_l(t) - \frac{\gamma}{4}V_{l+2}(t) \end{aligned} \tag{37}$$

where use successively (64), (32), Lemma 6 in Appendix C, and the positivity of the V_l. Inequality (37) is – after multiplication by $\gamma((V_l(t) - V_{l+2}(t))/2$ – identical with the desired monotonicity inequality

$$j_{l+1,1/2}(t) \geq j_{l,1/2}(t). \tag{38}$$

For later purposes we note that functions $j_{l,1/2}$ are symmetric about the origin. Next we will show that the energy density has its absolute minimum at the origin: to this end we simply show that the derivative of $j_{0,1/2}$ is nonnegative on the positive axis, if $\gamma \leq 2/(\pi/2 + 2/\pi)$ which is bigger than $4/\pi$. Since

$$|V_0(t) - V_1(t)| \leq \int_0^\infty (q_0(x) - q_1(x))\frac{dx}{x} = V_0(0) - V_1(0) = \frac{\pi}{2} - \frac{2}{\pi}$$

we have

$$-1 + \frac{\gamma}{2}(V_0(t) - V_1(t)) \leq 0 \tag{39}$$

and obviously we have

$$-1 - \frac{\gamma}{2}(V_0(t) - V_1(t)) \leq 0. \tag{40}$$

Thus the derivative of the energy $j_{0,1/2}$ is

$$\begin{aligned} j'_{0,1/2}(t) &= \frac{\gamma}{2}[-V'_0(t) - V'_1(t) + \frac{\gamma}{2}(V_0(t) - V_1(t))(V'_0(t) - V'_1(t))] \\ &= \frac{\gamma}{2}\{V'_0(t)[-1 + \frac{\gamma}{2}(V_0(t) - V_1(t))] + V'_1(t)[-1 - \frac{\gamma}{2}(V_0(t) - V_1(t))]\} \geq 0, \end{aligned} \tag{41}$$

since V_0 and V_1 are symmetrically decreasing about the origin (see Appendix C).

Finally, the polynomial

$$j_{0,1/2}(0) = 1 - \frac{\gamma}{2}\left(\frac{\pi}{2} + \frac{2}{\pi}\right) + \frac{\gamma^2}{8}\left(\frac{\pi}{2} - \frac{2}{\pi}\right)^2$$

is nonnegative for $\gamma \leq \gamma_c$ as defined in the hypothesis. Thus, we have

$$j_{l,s}(t) \geq j_{0,1/2}(0) \geq 0.$$

□

4 Lower Bound on the Energy According to Jansen and Hess

To distinguish the massive and the massless expressions we will indicate in this section the dependence their on the mass m by a superscript m, if it seems appropriate.

The goal of this section is to show Theorem 1 for the massive case. We proceed by enunciating the following lemmata.

Lemma 3 (Tix [18, 20]). *For all* $u \in C_0^\infty(\mathbb{R}^3) \otimes \mathbb{C}^2$,$m \geq 0$, *and* $\gamma \leq \gamma_c^B$ *then*

$$\mathcal{B}(u) \geq m(1-\gamma).$$

Lemma 4 (Tix [19]). *The expression* $|\mathcal{B}^m(u) - \mathcal{B}^0(u)|$ *is bounded for* $u \in C_0^\infty(\mathbb{R}^3) \otimes \mathbb{C}^2$.

Lemma 5. *For all* $m \geq 0$ *and for all* $u \in C_0^\infty(\mathbb{R}^3) \otimes \mathbb{C}^2$ *we have*

$$|\tilde{K}^m(u) - \tilde{K}^0(u)| \leq md\|u\|^2 \tag{42}$$

where $d := \sqrt{2}(12 + 2^{5/2})$.

We note that the first part of Theorem 1 follows from Lemmata 2, 4, and 5. The third part is a consequence of Lemmata 3 and 5.

Proof. First we remark that

$$\sup\{|\mathcal{J}^m(u) - \mathcal{J}^0(u)| \mid \|u\| = 1\} = m \sup\{|\mathcal{J}^1(u) - \mathcal{J}^0(u)| \mid \|u\| = 1\}.$$

Then it is enough to start bounding $|(u, \tilde{K}^1 u) - (u, \tilde{K}^0 u)|$: By the mean value theorem we have

$$|\tilde{K}^1(\mathfrak{p}, \mathfrak{p}') - \tilde{K}^0(\mathfrak{p}, \mathfrak{p}')| \leq \lambda |D(\mu, \mathfrak{p}, \mathfrak{p}')| \tag{43}$$

for some $\mu \in (0, \lambda)$ where $\lambda \in (0,1)$ is a deformation parameter and $D(\mu, \mathfrak{p}, \mathfrak{p}')$ is the derivative of $\tilde{K}^\mu(\mathfrak{p}, \mathfrak{p}')$ with respect to μ. Computing the derivative yields

$$|D(\mu, \mathfrak{p}, \mathfrak{p}')| = \left| \int d\mathfrak{p}'' F(\mu, \mathfrak{p}, \mathfrak{p}'', \mathfrak{p}') \right| \tag{44}$$

with

$$\begin{aligned} &F(\mu, \mathfrak{p}, \mathfrak{p}'', \mathfrak{p}') \\ &\quad := \frac{1}{2(2\pi^2)^2} \left(\frac{\partial C}{\partial \lambda}(T_1 + ... + T_4) + C \frac{\partial (T_1 + ... + T_4)}{\partial \lambda} \right) (\mu, \mathfrak{p}, \mathfrak{p}'', \mathfrak{p}') \end{aligned} \tag{45}$$

where C and $T_1, ..., T_4$ are defined right below (14). Note that $a(p)^2 \leq 1$ and $b(p)^2 \leq 1/2$, i.e., by the definition $T_1, ..., T_4 \leq 1/2$. Furthermore we note that

$$\begin{aligned} \frac{\partial C}{\partial \lambda} = \frac{-\lambda}{E(\mathfrak{p}'')} &\frac{1}{|\mathfrak{p} - \mathfrak{p}''|^2 |\mathfrak{p}'' - \mathfrak{p}'|^2} \\ &\left(\frac{1}{(E(\mathfrak{p}) + E(\mathfrak{p}''))E(\mathfrak{p})} + \frac{1}{(E(\mathfrak{p}'') + E(\mathfrak{p}'))E(\mathfrak{p}')} \right). \end{aligned} \tag{46}$$

First we treat $\frac{\partial C}{\partial \lambda}(T_1 + ... + T_4)$. We get using the above estimates on T_1 through T_4 and (46)

$$\left| \frac{\partial C}{\partial \lambda}(T_1 + ... + T_4)(\mu, \mathfrak{p}, \mathfrak{p}'', \mathfrak{p}') \right| \leq \frac{2}{p''} \frac{1}{|\mathfrak{p} - \mathfrak{p}''|^2 |\mathfrak{p}'' - \mathfrak{p}'|^2} \left(\frac{1}{p + p''} + \frac{1}{p'' + p'} \right) \tag{47}$$

Next we treat $C\frac{\partial(T_1+...+T_4)}{\partial\lambda}$. To this end we note

$$\left|\frac{\partial a}{\partial\lambda}(p)\right| = \frac{p^2}{4E(\mathfrak{p})^3}\sqrt{\frac{2E(\mathfrak{p})}{E(\mathfrak{p})+\lambda}} \leq \frac{\sqrt{2}}{4p} \tag{48}$$

and

$$\left|\frac{\partial b}{\partial\lambda}(p)\right| = p\sqrt{\frac{E(\mathfrak{p})+\lambda}{8E(\mathfrak{p})^5}} \leq \frac{1}{2p}. \tag{49}$$

Thus

$$\begin{aligned}&|C\frac{\partial(T_1+...+T_4)}{\partial\lambda}(\mu,\mathfrak{p},\mathfrak{p}'',\mathfrak{p}')|\\ &\qquad\leq \frac{3}{2^{3/2}}\frac{1}{|\mathfrak{p}-\mathfrak{p}''|^2|\mathfrak{p}''-\mathfrak{p}'|^2}\left(\frac{1}{p+p''}+\frac{1}{p''+p'}\right)\left(\frac{1}{p}+\frac{2}{p''}+\frac{1}{p'}\right).\end{aligned} \tag{50}$$

We now bound the integral operator $\tilde{K}^1 - \tilde{K}^0$ by a multiplication operator: First pick $\alpha \in \mathbb{R}$. Then we have — using the symmetry of $F(\mu,\mathfrak{p},\mathfrak{p}'',\mathfrak{p}')$ in $\mathfrak{p}$ and $\mathfrak{p}'$ for fixed $\mathfrak{p}''$ —

$$\begin{aligned}|(u,(\tilde{K}^1-\tilde{K}^0)u)| &= \left|\int d\mathfrak{p}''\int d\mathfrak{p}\int d\mathfrak{p}' u(\mathfrak{p})^* F(\mu,\mathfrak{p},\mathfrak{p}'',\mathfrak{p}')u(\mathfrak{p}')\right|\\ &\leq \int d\mathfrak{p}''\int d\mathfrak{p}|u(\mathfrak{p})|^2\int d\mathfrak{p}'\left|\frac{p}{p'}\right|^\alpha |F(\mu,\mathfrak{p},\mathfrak{p}'',\mathfrak{p}')|\end{aligned} \tag{51}$$

where we used the Schwarz inequality in the measure $d\mathfrak{p}d\mathfrak{p}'$ in the last step for fixed $\mathfrak{p}''$. Now using the estimates (47) and (50) and collecting similar terms yields

$$\begin{aligned}|(u,(\tilde{K}^1-\tilde{K}^0)u)| \leq \frac{1}{2^{5/2}(2\pi^2)^2}&\int d\mathfrak{p}|u(\mathfrak{p})|^2\int d\mathfrak{p}''\int d\mathfrak{p}'\left|\frac{p}{p'}\right|^\alpha\\ \frac{1}{|\mathfrak{p}-\mathfrak{p}''|^2|\mathfrak{p}''-\mathfrak{p}'|^2}&\left(\frac{1}{p+p''}+\frac{1}{p''+p'}\right)\left(\frac{3}{p}+\frac{2^{\frac{5}{2}}+6}{p''}+\frac{3}{p'}\right)\end{aligned} \tag{52}$$

where we claim the last line to be bounded by $32(12+2^{5/2})\pi^4$, i.e.,

$$|(u,(\tilde{K}^1-\tilde{K}^0)u)| \leq \sqrt{2}\int d\mathfrak{p}|u(\mathfrak{p})|^2(12+2^{5/2}). \tag{53}$$

To show the above bound we break the integral into three parts

$$\begin{aligned}I &:= \int d\mathfrak{p}''\int d\mathfrak{p}'\left(\frac{p}{p'}\right)^\alpha \frac{1}{|\mathfrak{p}-\mathfrak{p}''|^2|\mathfrak{p}''-\mathfrak{p}'|^2}\left(\frac{1}{p+p''}+\frac{1}{p''+p'}\right)\frac{1}{p},\\ I'' &:= \int d\mathfrak{p}''\int d\mathfrak{p}'\left(\frac{p}{p'}\right)^\alpha \frac{1}{|\mathfrak{p}-\mathfrak{p}''|^2|\mathfrak{p}''-\mathfrak{p}'|^2}\left(\frac{1}{p+p''}+\frac{1}{p''+p'}\right)\frac{1}{p''},\\ I' &:= \int d\mathfrak{p}''\int d\mathfrak{p}'\left(\frac{p}{p'}\right)^\alpha \frac{1}{|\mathfrak{p}-\mathfrak{p}''|^2|\mathfrak{p}''-\mathfrak{p}'|^2}\left(\frac{1}{p+p''}+\frac{1}{p''+p'}\right)\frac{1}{p'}.\end{aligned} \tag{54}$$

We will also use the following integral (see [13], p.124)

$$\Upsilon(\beta) := \int_{\mathbb{R}^3} d\mathfrak{p} \frac{1}{|\mathfrak{e}-\mathfrak{p}|^2} \frac{1}{p^\beta} = \pi^2 \frac{\Gamma(\frac{\beta-1}{2})\Gamma(1-\frac{\beta-1}{2})}{\Gamma(2-\frac{\beta}{2})\Gamma(\frac{\beta}{2})}, \tag{55}$$

where $\mathfrak{e}$ is an (arbitrary) unit vector in $\mathbb{R}^3$ and $\beta \in (1,3)$. We observe that each of the integrals in (54) do not depend on the value of p (what becomes evident after substitution of $\mathfrak{p}' \to p\mathfrak{p}'$ and $\mathfrak{p}'' \to p\mathfrak{p}''$). So picking $p = 1$ and doing $\mathfrak{p}' \to p''\mathfrak{p}'$ in each integral in (54) we find

$$\begin{aligned}
I &= \int d\mathfrak{p}'' \int d\mathfrak{p}' \left(\frac{1}{p'p''}\right)^\alpha \frac{1}{|\mathfrak{u}-\mathfrak{p}''|^2|\mathfrak{u}''-\mathfrak{p}'|^2} \left\{\frac{p''}{1+p''} + \frac{1}{1+p'}\right\} \le 2\Upsilon(\alpha)^2,\\
I'' &= \int d\mathfrak{p}'' \int d\mathfrak{p}' \left(\frac{1}{p'p''}\right)^\alpha \frac{1}{|\mathfrak{u}-\mathfrak{p}''|^2|\mathfrak{u}''-\mathfrak{p}'|^2} \left\{\frac{1}{1+p''} + \frac{1}{p''(1+p')}\right\}\\
&\quad \le \Upsilon(\alpha)^2 + \Upsilon(\alpha)\Upsilon(\alpha+1),\\
I' &= \int d\mathfrak{p}'' \int d\mathfrak{p}' \left(\frac{1}{p'p''}\right)^\alpha \frac{1}{|\mathfrak{u}-\mathfrak{p}''|^2|\mathfrak{u}''-\mathfrak{p}'|^2} \left\{\frac{1}{p'(1+p'')} + \frac{1}{p'p''(1+p')}\right\}\\
&\quad \le 2\Upsilon(\alpha+1)^2,
\end{aligned} \tag{56}$$

We choose $\alpha = 3/2$ and using (55) we obtain the same bound for each integral, namely $32\pi^4$. Equation (53) proves Lemma 5 and follows by using the latter bound in (52). □

A Some Useful Integral Identities

Suppose $f(x) = f(1/x)$ and suppose $f(x)/(1+x)$ is integrable on $(0,\infty)$. Then

$$\int_0^\infty \frac{f(x)}{1+x} dx = \int_0^1 \frac{f(x)}{x} dx = \frac{1}{2}\int_0^\infty \frac{f(x)}{x} dx \tag{57}$$

To show (57) we split the first integral

$$\begin{aligned}
\int_0^1 \frac{dx}{x} f(x) \frac{x}{1+x} + \int_1^\infty \frac{dx}{x} f(x) \frac{x}{1+x} &= \int_0^1 \frac{dx}{x} f(x)\\
= \int_0^\infty \frac{dx}{x} f(x) - \int_1^\infty \frac{dx}{x} f(x) &= \int_0^\infty \frac{dx}{x} f(x) - \int_0^1 \frac{dx}{x} f(x).
\end{aligned} \tag{58}$$

where we used the invariance under inversion of f for the first and third equality. Next we wish to simplify the kernel $j_{l,s}$. To this end we use again the abbreviation $q_l(x) := Q_l\left(\frac{1}{2}\left(x+\frac{1}{x}\right)\right)$ as in (26). We claim

$$\begin{aligned} &I(p,p') \\ &:= \int_0^\infty \frac{dp''}{p''}\left(q_l(\frac{p}{p''})q_m(\frac{p''}{p'}) + q_m(\frac{p}{p''})q_l(\frac{p''}{p'})\right)\left(\frac{p''}{p+p''}+\frac{p''}{p''+p'}\right) \\ &= \int_0^\infty \frac{dp''}{p''}\left(q_l(\frac{p}{p''})q_m(\frac{p''}{p'}) + q_m(\frac{p}{p''})q_l(\frac{p''}{p'})\right) \end{aligned} \tag{59}$$

To prove this we take the integral with the complete first factor times the first summand of the second factor –we name I_1– and the integral over the complete first factor times the second summand of the second factor, I_2. In I_1 we substitute $p'' \to pp''$ whereas in I_2 we substitute $p'' \to p'p''$. This yields using (57)

$$\begin{aligned} I(p,p') = I_1 + I_2 = \frac{1}{2}\int_0^\infty \frac{dp''}{p''}\Bigg[q_l\left(p''\right)q_m\left(\frac{p''p}{p'}\right) \\ + q_m(p'')q_l\left(p''\frac{p}{p'}\right) + q_l\left(\frac{p''p'}{p}\right)q_m(p'') + q_m\left(p''\frac{p'}{p}\right)q_l(p'')\Bigg]. \end{aligned} \tag{60}$$

Undoing the substitutions yields the desired result.

B The Mellin Transform

The Mellin transform is a unitary map from $L^2(\mathbb{R}^+)$ to $L^2(\mathbb{R})$ given by the formula

$$f^\#(s) := \frac{1}{\sqrt{2\pi}}\int_0^\infty f(p)p^{-\frac{1}{2}-is}dp.$$

The Mellin convolution of two function f and g is defined as

$$(f \star g)(p) = \int_0^\infty f\left(\frac{p}{q}\right)g(q)\frac{dq}{q}. \tag{61}$$

If $f \in C_0^\infty(\mathbb{R}^+)$, then $f^\#$ extends to an entire function, and we have

$$(p^\alpha f)^\#(s) = f^\#(s+i\alpha). \tag{62}$$

We also have

$$(f \star g)^\#(s) = \sqrt{2\pi} f^\#(s)g^\#(s). \tag{63}$$

Both, (62) and (63), can be verified by direct computation.

C Some Properties Related to the Partial Wave Analysis of the Coulomb potential in Mellin Space

We first remark the follow property on the difference of V_l and V_{l+2}.

Lemma 6. *For $l = 0, 1, 2, ...$ and $t \in \mathbb{R}$ we have $V_{l+2}(t) < V_l(t)$.*

Proof. From the definition of V_l in (30) we see that the claim is equivalent to

$$\left|\frac{\Gamma\left(\frac{l+1-it}{2}\right)}{\Gamma\left(\frac{l+2-it}{2}\right)}\right|^2 > \left|\frac{\Gamma\left(\frac{l+3-it}{2}\right)}{\Gamma\left(\frac{l+4-it}{2}\right)}\right|^2.$$

This, however, can be easily verified using the functional equation $\Gamma(x+1) = x\Gamma(x)$ of the Gamma function in the numerator and denominator of the right hand side with $x = (l+1-it)/2$ and $x = (l+2-it)/2$. $\square$

From the definition of the V_l and from Formulae 8.332.2 and 8.333.3 in [7] one finds V_0 and V_1 in terms of the hyperbolic tangent and cotangent:

$$V_0(t) = \frac{\mathfrak{Tg}(\pi t/2)}{t} \tag{64}$$

$$V_1(t) = \frac{t}{1+t^2}\mathfrak{Ctg}(\pi t/2). \tag{65}$$

Moreover, both of these functions are decreasing symmetricly about the origin.

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References

[1] Hans A. Bethe and Edwin E. Salpeter. Quantum mechanics of one- and two-electron atoms. In S. Flügge, editor, *Handbuch der Physik, XXXV*, pages 88–436. Springer, Berlin, 1 edition, 1957.

[2] G. E. Brown and D. G. Ravenhall. On the interaction of two electrons. *Proc. Roy. Soc. London Ser. A.*, 208:552–559, 1951.

[3] Raymond Brummelhuis, Norbert Röhrl, and Heinz Siedentop. Stability of the relativistic electron-positron field of atoms in Hartree-Fock approximation: Heavy elements. *Doc. Math., J. DMV*, 6:1–8, 2001.

[4] Marvin Douglas and Norman M. Kroll. Quantum electrodynamical corrections to the fine structure of helium. *Annals of Physics*, 82:89–155, 1974.

[5] William Desmond Evans, Peter Perry, and Heinz Siedentop. The spectrum of relativistic one-electron atoms according to Bethe and Salpeter. *Commun. Math. Phys.*, 178(3):733–746, July 1996.

[6] Siegfried Flügge. *Practical Quantum Mechanics I*, volume 177 of *Grundlehren der mathematischen Wissenschaften*. Springer-Verlag, Berlin, 1 edition, 1982.

[7] I.S. Gradshteyn and I.M. Ryzhik. *Table of Integrals, Series, and Products*. Academic Press, 4th edition, 1980.

[8] Walter Greiner. *Relativistic Quantum Mechanics*, volume 3 of *Theoretical Physics – Text and Excercise Books*. Springer, Berlin, 1 edition, 1990.

[9] G. Hardekopf and J. Sucher. Relativistic wave equations in momentum space. *Phys. Rev. A*, 30(2):703–711, August 1984.

[10] Dirk Hundertmark, Norbert Röhrl, and Heinz Siedentop. The sharp bound on the stability of the relativistic electron-positron field in Hartree-Fock approximation. *Commun. Math. Phys.*, 211(3):629–642, May 2000.

[11] Georg Jansen and Bernd A. Heß. Revision of the Douglas-Kroll transformation. *Physical Review A*, 39(11):6016–6017, June 1989.

[12] V. Kellö, A. J. Sadlej, and B. A. Hess. Relativistic effects on electric properties of many-electron systems in spin-averaged Douglas-Kroll and Pauli approximations. *Journal of Chemical Physics*, 105(5):1995–2003, August 1996.

[13] Elliott H. Lieb and Michael Loss. *Analysis*. Number 14 in Graduate Studies in Mathematics. American Mathematical Society, Providence, 1 edition, 1996.

[14] Albert Messiah. *Mécanique Quantique*, volume 1. Dunod, Paris, 2 edition, 1969.

[15] G. Nenciu. Self-adjointness and invariance of the essential spectrum for Dirac operators defined as quadratic forms. *Commun. Math. Phys.*, 48:235–247, 1976.

[16] Irene A. Stegun. Legendre functions. In Milton Abramowitz and Irene A. Stegun, editors, *Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables*, chapter 8, pages 331–353. Dover Publications, New York, 1965.

[17] J. Sucher. Foundations of the relativistic theory of many-electron atoms. *Phys. Rev. A*, 22(2):348–362, August 1980.

[18] C. Tix. Lower bound for the ground state energy of the no-pair Hamiltonian. *Phys. Lett. B*, 405(3-4):293–296, 1997.

[19] C. Tix. Self-adjointness and spectral properties of a pseudo-relativistic Hamiltonian due to Brown and Ravenhall. *Preprint*, mp-arc: 97-441, 1997.

[20] C. Tix. Strict positivity of a relativistic Hamiltonian due to Brown and Ravenhall. *Bull. London Math. Soc.*, 30(3):283–290, 1998.

[21] E. T. Whittaker and G. N. Watson. *A Course of Modern Analysis; An Introduction to the General Theory of Infinite Processes and of Analytic Functions, with an Account of the Principal Transcendental Functions.* Cambridge University Press, Cambridge, 4 edition, 1927.

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