STRICT POSITIVITY OF A RELATIVISTIC HAMILTONIAN DUE TO BROWN AND RAVENHALL

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Abstract. We prove that the spectrum of a suitably projected Dirac operator - sometimes called no-pair operator – introduced by Brown and Ravenhall is bounded from below by some positive constant when the nuclear charge is below some critical charge. This bound improves a result obtained recently by Evans et al and disproves a conjecture made by Hardekopf and Sucher.

1. Introduction

Relativistic kinematic of spin–1/2 particles is usually described with the Dirac-Operator. But this operator is unbounded from below and therefore problematic to extend to the multi-particle case. A solution to this problem is – according to Brown and Ravenhall [2] – to consider the operator

$$B := \Lambda_+ \left(D_0 - \frac{e^2 Z}{|\boldsymbol{x}|} \right) \Lambda_+ \tag{1}$$

in the Hilbert space $\mathfrak{H} = \Lambda_+ \left(L^2(\mathbb{R}^3) \otimes \mathbb{C}^4 \right)$ for a relativistic electron in the field of a nucleus, see also [1] and for a more recent review article [15]. Here D_0 is the Dirac operator $D_0 := \sum_{j=1}^3 \boldsymbol{\alpha}_j c \frac{\hbar}{i} \nabla_j + \boldsymbol{\beta} mc^2$. The constants $\hbar$, Planck's constant divided by 2π, the electron mass m, and e, the absolute value of the electron charge, are all positive. As usual we set $\alpha := e^2/(\hbar c)$, the Sommerfeld fine structure constant. The 4×4-matrices $\boldsymbol{\alpha}_j$ and $\boldsymbol{\beta}$ are the four Dirac matrices in standard representation and

$$\Lambda_+ := \chi_{(0,\infty)}(D_0)$$

is the projection on the positive spectral subspace of the free Dirac operator.

The operator (1) and its multi-particle analogon is widely used to describe relativistic effects in atoms and molecules, see, e.g., [7, 8], and in this context called no-pair operator. It appears – usually with different potentials – as a "reduced Salpeter operator" in the description of meson models with fermionic constituents, see, e.g., [11], and attracted recently attention in connection with the "stability of relativistic matter"–question [9].

The first mathematical investigation of the operator (1) was done by Evans et al [3]. They proved that the energy $\mathcal{E}[\psi] := (\psi, B\psi)$ associated with B is bounded from below by $\alpha Z(1/\pi - \pi/4)mc^2$ on the set of normalized rapidly decaying smooth spinors in the electron Hilbert space $\mathfrak{H}$, if the nuclear charge does not exceed the critical charge $Z_c := 2/[(\pi/2 + 2/\pi)\alpha]$. This allows to realize the operator self-adjointly as the Friedrichs extension in $\mathfrak{H}$. Note that this bound is always negative and yields for the physical value of the fine structure constant $\alpha = 1/137$ roughly $-0.42\, mc^2$ for $Z = Z_c$. Earlier Hardekopf and Sucher [5, 6] investigated the operator numerically and claimed that, as for the Dirac equation, the ground state energy vanishes for $Z = Z_c$ [6, p. 2025]. Obviously, there is need to clarify whether the bound of Evans et al can be sharpened and if the operator has a similar structure as the Dirac operator and therefore a vanishing ground state energy. However, here

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we prove that $\mathcal{E}[\psi]$ is *strictly* positive for $Z \le Z_c$ by using a better "trial function" than Evans et al. We expect this bound to be quite good and therefore to be also useful for the test of the accuracy of numerical calculations.

In Section 2 we state the theorem and point out the proof. In the appendices some integrals are calculated and some estimates are given.

2. Positivity of the operator

Theorem 1.

$$\inf_{\substack{\psi\in\mathfrak{H}\cap\left(H^{1/2}(\mathbb{R}^3)\otimes\mathbb{C}^4\right)\\ \|\psi\|=1}} \mathcal{E}[\psi] \ge mc^2\left(1-\alpha Z - 0.002\frac{Z}{Z_c}\right) \tag{2}$$

for $Z \le Z_c$, i.e., the energy of the operator B is strictly positive for nuclear charges below or equal the critical charge.

We remark the following:

- For the critical charge Z_c we obtain roughly 0.09 as a lower bound. This bound is presumably quite sharp for $Z = Z_c$ and rather bad for small Z.
- the kinetic energy of B, i.e., the expectation of D_0 in $\mathfrak{H}$ is equal to $\left(\psi, \sqrt{-c^2\hbar^2\Delta + m^2c^4}\,\psi\right)$. This suggest a similar "trial function" than the one that was used by Raynal et al [13] for the Herbst operator $H = \sqrt{-c^2\hbar^2\Delta+m^2c^4} - e^2Z/|\boldsymbol{x}|$. They obtained excellent upper and lower bounds for the ground state of H by using a local energy criterion, see [16, p. 140], and proved that $H > 0$ for $Z \le 2/(\pi\alpha)$, which is the critical Z for this operator. However, the derivation of the bounds includes some numerical calculations.
- As can be seen from (5) the Herbst operator H with charge $Z/2$ is an upper bound for the operator B with charge Z. This ensures the existence of an eigenvalue by using the bounds given in [10, 13] since $\sigma_{\mathrm{ess}}(B) = [1,\infty)$ [3] but leads to the poor upper bound of about 0.9 for the ground state energy.

Proof. We will follow the basic strategy of Evans et al until (9) which we include here to be self-consistent.

According to [3], elements $\widehat{\psi}$ in $\widehat{\mathfrak{H}}$, the image of $\mathfrak{H}$ under the Fourier transform, can be written as

$$\widehat{\psi}(\boldsymbol{p}) = \frac{1}{N(\boldsymbol{p})}\begin{pmatrix}(E_0+E(\boldsymbol{p}))\,u(\boldsymbol{p})\\ c\boldsymbol{p}\cdot\boldsymbol{\sigma}u(\boldsymbol{p})\end{pmatrix} \tag{3}$$

with $u \in L^2(\mathbb{R}^3)\otimes\mathbb{C}^2$, i.e., a Pauli spinor, $\boldsymbol{\sigma} = (\boldsymbol{\sigma}_1,\boldsymbol{\sigma}_2,\boldsymbol{\sigma}_3)^*$ with the Pauli-matrices $\boldsymbol{\sigma}_j$ and $E(\boldsymbol{p}) := (c^2\boldsymbol{p}^2+m^2c^4)^{1/2}$, $E_0 := E(\boldsymbol{0})$, $N(\boldsymbol{p}) = [2E(\boldsymbol{p})(E(\boldsymbol{p})+E_0)]^{1/2}$. Conversely, any Dirac spinor of the form (3) is in $\widehat{\mathfrak{H}}$. Substituting this expression for ψ turns $(\psi, B\psi)$ into

$$\int_{\mathbb{R}^3} E(\boldsymbol{p})|u(\boldsymbol{p})|^2 d\boldsymbol{p} - \frac{\alpha c Z}{2\pi^2}\int_{\mathbb{R}^6} u(\boldsymbol{p}')^* K(\boldsymbol{p}',\boldsymbol{p}) u(\boldsymbol{p}) d\boldsymbol{p} d\boldsymbol{p}'$$

where K is given by

$$K(\boldsymbol{p}',\boldsymbol{p}) = \frac{(E(\boldsymbol{p}')+E_0)(E(\boldsymbol{p})+E_0) + c^2(\boldsymbol{p}'\cdot\boldsymbol{\sigma})(\boldsymbol{p}\cdot\boldsymbol{\sigma})}{N(\boldsymbol{p}')|\boldsymbol{p}'-\boldsymbol{p}|^2 N(\boldsymbol{p})}. \tag{4}$$

Note that it suffices to prove (2) for $\hbar = m = c = 1$ when $m > 0$ because of scaling. We shall assume this in the following.

From the partial wave analysis of the operator B, see [3], Lemma 1 and its proof, we know that the minimizer of (u, bu) occurs for spinors of the form $u_a(\boldsymbol{p}) =$

$a(|\boldsymbol{p}|)(\sqrt{4\pi}|\boldsymbol{p}|)^{-1}(1,0)^*$ where $a \in L^2(\mathbb{R}_+,(1+p^{1/2})dp)$ and $a(p) \geq 0$ for $p \in \mathbb{R}_+$. We write for the quadratic form in a obtained by taking spinors of this form

$$(5)\quad (a, b_0 a) := (u_a, b u_a) = \int_0^\infty e(p)a(p)^2 dp - \frac{\alpha Z}{2\pi}\int_0^\infty\int_0^\infty a(p')k(p',p)a(p)dpdp'$$

with $n(p) := N(\boldsymbol{p})$, $e(p) := E(\boldsymbol{p})$, $k := k_1 + k_2$ and

$$(6)\qquad k_j(p',p) := \sqrt{1+\frac{(-1)^j}{e(p)}}\, Q_j\left(\frac{p}{2p'}+\frac{p'}{2p}\right)\sqrt{1+\frac{(-1)^j}{e(p')}}.$$

The functions Q_l are Legendre functions of the second kind, i.e., $Q_l(z) = \frac{1}{2}\int_{-1}^1 \frac{P_l(t)}{z-t}dt$ where the P_l are Legendre polynomials (see [14] for the notation).

Introducing functions $h_j(p) > 0$, $j = 0,1$, using the Schwarz inequality and omitting the argument of Q_0 we obtain

$$\begin{aligned}
&\int_0^\infty\int_0^\infty a(p')k_0(p',p)a(p)dpdp' \\
&= \int_0^\infty\int_0^\infty a(p')\sqrt{1+\frac{1}{e(p')}}\sqrt{Q_0}\,\sqrt{\frac{h_0(p)}{h_0(p')}}\sqrt{\frac{h_0(p')}{h_0(p)}}\,\sqrt{Q_0}\; a(p)\sqrt{1+\frac{1}{e(p)}}\,dpdp' \\
&\qquad\qquad \leq \int_0^\infty a(p)^2\left(1+\frac{1}{e(p)}\right)\frac{I[h_0](p)}{h_0(p)}\,dp.
\end{aligned}$$

and similarly

$$\int_0^\infty\int_0^\infty a(p')k_1(p',p)a(p)dpdp' \leq \int_0^\infty a(p)^2\left(1-\frac{1}{e(p)}\right)\frac{I[h_1](p)}{h_1(p)}\,dp$$

with

$$(7)\qquad I[h_j](p) := \int_0^\infty h_j(p')Q_j\left(\frac{p}{2p'}+\frac{p'}{2p}\right)dp'.$$

Putting all together we have the lower bound

$$(8)\qquad (a, b_0 a) \geq \inf_{p\in\mathbb{R}+}\mathcal{E}[h_0,h_1](p)\int_0^\infty a^2(p)\,dp$$

for all functions $h_j(p) > 0$ where

$$(9)\quad \mathcal{E}[h_0,h_1](p) = e(p) - \frac{\alpha Z}{2\pi}\left(\left(1+\frac{1}{e(p)}\right)\frac{I[h_0](p)}{h_0(p)} + \left(1-\frac{1}{e(p)}\right)\frac{I[h_1](p)}{h_1(p)}\right).$$

If we choose $h_j(p)$ to be proportional to the ground state wave function of b_0, (8) becomes an equality and our lower bound would be sharp. To obtain a better bound than Evans et al we have to alter their strategy at this point. They used $h_j(p) = 1/p$ which should be correct for large values of p but is obviously not correct for small values of p. Our choice of h_j is motivated by this asymtotics and from the trial function which was used for the Herbst operator by Raynal et al [13], i.e., our choice of h_j is connected with the Fourier transform of $|\boldsymbol{x}|^{\beta-1}e^{-\mu|\boldsymbol{x}|}$. From

$$(10)\qquad h_{0,\beta,\mu_0}(p) := \Gamma(\beta+1)(\mu_0^2+p^2)^{-(\beta+1)/2}\sin[(\beta+1)\arctan(p/\mu_0)]$$

for $p > 0$ with $\mu_0 > 0$ and $-1 < \beta < 1$ (this ensures $h_0(p) > 0$) we find (see appendix A)

$$(11)\qquad I[h_{0,\beta,\mu_0}](p) = \pi\Gamma(\beta)(\mu_0^2+p^2)^{-\beta/2}\sin\left[\beta\arctan(p/\mu_0)\right].$$

The second "trial function" is chosen to be

$$(12)\qquad h_{1,\beta,\mu_1}(p) := p^{1/2}(\mu_1^2+p^2)^{-(\beta+3/2)/2}\Gamma(3+\beta)\,P_{\beta+1/2}^{-3/2}\left(\frac{\mu_1}{\sqrt{\mu_1^2+p^2}}\right)$$

for $p > 0$ and yields (see appendix A)

$$I[h_{1,\beta,\mu_1}](p) = \pi p^{1/2}(\mu_1^2 + p^2)^{-(\beta+1/2)/2}\Gamma(2+\beta)\, P^{-3/2}_{\beta-1/2}\left(\frac{\mu_1}{\sqrt{\mu_1^2+p^2}}\right). \tag{13}$$

From the integral representation of the associated Legendre functions $P^\mu_\nu(\cos\phi)$ with $\mathrm{Re}(\mu) < 1/2$ and $0 < \phi < \pi$ [4, p. 1002]

$$P^\mu_\nu(\cos\phi) = \sqrt{\frac{2}{\pi}}\frac{\sin^\mu\phi}{\Gamma(1/2-\mu)}\int_0^\phi \frac{\cos[(\nu+1/2)t]\,dt}{(\cos t - \cos\phi)^{\mu+1/2}} \tag{14}$$

we find that $h_{1,\beta,\mu_1}(p) > 0$ at least for $-1 < \beta \le 0$. Collecting all terms gives

(15)

$$\begin{aligned}\mathcal{E}[h_{0,\beta,\mu_0}, h_{1,\beta,\mu_1}](p) = e(p) &- \frac{\alpha Z}{2}\frac{\sqrt{p^2+\mu_0^2}}{\beta}\frac{\sin[\beta\arctan(p/\mu_0)]}{\sin[(\beta+1)\arctan(p/\mu_0)]}\left(1+\frac{1}{e(p)}\right)\\ &- \frac{\alpha Z}{2}\left(1-\frac{1}{e(p)}\right)\frac{\sqrt{p^2+\mu_1^2}}{\beta+2}\frac{P^{-3/2}_{\beta-1/2}\left(\mu_1(p^2+\mu_1^2)^{-1/2}\right)}{P^{-3/2}_{\beta+1/2}\left(\mu_1(p^2+\mu_1^2)^{-1/2}\right)}\end{aligned}$$

and therefore

$$(a, b_0 a) \ge \sup_{\substack{-1<\beta\le 0\\ \mu_0,\mu_1>0}} \inf_{p\in\mathbb{R}+} \mathcal{E}[h_{0,\beta,\mu_0}, h_{1,\beta,\mu_1}](p)\int_0^\infty a^2(p)\,dp. \tag{16}$$

Since we are not able to evaluate (16) in general we choose $\mu_0 = \mu_1 = 1$ and $\beta = 0$ and use (14) to obtain for $\mathcal{E}_Z(p) := \mathcal{E}[h_{0,0,1}, h_{1,0,1}](p)$

$$e(p) - \frac{\alpha Z}{2}\left(\arctan(p)\frac{e(p)}{p}(e(p)+1) + (e(p)-1)\frac{p-\arctan p}{e(p)\arctan p - p/e(p)}\right). \tag{17}$$

But note that the evaluation of the integral (14) is elementary for all β.

The choice of $\beta = 0$ cancels the large momentum terms for $Z = Z_c$ and we find $\lim_{p\to\infty}\mathcal{E}_Z(p) = \pi^{-1}(4\pi^2 + 4\pi - 16 - \pi^3)/(4+\pi^2)$ and $\lim_{p\to 0}\mathcal{E}_Z(p) = 1 - \alpha Z$. The tedious calculations to bound $\mathcal{E}_Z(p)$ for $Z = Z_c$ can be found in appendix B, we obtain

$$\inf_{p\in\mathbb{R}+}\mathcal{E}_{Z_c}(p) = \lim_{p\to 0}\mathcal{E}_{Z_c}(p) - 0.002 = 1 - \alpha Z_c - 0.002. \tag{18}$$

Note that $e(p)$ is a monotone increasing function and from this the bound given in (2) easily follows for all positive Z which are smaller or equal Z_c. $\square$

Appendix A. Calculation of the integrals

Before doing the integration in (11) we remark the following: the inverse Fourier transform of

$$h(p) = \sqrt{\frac{2}{\pi}}\Gamma(\beta+1)p^{-1}(\mu^2+p^2)^{-(\beta+1)/2}\sin[(\beta+1)\arctan(p/\mu)],$$

with $p = |\boldsymbol{p}|$, $\mu > 0$ and $\beta > -2$ is given by

$$\check{h}(r) = \frac{1}{(2\pi)^{3/2}}\int_{\mathbb{R}^3} h(|\boldsymbol{p}|)e^{i\boldsymbol{p}\cdot\boldsymbol{x}}d\boldsymbol{p} = r^{\beta-1}e^{-\mu r} \tag{19}$$

with $r = |\boldsymbol{x}|$. Furthermore, the Fourier transform of $\check{h}(r)/r$ can be written as

$$\begin{aligned}\left(\frac{1}{|\cdot|}\check{h}(|\cdot|)\right)^{\widehat{}}(\boldsymbol{p}) &= \frac{1}{(2\pi)^{3/2}}\left(\widehat{\frac{1}{|\cdot|}} * h(|\cdot|)\right)(\boldsymbol{p})\\ &= \frac{1}{2\pi^2}\int_{\mathbb{R}^3} d\boldsymbol{p}'\frac{h(p')}{|\boldsymbol{p}-\boldsymbol{p}'|^2} = (\pi p)^{-1}\int_0^\infty dp'\, Q_0\left(\frac{p}{2p'}+\frac{p'}{2p}\right)p' h(p'),\end{aligned} \tag{20}$$

where the last equality is obtained by performing the angular integration and the $*$ denotes convolution. If we choose h as in (10) we obtain from (19) and (20) the desired integral (11).

We proceed similarly to find a trial function h_1 for which we are able to calculate $I[h_1]$. Again, we write the Fourier transform of $p^{-1}g(p)Y_{1,0}(\boldsymbol{p}/|\boldsymbol{p}|)$ as a convolution, where g is a function such that the Fourier transform of $gY_{1,0}$ exists and $Y_{1,0}$ is a spherical harmonic:

$$\left[\frac{1}{|\cdot|}g(|\cdot|)Y_{1,0}(\cdot/|\cdot|)\right]^{\widehat{}} = \frac{1}{(2\pi)^{3/2}}\widehat{\frac{1}{|\cdot|}} * [g(|\cdot|)Y_{1,0}(\cdot/|\cdot|)]^{\widehat{}}. \tag{21}$$

Note that the Fourier transform of $gY_{1,0}$ reproduce the spherical harmonic:

$$[g(|\cdot|)Y_{1,0}(\cdot/|\cdot|)]^{\widehat{}}(\boldsymbol{p}) = \mathcal{H}\{g\}(p)Y_{1,0}(\boldsymbol{p}/|\boldsymbol{p}|)$$

with $\mathcal{H}\{g\}(p) = i^{-1}p^{-1/2}\int_0^\infty J_{3/2}(pr)r^{3/2}g(r)\,dr$, see [4, p. 951] for the notation of the Bessel function of the first kind $J_{3/2}$. We get by performing the remaining angular integration in (21)

$$\left[\frac{1}{|\cdot|}g(|\cdot|)Y_{1,0}(\cdot/|\cdot|)\right]^{\widehat{}}(\boldsymbol{p}) = (\pi p)^{-1}Y_{1,0}(\boldsymbol{p}/|\boldsymbol{p}|)\int_0^\infty dp'\,p'\mathcal{H}\{g\}(p')\,Q_1\left(\frac{p}{2p'}+\frac{p'}{2p}\right). \tag{22}$$

From [4, p. 711] we find for $\mu_1 > 0$ and $\beta > -3$

$$\mathcal{H}\{(\cdot)^{\beta-1}e^{-\mu_1\cdot}\}(p) = i^{-1}p^{-1/2}(\mu_1^2+p^2)^{-(\beta+3/2)/2}\Gamma(3+\beta)\,P_{\beta+1/2}^{-3/2}\left(\frac{\mu_1}{\sqrt{\mu_1^2+p^2}}\right). \tag{23}$$

Choosing the trial function as done in (12), we find from (22) and (23) the result (13).

Appendix B. Estimating $\mathcal{E}_{Z_c}(p)$

We begin to estimate $\mathcal{E}_{Z_c}(p)$ from below for $p \geq p_0 := 7$. From $\arctan(p) = \int_0^p (x^2+1)^{-1}dx$, $1-x^2 \leq (x^2+1)^{-1} \leq 1$ and $\arctan(p)+\arctan(1/p) = \pi/2$ we obtain the upper and lower bound $\pi/2 - p^{-1} \leq \arctan(p) \leq \pi/2 - p^{-1} + p^{-3}/3$ for $p > 0$. Furthermore we use the estimates $p + p^{-1}/2 - p^{-3}/8 \leq e(p) \leq p + p^{-1}/2$ and $p/e(p) \leq 1 - p^{-1}/2 + 3p^{-4}/8$. This yields

$$\begin{aligned}\mathcal{E}_{Z_c}(p) \geq p + \frac{1}{2p} - \frac{1}{8p^3} - \frac{\alpha Z_c}{2}\Bigg[&\frac{\pi p}{2} - 1 + \frac{\pi}{2} + \frac{\pi/2-1}{p} + \frac{\pi/4-2/3}{p^2} - \frac{1}{6p^3} + \frac{1}{3p^4} \\ &+ \frac{1}{6p^5} + \frac{p^2 - (\pi/2+1)p + 3/2 + \pi/2 - (\pi/4+1)p^{-1} + p^{-2}/2}{\pi p/2 - 2 + \pi p^{-1}/4 - \pi p^{-3}/16 - p^{-4}/4}\Bigg].\end{aligned}$$

Estimating $\pi p/2 - 2 + \pi p^{-1}/4 - \pi p^{-3}/16 - p^{-4}/4$ from below by $\pi p/2 - 2 + \pi p^{-1}/4 - \pi p_0^{-3}/16 - p_0^{-4}/4$ and observing that this lower bound is still positive for $p \geq p_0$, we can bound all remaining terms of the form p^{-j} for $j \leq -2$ by either p_0^{-j} or by 0. With this procedure $\mathcal{E}_{Z_c}(p)$ is estimated from below by some function $\mathcal{E}_{Z_c,p_0}(p)$. The equation $\mathcal{E}'_{Z_c,p_0}(p) = 0$ is equivalent with solving a polynomial equation of degree four because the highest order of p is canceling. Since $\mathcal{E}'_{Z_c,p_0}(p) = 0$ possesses no solutions for $p \geq p_0$ and $\mathcal{E}'_{Z_c,p_0}(p_0) > 0$, we conclude that $\inf_{p\geq p_0}\mathcal{E}_{Z_c}(p) \geq \inf_{p\geq p_0}\mathcal{E}_{Z_c,p_0}(p) = \mathcal{E}_{Z_c,p_0}(p_0) \geq 0.097$.

Since $\lim_{p\to 0}\mathcal{E}_{Z_c}(p) = 1 - \alpha Z_c < 0.097$, it remains to find the infimum of $\mathcal{E}_{Z_c}(p)$ in the compact interval $[0, p_0]$. But since $\mathcal{E}_{Z_c}(p)$ is a smooth function this can confidently be done on a computer. However, we do not know any algorithm who can find the global minimum of a function even in a bounded region. But the second algorithm of Remes (see [12] for details) leads for $f \in C[a,b]$ to a series of polynomials $P_n^{(j)}$ of degree n which uniformly converge to the minimizing polynomial P_n of degree n of the Chebyshev norm $\|f - p_n\|_\infty$. Here $\|f\|_\infty = \max_{p\in[a,b]} |f(p)|$ and p_n is any polynomial of degree n. We choose $n = 3$, $a = 0$, $b = p_0$ and $f = \mathcal{E}_{Z_c}$ and obtain numerically the minimizer $P_3(p) = 0.09325640 + 0.007174570p - 0.0008136597p^2 + 0.00002323894p^3$ with $\|\mathcal{E}_{Z_c} - P_n\|_\infty \leq 0.001$. From $\min_{p\in[0,7]} P_3(p) = P_3(0)$ we finally get (18).

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