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The Spectrum of Relativistic One-Electron Atoms According to Bethe and Salpeter

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Abstract: Bethe and Salpeter introduced a relativistic equation – different from the Bethe–Salpeter equation – which describes relativistic multi-particle systems. Here we will begin some basic work concerning its mathematical structure. In particular we show self-adjointness of the one-particle operator which will be a consequence of a sharp Sobolev type inequality yielding semi-boundedness of the corresponding sesquilinear form. Moreover we locate the essential spectrum of the operator and show the absence of singular continuous spectrum.

1. Introduction

It is well known that the extension of the Dirac equation to multi-particle systems in analogy with the multi-particle Schrödinger equation is problematic. Already the operator describing two non-interacting electrons in the electric field of a nucleus can be easily seen to have the whole real line as spectrum. The situation does not improve when the interaction between the electrons is taken into account. This trivial but important remark was seemingly made rather late (Brown and Ravenhall [2]) and is known in the physics literature as continuum dissolution.

Bethe and Salpeter [1] proposed an equation that overcomes this difficulty by projecting to the electron subspace only. Note that the Dirac equation really describes two different particles, namely electrons and positrons. Although their intention is clearly to treat the multi-particle problem, it is mathematically interesting to discuss the one-particle operator first, since its properties are basic for the N-body situation. The Hamiltonian B of Bethe and Salpeter – we will henceforth use the term Bethe–Salpeter operator – for an electron of charge $-e$ in the magnetic vector potential $\mathfrak{A}$ and the electric potential φ is

$$B = \Lambda_+ \left(c\boldsymbol{\alpha} \cdot \left(\frac{\hbar}{i} \mathrm{grad} + e\mathfrak{A} \right) + mc^2\beta - e\varphi \right) \Lambda_+ \,, \tag{1}$$

where $\Lambda_+ := \chi_{(0,\infty)}(c\boldsymbol{\alpha}\cdot\frac{\hbar}{i}\mathrm{grad} + mc^2\beta)$ is the projection onto the positive spectral subspace of the free Dirac operator, and $\boldsymbol{\alpha} := (\alpha_1, \alpha_2, \alpha_3)$, and β are the four Dirac matrices, explicitly

$$\boldsymbol{\alpha} = \begin{pmatrix} 0 & \boldsymbol{\sigma} \\ \boldsymbol{\sigma} & 0 \end{pmatrix},$$

$\boldsymbol{\sigma}$ denoting the three Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

and

$$\beta = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}.$$

We note that $\alpha_1, \alpha_2, \alpha_3$, and β anti-commute and yield the unit matrix upon squaring. Furthermore m, the rest mass of the electron, and c, the velocity of light, are positive constants. The underlying Hilbert space is

$$\mathfrak{H} = \Lambda_+(L^2(\mathbb{R}^3) \otimes \mathbb{C}^4).$$

We wish to emphasize that this operator is not to be confused with the operator occurring in the Bethe–Salpeter equation also put forward by Bethe and Salpeter [1], which is intended to describe a similar physical setting.

The operator B and its multi-particle analogue have been rediscovered and discussed under various aspects in the recent physics literature (see, e.g., Sucher [14, 15]); a mathematical discussion, however, has not yet been given. In this paper we take a first step in this direction in the case without magnetic field, i.e., from now on we will assume $\mathfrak{A} = 0$.

It is obvious that B may be self-adjointly realized in this space, when the electric potential is relatively compact with respect to $(-\Delta + 1)^{1/2}$ with domain $\Lambda_+(H^1(\mathbb{R}^3) \otimes \mathbb{C}^4)$. Note that $\Lambda_+(c\boldsymbol{\alpha}\cdot\frac{\hbar}{i}\mathrm{grad} + mc^2\beta)\Lambda_+ = \sqrt{-(\hbar c)^2\Delta + m^2c^4}\,\Lambda_+$ holds. We are, however, interested in the critical potentials $\varphi(\mathfrak{r}) = Ze/|\mathfrak{r}|$. In particular we are interested in finding the largest nuclear charge Z such that the sesquilinear form $(\psi, B\psi)$ for $\psi \in \mathfrak{S} \otimes \mathbb{C}^4$, i.e., the expectation of B in the state ψ, where ψ is a smooth rapidly decaying Dirac spinor, is bounded from below. This will be done in Sect. 2. In Sect. 3 we will locate the essential spectrum of B and show that there is no singular continuous spectrum for Coulomb potentials.

2. The Semi-Boundedness of the Bethe–Salpeter Operator

2.1. Reduction to Pauli Spinors. The eigenvalue equation for the Bethe–Salpeter operator may be reduced from a four-component (Dirac spinor) to a two-component one (Pauli spinor). Although this can be essentially extracted already from [1] we will make it explicit here again for the sake of establishing some notation and the convenience of the reader.

To fix the notation, we denote by

$$(\mathscr{F}f)(\mathfrak{p}) := \int_{\mathbb{R}^3} e^{-i\mathfrak{p}\cdot\mathfrak{r}/\hbar} f(\mathfrak{r})\, d\mathfrak{r}/(2\pi\hbar)^{3/2}$$

the – appropriately normalized – Fourier transform. Since the free Dirac operator becomes the 4×4 matrix multiplication operator

$$D_0 = c\boldsymbol{\alpha} \cdot \mathfrak{p} + mc^2\beta$$

after conjugating with the Fourier transform $\mathscr{F}$, the projection Λ_+ – known as the Casimir projection operator – is easiest expressed in momentum space. It also becomes a matrix multiplication operator for which we write – with slight abuse of notation – $\Lambda_+(\mathfrak{p})$. Note that we normalize the Fourier transform such that it is unitary.

To proceed, we find the positive eigenvalues of D_0 and the corresponding eigenvectors. For fixed $\mathfrak{p}$ two orthonormal eigenvectors with eigenvalue $E(\mathfrak{p}) = (c^2\mathfrak{p}^2 + m^2c^4)^{1/2}$ are

$$\frac{1}{N(\mathfrak{p})}\begin{pmatrix} (E_0 + E(\mathfrak{p}))\begin{pmatrix}1\\0\end{pmatrix} \\ c\mathfrak{p}\cdot\boldsymbol{\sigma}\begin{pmatrix}1\\0\end{pmatrix}\end{pmatrix} \quad \text{and} \quad \frac{1}{N(\mathfrak{p})}\begin{pmatrix} (E_0 + E(\mathfrak{p}))\begin{pmatrix}0\\1\end{pmatrix} \\ c\mathfrak{p}\cdot\boldsymbol{\sigma}\begin{pmatrix}0\\1\end{pmatrix}\end{pmatrix}, \tag{2}$$

where $E_0 := E(0)$ and $N(\mathfrak{p}) = [2E(\mathfrak{p})(E(\mathfrak{p}) + E_0)]^{1/2}$. Any spinor ψ in the positive spectral subspace of D_0 can be written as

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

with $u \in L^2(\mathbb{R}^3) \otimes \mathbb{C}^2$, i.e., a Pauli spinor. Conversely, any Dirac spinor of the form (3) is in the image of $\mathfrak{H}$ under the Fourier transform. We note that two Dirac spinors are orthonormal, if and only if the corresponding Pauli spinors u are orthonormal.

The projection in Fourier space is given as

$$\Lambda_+(\mathfrak{p}) = \frac{1}{2} + \frac{c\boldsymbol{\alpha}\cdot\mathfrak{p} + mc^2\beta}{2E(\mathfrak{p})} \tag{4}$$

which follows from the fact that $\Lambda_+(\mathfrak{p})$ is Hermitian, idempotent, reproduces the vectors (2), and annihilates any vector orthogonal to (2).

Eventually we will need the Fourier transform of the Coulomb potential, namely

$$\mathscr{F}\frac{1}{|\cdot|} = \sqrt{\frac{2\hbar}{\pi}}\frac{1}{|\cdot|^2}\,.$$

Using these facts we obtain for any ψ in the positive spectral subspace, on writing $(\cdot,\cdot)$ for the inner product in $L^2(\mathbb{R}^3)\otimes\mathbb{C}^4$ or $L^2(\mathbb{R}^3)\otimes\mathbb{C}^2$ as appropriate, that

$$(\psi, B\psi) = (u, bu) := \int_{\mathbb{R}^3} E(\mathfrak{p})|u(\mathfrak{p})|^2 d\mathfrak{p} - \alpha c\frac{Z}{2\pi^2}\int_{\mathbb{R}^6} u(\mathfrak{p}')^* K(\mathfrak{p}',\mathfrak{p})u(\mathfrak{p})\,d\mathfrak{p}\,d\mathfrak{p}'\,, \tag{5}$$

where * denotes the Hermitian conjugate, $|u(\mathfrak{p})|^2 = u(\mathfrak{p})^*u(\mathfrak{p})$, $\alpha := e^2/(\hbar c)$ is Sommerfeld's fine structure constant which is about 1/137.037 and the kernel K

is given by

$$K(\mathfrak{p}',\mathfrak{p}) = \frac{(E(\mathfrak{p}')+E_0)(E(\mathfrak{p})+E_0)+c^2(\mathfrak{p}'\cdot\boldsymbol{\sigma})(\mathfrak{p}\cdot\boldsymbol{\sigma})}{N(\mathfrak{p}')|\mathfrak{p}'-\mathfrak{p}|^2N(\mathfrak{p})}\,. \tag{6}$$

The right-hand side of (5) defines a self-adjoint operator b, if we can show that the form (u,bu) is bounded from below. We also call this operator the Bethe–Salpeter operator. This is justified, since the sesquilinear form $(\psi,B\psi)$ is bounded from below if and only if (u,bu) is bounded from below, and the operators B, and b, defined as the corresponding Friedrichs extensions, are unitarily equivalent because of (3).

2.2. Partial Wave Decomposition. To obtain a sharp estimate for the potential energy we decompose the operator 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 $\mathfrak{J} = \frac{1}{2}(\mathfrak{r}\times\mathfrak{p}+\sigma)$ commutes with b. In fact this has been partially carried through earlier by Hardenkopf and Sucher [5].

We begin by observing that those of the spherical spinors

$$\Omega_{l,m,s}(\omega) := \begin{cases} \begin{pmatrix} \sqrt{\frac{l+s+m}{2(l+s)}}Y_{l,m-\frac{1}{2}}(\omega) \\ \sqrt{\frac{l+s-m}{2(l+s)}}Y_{l,m+\frac{1}{2}}(\omega) \end{pmatrix} & s=\frac{1}{2} \\ \begin{pmatrix} -\sqrt{\frac{l+s-m+1}{2(l+s)+2}}Y_{l,m-\frac{1}{2}}(\omega) \\ \sqrt{\frac{l+s+m+1}{2(l+s)+2}}Y_{l,m+\frac{1}{2}}(\omega) \end{pmatrix} & s=-\frac{1}{2} \end{cases} \tag{7}$$

with $l=0,1,2,\dots$ and $m=-l-\frac{1}{2},\dots,l+\frac{1}{2}$, 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., [11], p. 421) with the convention that $Y_{l,k}=0$, if $|k|>l$. We denote the corresponding index set by I, i.e., $I := \{(l,m,s)|l\in\mathbb{N}_0, m=-l-\frac{1}{2},\dots, l+\frac{1}{2}, s=\pm\frac{1}{2}, \Omega_{l,m,s}\neq 0\}$. Thus any $u\in L^2(\mathbb{R}^3)\otimes\mathbb{C}^2$ can be written as

$$u(\mathfrak{p}) = \sum_{(l,m,s)\in I} p^{-1}a_{l,m,s}(p)\Omega_{l,m,s}(\omega)\,,$$

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

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

Inserting this expansion into (5) yields

$$\begin{aligned}(u,bu) = \sum_{(l,m,s)\in I}(a_{l,m,s},b_{l,s}a_{l,m,s}) := \sum_{(l,m,s)\in I}\Bigg(&\int_0^\infty e(p)|a_{l,m,s}(p)|^2dp \\ &- \alpha c\frac{Z}{\pi}\int_0^\infty\int_0^\infty \overline{a_{l,m,s}(p')}k_{l,s}(p',p)a_{l,m,s}(p)\,dp\,dp'\Bigg)\end{aligned} \tag{8}$$

with $n(p) := N(\mathfrak{p}), e(p) := E(\mathfrak{p})$, and

$$k_{l,s}(p',p) = \frac{(e(p')+E_0)Q_l(\frac{1}{2}(\frac{p}{p'}+\frac{p'}{p}))(e(p)+E_0)+c^2p'Q_{l+2s}(\frac{1}{2}(\frac{p}{p'}+\frac{p'}{p}))p}{n(p')n(p)} . \tag{9}$$

The functions Q_l are Legendre functions of the second kind, i.e.,

$$Q_l(z) = \frac{1}{2}\int_{-1}^{1} \frac{P_l(t)}{z-t}dt , \tag{10}$$

where the P_l are Legendre polynomials. [See Stegun [13] for the notation and some properties of these special functions. 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 [3], Problem 77).] To obtain (8), we also use that $(\mathfrak{p}\cdot\boldsymbol{\sigma})\Omega_{l,m,s}(\omega) = -p\Omega_{l+2s,m,s}(\omega)$ (see, e.g., Greiner [4], p. 171, (12)). The operators $b_{l,s}$ defined by the sesquilinear form (8) are the reduced Bethe–Salpeter operators on the corresponding angular momentum subspaces.

We close this subsection with the following useful result:

Lemma 1.

$$\begin{aligned}&\inf\{(u,bu)|(1+p^{1/2})|u| \in L^2(\mathbb{R}^3), \|u\| = 1\}\\ &= \inf\{(f,b_{0,\frac{1}{2}}f)|(1+p^{1/2})|f| \in L^2(\mathbb{R}^+), \|f\| = 1\} .\end{aligned} \tag{11}$$

Proof. To see which of the angular momentum channels is yielding the lowest energy, we first note that for any given $a \in L^2(\mathbb{R}_+, dp)$ the inequality

$$\begin{aligned}(a,b_{l,s}a) &= \int_0^\infty e(p)|a(p)|^2dp - \alpha c\frac{Z}{\pi}\int_0^\infty\int_0^\infty \overline{a(p')}k_{l,s}(p',p)a(p)dpdp'\\ &\geqq \int_0^\infty e(p)|a(p)|^2dp - \alpha c\frac{Z}{\pi}\int_0^\infty\int_0^\infty \overline{|a(p')|}k_{l,s}(p',p)|a(p)|dpdp'\\ &= (|a|,b_{l,s}|a|)\end{aligned}$$

holds, since all the Legendre functions of the second kind $Q_l(t)$ are positive for $t > 1$, which is an immediate consequence of the integral representation [13], Formula 8.8.2. Thus we may and shall restrict ourselves to positive functions when minimizing $(a, b_{l,s}a)$.

Next we observe the following chain of inequalities:

$$Q_0(t) \geqq \cdots \geqq Q_l(t) \geqq \cdots \geqq 0 \tag{12}$$

for all $t > 1$ which follows from the integral representation

$$Q_l(t) = \int_{t+(t^2-1)^{\frac{1}{2}}}^{\infty} \frac{z^{-l-1}dz}{\sqrt{1-2tz+z^2}}$$

(Whittaker and Watson [16], p. 334, Chapter XV, Sect. 32).

We now resume our main argument by inferring from (12) that we may assume that coefficients $a_{l,m,s}$ are zero unless $(l,m,s) = (0,1/2,1/2)$ or $(l,m,s) = (1,1/2,-1/2)$ when minimizing. Finally we show that we can pick $a_{1,1/2,-1/2} = 0$ as well: we have

$$
\begin{aligned}
&n(p)n(p')k_{1,-\frac{1}{2}}(p',p)\\
&= (e(p')+E_0)Q_1\left(\frac{1}{2}\left(\frac{p}{p'}+\frac{p'}{p}\right)\right)(e(p)+E_0)+c^2p'Q_0\left(\frac{1}{2}\left(\frac{p}{p'}+\frac{p'}{p}\right)\right)p\\
&= (e(p')+E_0)(e(p)+E_0)Q_0+c^2p'pQ_1\\
&\quad+[(e(p')+E_0)(e(p)+E_0)-c^2pp'](Q_1-Q_0)\\
&\leqq (e(p')+E_0)(e(p)+E_0)Q_0+c^2p'pQ_1=n(p)n(p')k_{0,\frac{1}{2}}(p',p)\,,
\end{aligned}
$$

where we used (12). This shows that we gain by putting all the weight into the channel $l=0, s=\frac{1}{2}$ and picking $a_{1,m,-\frac{1}{2}}=0$. □

From now on we will drop the indices in $a_{l,m,s}$ and write merely a.

2.3. Critical Coupling Constant. Our main result is

Theorem 1. *Set $Z_c := 2/[(\frac{\pi}{2}+\frac{2}{\pi})\alpha]$. If $Z \leqq Z_c$, then*

$$(u, bu) \geqq -\alpha Z\left(\frac{\pi}{4}-\frac{1}{\pi}\right)mc^2$$

on $[L^2(\mathbb{R}^3,(1+|\mathfrak{p}|^2)^{1/2}d\mathfrak{p})]^2$; if, however, $Z > Z_c$, then (u, bu) is unbounded from below. Moreover, if $Z < Z_c$ then the operator $v_{l,s}$ defined by the kernel $-\frac{\alpha c}{\pi}k_{l,s}$ is relatively form bounded with respect to cp on $L^2(\mathbb{R}^+, pdp)$ with form bound less than one.

We remark the following:

- The claim of this theorem was predicted by Hardenkopf and Sucher [6] based on the asymptotic behavior of the eigenfunctions of $b_{l,s}$ and on numerical evidence. Hardenkopf and Sucher assume that Z_c is given when the lowest eigenvalue reaches zero from above. In particular all eigenvalues are non negative according to this assumption. In general, we have to leave this question open except for two cases:
  - If $m = 0$ our bound shows positivity directly.
  - If $Z \leqq 2/(\pi\alpha)$, B is positive. This follows from the identity

$$(\psi, B\psi) = (\psi, (\sqrt{-(\hbar c)^2\Delta + m^2c^4} - Ze^2/|\cdot|)\psi)\,.$$

  The right-hand side is positive by Kato's inequality (see below) regardless of whether ψ is in the positive spectral subspace or not.
- The numerical value of Z_c is roughly 124.2, i.e., bigger than 111, the heaviest element known today (Hofmann et al. [8]), as opposed to the critical value $2/(\pi\alpha)$ of the operator $(-(c\hbar)^2\Delta + m^2c^4)^{1/2} - Ze^2/|\mathfrak{r}|$ which is about 87.2 and thus covers not even all natural elements.
- A lower bound on the critical coupling constant Z_c can be directly extracted from the inequality $(-\Delta)^{1/2} \geqq \frac{2}{\pi}\frac{1}{|\mathfrak{r}|}$ (Kato [9], p. 307) by simply omitting the projections Λ_+. However, this gives $Z_c \geqq 2/(\pi\alpha)$, i.e., is not optimal.

- One might also think of using a similar estimate as Lieb and Yau [10] directly for the kernel K in (6). This, however, is also problematic, since the second summand contains terms that change their sign according to the mutual orientation of $\mathfrak{p}$ and $\mathfrak{p}'$.

Proof. We begin by showing that (u, bu) is bounded from below by some constant, if $Z \leqq Z_c$. According to Lemma 1 we need to look at the $l = 0$, $s = 1/2$-channel only. Set $h(p) = 1/p$, split the kernel $k_{0,1/2} := k^{(1)} + k^{(2)}$ into two parts and use the Schwarz inequality:

$$\int_0^\infty \int_0^\infty a(p') \frac{e(p') + E_0}{n(p')} Q_0 \left(\frac{1}{2}\left(\frac{p}{p'} + \frac{p'}{p}\right)\right) \frac{e(p) + E_0}{n(p)} a(p) dp dp'$$

$$= \int_0^\infty \int_0^\infty a(p') \frac{e(p') + E_0}{n(p')} \sqrt{Q_0 \left(\frac{1}{2}\left(\frac{p}{p'} + \frac{p'}{p}\right)\right)} \sqrt{\frac{h(p)}{h(p')}}$$

$$\cdot \sqrt{\frac{h(p')}{h(p)}} \sqrt{Q_0 \left(\frac{1}{2}\left(\frac{p}{p'} + \frac{p'}{p}\right)\right)} a(p) \frac{e(p) + E_0}{n(p)} dp dp'$$

$$\leqq \int_0^\infty a(p)^2 \frac{(e(p) + E_0)^2}{n(p)^2} \int_0^\infty \frac{h(p')}{h(p)} Q_0 \left(\frac{1}{2}\left(\frac{p}{p'} + \frac{p'}{p}\right)\right) dp' dp \,. \tag{13}$$

Similarly

$$\int_0^\infty \int_0^\infty a(p') \frac{p'}{n(p')} Q_1 \left(\frac{1}{2}\left(\frac{p}{p'} + \frac{p'}{p}\right)\right) \frac{p}{n(p)} a(p) dp dp'$$

$$\leqq \int_0^\infty a(p)^2 \frac{p^2}{n(p)^2} \int_0^\infty \frac{h(p')}{h(p)} Q_1 \left(\frac{1}{2}\left(\frac{p}{p'} + \frac{p'}{p}\right)\right) dp dp' \tag{14}$$

with $h(p) := p^{-1}$. Note that $h(p) = p^{-1}$ is the optimal power function in (13) and (14). Evaluating the p' integral gives

$$\int_0^\infty dp' \frac{h(p')}{h(p)} Q_l \left(\frac{1}{2}\left(\frac{p}{p'} + \frac{p'}{p}\right)\right) = p \begin{cases} \frac{\pi^2}{2} & \text{for } l = 0 \\ 2 & \text{for } l = 1 \end{cases} .$$

Putting all together thus gives

$$\alpha c \frac{Z}{\pi} \int_0^\infty dp \int_0^\infty dp' a(p') k_{0,1/2}(p', p) a(p)$$

$$\leqq \alpha c \frac{Z}{\pi} \int_0^\infty p \left(\frac{\pi^2}{2} \frac{(e(p) + E_0)^2}{n(p)^2} + 2 \frac{c^2 p^2}{n(p)^2}\right) a(p)^2 dp$$

$$\leqq \alpha \frac{Z}{2} \left(\frac{\pi}{2} + \frac{2}{\pi}\right) \int_0^\infty \left(cp + \frac{\pi^2 - 4}{\pi^2 + 4} E_0\right) a(p)^2 dp \,,$$

i.e., we have the following lower bound on the Bethe operator

$$B \geqq -\alpha Z\left(\frac{\pi}{4}-\frac{1}{\pi}\right)E_0$$

provided $Z \leqq 2/[(\pi/2+2/\pi)\alpha]$, thus giving the desired lower bound on Z_c, and we have proven the claimed form boundedness as well.

To show that (u, bu) is unbounded from below when $Z > Z_c$, we will just do a variational calculation. We pick the trial function

$$a(p) := \begin{cases} \frac{1}{p} & p \in (\tilde{c}, \tilde{d}) \\ 0 & p \in \mathbb{R}_+ \setminus (\tilde{c}, \tilde{d}) \end{cases}, \tag{15}$$

where $\tilde{c}, \tilde{d}$, and $\gamma := \tilde{d}/\tilde{c}$ are positive numbers which we will choose later sufficiently large, and evaluate. Firstly, we note that for $t > 1$,

$$Q_0(t) = \frac{1}{2}\log\left(\frac{t+1}{t-1}\right) \quad \text{and} \quad Q_1(t) = \frac{t}{2}\log\left(\frac{t+1}{t-1}\right) - 1 \tag{16}$$

(Stegun [13]). Secondly, we evaluate three integrals

$$I(v) := \int_{\tilde{c}}^{\tilde{d}}\int_{\tilde{c}}^{\tilde{d}} p'^{-1}p^{-1}\left(\frac{p}{p'}\right)^{v} Q_0\left(\frac{1}{2}\left(\frac{p}{p'}+\frac{p'}{p}\right)\right) dp\, dp'$$

for $v = 0, \pm 1$. By symmetry we have $I(v) = I(-v)$. To estimate these integrals we distinguish the regions where $p > p'$ and $p' > p$. The results are as $\tilde{c}, \tilde{d}$, and γ tend to infinity:

$$I(0) = \frac{\pi^2}{2}\log\gamma + O(1)\,, \tag{17}$$

$$I(\pm 1) = (\log\gamma)^2 + 2\log\gamma + O(1)\,. \tag{18}$$

Next we observe that for $p, p' \in \operatorname{supp}(a)$,

$$k^{(1)}(p', p) \geqq \frac{1}{2}Q_0\left(\frac{1}{2}\left(\frac{p}{p'}+\frac{p'}{p}\right)\right), \tag{19}$$

$$k^{(2)}(p', p) \geqq \frac{1}{2}Q_1\left(\frac{1}{2}\left(\frac{p}{p'}+\frac{p'}{p}\right)\right)(1-\mathrm{const}/\tilde{c})\,. \tag{20}$$

Thus using the definition of $k_{1,-1/2}$, (19), (20), and (16),

$$\begin{aligned} &\frac{Z}{\pi}\int_0^\infty\int_0^\infty a(p')k_{1,-1/2}a(p)\,dp\,dp' \\ &\geqq \frac{Z}{\pi}\left[\frac{1}{2}I(0) + \left(\frac{1}{4}I(1)+\frac{1}{4}I(-1)-\frac{1}{2}(\log\gamma)^2\right)(1-\mathrm{const}/\tilde{d})\right] \\ &\geqq c\frac{Z}{\alpha Z_c}\log\gamma(1-\mathrm{const}/\tilde{c})\,. \end{aligned} \tag{21}$$

Moreover we get for the kinetic energy

$$\int_0^\infty e(p)a(p)^2\,dp = c\log\gamma + O(1)\,. \tag{22}$$

Thus subtracting (21) from (22) shows that

$$(a, b_{0,1/2}a) \leqq \left[1 - \frac{Z}{Z_c}(1 - \mathrm{const}/\tilde{c})\right] c\log\gamma + \mathrm{const} \to -\infty\,,$$

if we pick $\tilde{c}$ so small – but positive – that the term in brackets is negative, which is possible, since $Z > Z_c$, and tend γ to infinity. Since $\|a\|^2 = \frac{1}{\tilde{c}} - \frac{1}{\tilde{d}} \leqq 1$ for $\tilde{c} \geqq 1$ the assertion follows. □

3. The Essential Spectrum

Our result is

Theorem 2. *Assume that* $Z < Z_c$. *Then* $\sigma_{\mathrm{ess}}(B) = [mc^2, \infty)$ *and* $\sigma_{\mathrm{sc}}(B) = \emptyset$.

Proof. Let $\mathfrak{H} = \Lambda_+(L^2(\mathbb{R}^3) \otimes \mathbb{C}^4)$, and let

$$B_0 = \Lambda_+(c\boldsymbol{\alpha} \cdot \mathfrak{p} + mc^2\beta)\Lambda_+\,,$$

$$W(\mathfrak{r}) = Ze^2/|\mathfrak{r}|\,,$$

and

$$C = -\Lambda_+ W \Lambda_+\,.$$

For $Z < Z_c$, the operator $B = B_0 + C$, defined in Sect. 2 using the Friedrichs extension, may also be defined via quadratic forms since C is B_0-form bounded with relative bound less than one for such C. The resulting self-adjoint extensions are equal and in what follows we will therefore regard B as a form sum. By Theorem 1, the estimate

$$(\phi, (B + \gamma)\phi) \geqq \|\phi\|^2$$

holds for all ϕ in $Q(B_0)$, the form domain of B_0, so long as

$$\gamma > \alpha Z\left(\frac{\pi}{4} - \frac{1}{\pi}\right) mc^2 + 1\,.$$

To prove the first claim, we will show that $(B + \gamma)^{-1} - (B_0 + \gamma)^{-1}$ is compact as an operator on $L^2(\mathbb{R}^3) \otimes \mathbb{C}^4$, and hence as an operator on $\mathfrak{H}$. It will then follow from Theorem XIII.14 of Reed–Simon [12] that $\sigma_{\mathrm{ess}}(B) = \sigma_{\mathrm{ess}}(B_0) = [mc^2, \infty)$. To this end we factor (in $L^2(\mathbb{R}^3) \otimes \mathbb{C}^4$)

$$\begin{aligned}(B + \gamma)^{-1} - (B_0 + \gamma)^{-1} &= -(B_0 + \gamma)^{-1} C (B + \gamma)^{-1} \\ &= [(B_0 + \gamma)^{-1}\Lambda_+ W^{1/2}][W^{1/2}\Lambda_+(B + \gamma)^{-1}]\,. \end{aligned} \tag{23}$$

The first factor in (23) may be written

$$(B_0 + \gamma)^{-1}\Lambda_+ W^{1/2} = \Lambda_+(B_{00} + \gamma)^{-1} W^{1/2}\,,$$

where

$$B_{00} = \sqrt{\mathfrak{p}^2 c^2 + m^2 c^4}\,.$$

By Lemma 2.6 of [7], the operator $(B_{00}+1)^{-1}W^{1/2}$ is compact, so the first factor in (23) is compact. To show that the second factor in (23) is bounded, we write

$$W^{1/2}\Lambda_+(B+\gamma)^{-1} = [W^{1/2}\Lambda_+(B_0+\gamma)^{-1/2}][(B_0+\gamma)^{1/2}(B+\gamma)^{-1}]\,. \tag{24}$$

The second factor in (24) is bounded by the closed graph theorem since B is a form-bounded perturbation of B_0 and $(B+\gamma)^{-1}$ maps into $\mathscr{D}(B) \subset \mathcal{Q}(B_0)$. To show that the first factor in (24) is bounded, we write

$$\begin{aligned} W^{1/2}\Lambda_+(B_0+\gamma)^{-1/2} &= W^{1/2}(B_{00}+\gamma)^{-1}\Lambda_+ \\ &= [W^{1/2}(|\mathfrak{p}|^{1/2}+1)^{-1}][(|\mathfrak{p}|^{1/2}+1)(B_{00}+\gamma)^{-1}\Lambda_+]\,. \end{aligned} \tag{25}$$

The second right-hand factor is trivially bounded; to bound the first we appeal to Kato's inequality which bounds $r^{-1/2}(|\mathfrak{p}|^{1/2}+1)^{-1}$. This shows that $W^{1/2}\Lambda_+ (B_0+\gamma)^{-1}$ is a bounded operator so that the first factor in (24) is also bounded. Thus $(B+\gamma)^{-1}-(B_0+\gamma)^{-1}$ is the product of a compact operator and a bounded operator, proving the required compactness.

To prove the second claim we will use the complex scaling methods of Aguilar, Balslev, and Combes (see [12] for discussion and references). Let $\mathscr{U}(\theta)f(\mathfrak{r}) = e^{3\theta/2}f(e^\theta \mathfrak{r})$ be the usual dilation group on $L^2(\mathbb{R}^3)$ (trivially extended to the spinor space $L^2(\mathbb{R}^3)\otimes\mathbb{C}^2$). This group of dilations projects under partial wave decomposition and Fourier transformation to the group of dilations $U(\theta)f(p) = e^{-\theta/2}f(e^{-\theta}p)$ on $L^2(\mathbb{R}^+, dp)$. We will write $b_{l,s} = b_0 + v_{l,s}$, where $(b_0\phi)(p) = e(p)\phi(p)$ is the "free" Hamiltonian, and show that each $b_{l,s}$ has empty singular spectrum. Let D be the disc $\{\theta \in \mathbb{C} : |\theta| < \theta_0\}$ for a $\theta_0 > 0$ to be chosen. The operator

$$b_0(\theta) = U(\theta)b_0U(\theta)^{-1} = \sqrt{e^{-2\theta}c^2p^2 + m^2c^4}$$

(choosing the branch of the square root with branch cut on $(-\infty, 0]$ and $-\pi < \arg(z) < \pi$) is an unbounded normal operator with domain equal to the domain of b_0 and with essential spectrum on the parametric complex curve

$$g_\theta(t) = \sqrt{m^2c^4 + t\,\cos(2\phi) - it\,\sin(2\phi)}\,,$$

where $\phi = \Im(\theta)$ and $t \in \mathbb{R}^+$. For $\phi > 0$, this curve intersects the real axis at $t = 0$; for $t > 0$ we have $\arg g_\theta(t) < 0$.

We want to study the spectra of the operators $b_{l,s}$ by studying the associated family $b_{l,s}(\theta) = U(\theta)b_{l,s}U(\theta)^{-1}$. In order to apply the complex scaling method, we need to show that

(1) for all $\theta \in D$, $v_{l,s}(\theta) = U(\theta)v_{l,s}U(\theta)^{-1}$ is b_0-form bounded with relative bound less than one, so that $b_{l,s}(\theta)$ may be defined as a form sum of $b_0(\theta)$ and $v_{l,s}(\theta)$,

(2) for suitable $\gamma > 0$, the operators $(b_{l,s}(\theta)+\gamma)^{-1} - (b_0(\theta)+\gamma)^{-1}$ are compact, and

(3) the family of operators $(b_0+1)^{1/2} v_{l,s}(\theta)(b_0+1)^{-1/2}$, initially defined for $\theta \in D \cap \mathbb{R}$, extends to an analytic operator-valued function in D.

Note that (2) differs slightly from the usual definition of dilation-analytic potentials in [12] (see Sect. XIII.10, p. 184) since $v_{l,s}$ is too singular to be b_0-form compact. However this weaker compactness condition suffices to prove that the essential spectra of $b_{l,s}(\theta)$ and $b_0(\theta)$ coincide, as may be seen as follows (cf. Herbst [7]). By (1) and the fact that $b_0(\theta)$ defines a sectorial form, there is a $\gamma > 0$ (uniform in $\theta \in D$) so that $\Re(\phi, b^\#(\theta)\phi) \geqq -(\gamma-1)\|\phi\|^2$, where $b^\#$ is b_0 or $b_{l,s}$. Let $D = (b_0(\theta)+\gamma)^{-1}$ and let $E = (b_{l,s}(\theta)+\gamma)^{-1}$. The operator D is a bounded normal operator whose essential spectrum is a bounded arc in the complex plane. Thus $\sigma(D)$ has empty interior as a subset of $\mathbb{C}$, and its complement consists of a single connected component. Since the difference $D-E$ is compact and E has a nonempty resolvent set containing points of $\mathbb{C}\backslash\sigma(D)$, we can apply Lemma 3 of [12], Sect. XIII.4 to conclude that $\sigma_{\text{ess}}(D) = \sigma_{\text{ess}}(E)$. We now use the strong spectral mapping theorem (Lemma 2 in [12], Sect. XIII.4) to conclude that $\sigma_{\text{ess}}(b_{l,s}(\theta)) = \sigma_{\text{ess}}(b_0(\theta))$. Our application of complex scaling also differs from the Schrödinger case in that we assume analyticity in a disc rather than a strip, but this causes no essential difficulty so long as θ can have a small positive imaginary part. With these slight modifications, we can then mimic the arguments used to prove Theorem XIII.36(a)–(d) of [12] to conclude that the discrete spectrum of $b_{l,s}$ consists of (i) sub-continuum eigenvalues of $b_{l,s}$, (ii) eigenvalues of $b_{l,s}$ embedded in the continuous spectrum, and (iii) resonances. By Weyl's theorem applied to $b_{l,s}(\theta)$, eigenvalues of type (ii) can accumulate only at mc^2. Finally, using the existence of a dense set of analytic vectors for the dilation group $U(\theta)$ acting on $L^2(\mathbb{R}^+, dp)$, we can mimic the proof of Theorem XIII.36(e) in [12] to conclude that singular continuous spectrum is absent.

We now prove claims (1)–(3). To prove the relative boundedness statement we recall the explicit integral kernel for $v_{l,s}$, namely

$$k_{l,s}(p,q) = \frac{(e(p)+E_0)Q_l(\frac{1}{2}(\frac{p}{q}+\frac{q}{p}))(e(q)+E_0) + c^2 pq Q_{l+2s}(\frac{1}{2}(\frac{p}{q}+\frac{q}{p}))}{n(p)n(q)},$$

so that the kernel for $v_{l,s}(\theta)$ is

$$\begin{aligned} k_{l,s,\theta}(p,q) &= e^{-\theta} k_{l,s}(e^{-\theta}p, e^{-\theta}q) \\ &= e^{-\theta} \frac{(e_\theta(p)+E_0)Q_l(\frac{1}{2}(\frac{p}{q}+\frac{q}{p}))(e_\theta(q)+E_0) + c^2 e^{-2\theta} pq Q_{l+2s}(\frac{1}{2}(\frac{p}{q}+\frac{q}{p}))}{n_\theta(p)n_\theta(q)}, \end{aligned}$$

where

$$e_\theta(p) = \sqrt{e^{-2\theta}c^2p^2 + E_0^2}$$

and

$$n_\theta(p) = \sqrt{2e_\theta(p)(e_\theta(p)+E_0)}\,.$$

This kernel is holomorphic in θ for $|\Im\theta| < \pi/4$. Moreover, for any $\delta > 0$ there is a $\theta_0(\delta) > 0$ so that for $\theta \in D$,

$$(1-\delta)e(p) \leqq |e_\theta(p)| \leqq (1+\delta)e(p)\,.$$

It is not difficult to see that for $\theta \in D$, the estimate

$$|k_{l,s,\theta}(p,q)| \leqq \left(\frac{1+\delta}{1-\delta}\right)^2 k_{l,s}(p,q) \tag{26}$$

holds, so that choosing δ so small that

$$\frac{Z}{Z_c}\left(\frac{1+\delta}{1-\delta}\right)^2 < 1$$

guarantees that $v_{l,s}(\theta)$ is b_0 form-bounded with relative bound less than one. By choosing θ_0 smaller if necessary we can insure that $v_{l,s}(\theta)$ is $b_0(\theta)$-form bounded with relative bound less than one, so that $b_{l,s}(\theta)$ is well-defined as a form sum and gives rise to a sectorial form with

$$\Re(\phi, b_{l,s}(\theta)\phi) \geqq -(\gamma - 1)\|\phi\|^2$$

for a suitable $\gamma > 0$ and all ϕ belonging to the form domain of b_0.

To prove (ii), we will show that $(b_0+1)^{-1}v_{l,s}(\theta)(b_0+1)^{-1/2}$ is compact. Supposing this to be true for the moment, we then write

$$\begin{aligned}(b_{l,s}(\theta)+\gamma)^{-1} - (b_0(\theta)+\gamma)^{-1} &= (b_0(\theta)+\gamma)^{-1}v_{l,s}(\theta)(b_{l,s}(\theta)+\gamma)^{-1}\\ &= [(b_0(\theta)+\gamma)^{-1}(b_0+\gamma)][(b_0+\gamma)^{-1}v_{l,s}(\theta)(b_0+\gamma)^{-1/2}]\\ &\quad\times [(b_0+\gamma)^{1/2}(b_{l,s}(\theta)+\gamma)^{-1}]\,.\end{aligned}$$

The first factor in square brackets is bounded by explicit computation (each factor is a multiplication operator), the second factor is presumed compact, and the third factor is bounded by the closed graph theorem since $b_{l,s}(\theta)$ is a form-bounded perturbation of $b_0(\theta)$ and the form domains of $b_0(\theta)$ and b_0 coincide.

To prove that the second factor is compact, we note that for θ real, the operators $(b_0+\gamma)^{-1}v_{l,s}(\theta)(b_0+\gamma)^{-1/2}$ result from the partial wave decomposition in $L^2(\mathbb{R}^3)\otimes\mathbb{C}^2$ applied to the operators

$$(B_{00}+\gamma)^{-1}\mathscr{K}_\theta(B_{00}+\gamma)^{-1/2}\,,$$

where $\mathscr{K}_\theta$ is an operator with integral kernel

$$\mathscr{K}_\theta(\mathfrak{p}',\mathfrak{p}) = \mathscr{K}_\theta^{(1)}(\mathfrak{p},\mathfrak{p}') + \mathscr{K}_\theta^{(2)}(\mathfrak{p},\mathfrak{p}')$$

and

$$\mathscr{K}_\theta^{(1)}(\mathfrak{p}',\mathfrak{p}) = e^{-2\theta}\frac{E(e^{-\theta}\mathfrak{p}')+E_0}{N(e^{-\theta}\mathfrak{p}')}\frac{1}{|\mathfrak{p}-\mathfrak{p}'|^2}\frac{E(e^{-\theta}\mathfrak{p})+E_0}{N(e^{-\theta}\mathfrak{p})}\,,$$

$$\mathscr{K}_\theta^{(2)}(\mathfrak{p}',\mathfrak{p}) = e^{-\theta}\frac{\mathfrak{p}'\cdot\sigma}{N(e^{-\theta}\mathfrak{p}')}\frac{1}{|\mathfrak{p}-\mathfrak{p}'|^2}\frac{\mathfrak{p}\cdot\sigma}{N(e^{-\theta}\mathfrak{p})}\,.$$

Both $\mathscr{K}_\theta^{(1)}$ and $\mathscr{K}_\theta^{(2)}$ consist of bounded Fourier multipliers pre- and post-multiplying the operator with singular kernel $1/|\mathfrak{p}'-\mathfrak{p}|^2$. Up to constant factors, this kernel acts in x-space as multiplication by $|x|^{-1}$. Thus, to show that $(B_{00}+\gamma)^{-1}\mathscr{K}_\theta(B_{00}+\gamma)^{-1/2}$, is compact, it suffices to show that the operator

$$(B_{00}+1)^{-1}W(B_{00}+1)^{-1/2}$$

is compact. This follows from previous arguments since

$$(B_{00}+1)^{-1}W(B_{00}+1)^{-1/2} = [(B_{00}+1)^{-1}W^{1/2}][W^{1/2}(B_{00}+1)^{-1/2}]$$

and the first and second right-hand factors have already been shown to be, respectively, compact and bounded. This proves (2).

Claim (3) follows from the explicit expressions for the integral kernel of $v_{l,s}(\theta)$ together with the form bound proven above.

Putting claims (1)–(3) and the remarks following them together, we conclude that the singular continuous spectrum of $b_{l,s}$ is empty. □

We conclude with

Theorem 3. *If $m = 0$ and $Z \leqq Z_c$, then B has no eigenvalues.*

Proof. Let d_θ be the unitary dilation operator by a factor $1/\theta$, i.e., for any Pauli spinor u in the domain of b and $\theta \in \mathbb{R}^+$ let

$$(d_\theta u)(\mathfrak{p}) := u_\theta(\mathfrak{p}) = \theta^{-3/2}u(\mathfrak{p}/\theta)$$

which again is in the domain of b. Moreover we have

$$b_\theta := d_\theta^{-1} b d_\theta = b/\theta \,. \tag{27}$$

Equation (27) is easily verified in the quadratic form sense on $\mathfrak{S}(\mathbb{R}^3)\otimes\mathbb{C}^4$ which implies the operator identity for the Friedrichs extensions. If u were an eigenfunction of b with eigenvalue E, then $u_{1/\theta}$ would be an eigenfunction of b_θ with eigenvalue E and therefore $u_{1/\theta}$ is an eigenfunction of b with eigenvalue θE, i.e., any nonzero eigenvalue would imply the existence of a continuum of eigenvalues which contradicts the separability of $\mathfrak{H}$. This leaves the possibility of $E = 0$. Suppose there existed an eigenfunction u with eigenvalue zero. According to our partial wave analysis we may assume that $u = a\Omega_{0,m,1/2}/p$ with nonnegative a fulfilling the equation $b_{0,1/2}a = 0$. But the a_θ defined by $a_\theta(p) = \theta^{1/2}a(\theta p)$ would be another linearly independent eigenfunction of $b_{0,1/2}$, since the dilation operator has no eigenfunctions.

On the other hand we know from the proof of Lemma 1 that all ground states of any $b_{l,s}$ are non-negative. As the following argument shows, all ground states are in fact positive. Given this fact for the moment we see that the assumption that E is an eigenvalue is absurd.

Assume a to be a ground state, which is non-negative, that vanishes on a set M with non-zero measure. Let τ_v be the characteristic function of $(v, v+1)\cap M$. Then

$$\begin{aligned} 0 &= (\tau_v, b_{l,s}a) \\ &\leqq \int_0^\infty \tau_v(p)a(p)p\,dp - \alpha c\frac{Z}{\pi}\int_0^\infty dp' \int_0^\infty dp Q_l\left(\frac{1}{2}\left(\frac{p}{p'}+\frac{p'}{p}\right)\right)\tau_v(p')a(p)\,, \end{aligned}$$

and thus

$$\alpha c \frac{Z}{\pi} \int_0^\infty dp' \int_0^\infty dp Q_l \left(\frac{1}{2} \left(\frac{p}{p'} + \frac{p'}{p} \right) \right) \tau_\nu(p') a(p) \leqq \int_0^\infty \tau_\nu(p) a(p) p \, dp \, .$$

Summation over ν gives a positive value for the left-hand side, implying that M has zero measure. □

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Note added in Proof: On February 21, 1996 the Gesellschaft für Schwerionenforschung, Darmstadt, announced the discovery of element $Z = 112$.

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