Self-adjointness and spectral properties of a pseudo-relativistic Hamiltonian due to Brown and Ravenhall

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Abstract

Some properties of a pseudo-relativistic Hamiltonian describing a one electron atom - an appropriately projected Dirac operator with Coulomb potential - proposed by Brown and Ravenhall are proven. Self-adjointness is investigated and the explicit form of the Friedrichs extension is given. The behavior near the critical coupling constant Z_c is investigated and the essential spectrum is determined in the case of $Z = Z_c$.

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1 Introduction

To include relativistic effects in the description of a one electron atom with nuclear charge $Z > 0$, Brown and Ravenhall proposed the operator

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

acting in the Hilbert space $\mathfrak{H} = \Lambda_+ \left(L^2(\mathbb{R}^3) \otimes \mathbb{C}^4 \right)$. Here, $D_0 := -i\boldsymbol{\alpha} \cdot \nabla + \boldsymbol{\beta} m$ is the Dirac operator and $\Lambda_+ := \chi_{(0,\infty)}(D_0)$ the projection on the positive spectral subspace of D_0. The 4×4-matrices $\boldsymbol{\alpha}_j$, $j \in \{1, 2, 3\}$, and $\boldsymbol{\beta}$ are the four Dirac matrices in standard representation, the fine structure constant $\alpha = e^2 \approx 1/137$ and the electron mass $m \geq 0$.

The multi-particle analogon of the operator B attracted recently attention as a starting point for the extension of the "stability of matter" problem to relativistic systems [9]. Some of its basic properties from a physical point of view are reviewed in [1, 15]. Some newer references concerning the numerical treatment of the one or multi-particle operator can be found in [7].

Typical for such pseudo-relativistic Hamiltonians with Coulomb potential is the occurrence of a critical nuclear charge Z_c. Hardekopf and Sucher [4] obtained heuristically the value $Z_c = 2/[(\pi/2 + 2/\pi)\alpha]$ and Evans et al [3] proved that the energy $\mathcal{E}[\psi] := \langle \psi, B\psi \rangle$ is bounded from below by some negative constant times m on the set of normalized rapidly decaying smooth spinors in $\mathfrak{H}$ if $Z \leq Z_c$ and otherwise unbounded from below. Since $Z_c \approx 124$ the operator B allows - in contrast to other pseudo-relativistic Hamiltonians - to describe all known elements. In the case $Z < Z_c$, the essential spectrum is located to be $\sigma_{\text{ess}}(B) = [m, \infty)$ in [3] and the absence of singular continuous spectrum is proved.

¿From a physical point of view, the ground state energy is expected to be positive. Hardekopf and Sucher solved the eigenvalue equation numerically [5] and conjectured that $\inf[\sigma(B)] = 0$ for $Z = Z_c$. In [18] it was shown that the ground state energy is bounded by $m(1 - \alpha Z) > 0.09$ and therefore strictly positive and that the operator has an infinite discrete spectrum if $Z < Z_c$. A sharper lower bound for all nuclear charges $Z \leq Z_c$ was obtained with a computer assisted proof in [17].

All of the above mentioned results were obtained by performing a partial wave decomposition of the operator B, i.e. B can be decomposed in a sum of operators $b_{l,s}$ where l is the angular momentum channel and s the spin of the particle. The operator with the lowest angular momentum $b := b_{0,1/2}$ is basic for the understanding of B because its potential has the most severe singularity. Burenkov and Evans [2] calculated the norm of the Birman-Schwinger kernel of the potential of b. Using this norm they could proof that $\inf[\sigma(B)] \geq 0$.

Here we will explore some properties of b by using methods developed by Raynal et al [19] for the square root operator $H = \sqrt{\boldsymbol{p}^2 + m^2} - \alpha Z/|\boldsymbol{x}|$ acting in $L^2(\mathbb{R}^3)$ restricted to the lowest angular momentum channel. The results obtained for b can than easily be extended to all angular momentum channels and therefore to the operator B. Although the method can directly be applied on B with electron mass $m = 0$ the connection between the massless operator and the operator B with $m > 0$ is more complicated for B than for the square root operator.

We obtain the following main result: the operator b with its natural domain $D(b) = D(p) = L^2(\mathbb{R}, (1 + p^2)\, dp)$ is self-adjoint when the coupling constant $\alpha Z < \alpha Z_c' = 3/4$. For $\alpha Z = \alpha Z_c'$ the operator is essentially self-adjoint and for $\alpha Z_c' < \alpha Z \leq \alpha Z_c$ it is is symmetric and admits a one parametric family of self-adjoint extensions. The Friedrichs extension is considered as the physical relevant one and will be explicitly characterized. The operator $b_{1,-1/2}$ enjoys the same self-adjointness properties and the operators in the angular momentum channels $l > 1$ are all self-adjoint for $\alpha \leq \alpha_c$.

It is shortly noted that the Friedrichs extension of b forms a strict positive, self-adjoint holomorphic family of operators when considered as an operator depending on $\sqrt{Z_c - Z}$ (near Z_c) and that another self-adjoint extension exists when $Z_c' < Z \leq Z_c$. The ground state energy of this other extension reaches at least zero when $Z \to Z_c'$. But since we are not able to proof that this other self-adjoint extension is positive this result will not "explain" the strict positivity of b as this is the case for the square root operator in [19].

Finally we give an expression for the Friedrichs extension of B and localize the essential spectrum to be $\sigma_{\text{ess}}(B) = [m, \infty)$ when $Z = Z_c$, filling the gap left in [3].

In Section 2 we introduce the operator $b_{0,1/2}$. Then we show that the difference between the operator b with electron mass $m = 0$ and $m > 0$ is bounded. In Section 2, the adjoint operator of b (with $m = 0$) is characterized for different ranges of α and from this characterization self-adjointness properties and the explicit form of the Friedrichs extension are deduced. Then we will introduce a self-adjoint holomorphic family of operators which includes different extensions of b. Finally, in Section 4, the results are extended to the operator B and its essential spectrum is determined when $Z = Z_c$. In

Appendix A, the Mellin transform is introduced and some formulas in connection with b are given.

2 The operator restricted to its lowest angular momentum channel

In this Section we will introduce the operator B restricted to the lowest angular momentum channel denoted by b and show that the difference between the operator with $m = 0$ and $m > 0$ is bounded. This will allow to consider b with $m = 0$ when we are concerned with domain questions.

The operator B restricted to its lowest angular momentum channel can already be found in [5]. We will use the notation introduced in [3] and state the angular momentum decomposition of B. Using the special form of four spinors $\psi \in \mathfrak{H}$ and expanding them in an appropriate basis, the energy $\langle \psi, B\psi \rangle$ is obtained to be

$$\sum_{(l,m,s)\in I} \langle \psi_{l,m,s}, b_{l,s}\psi_{l,m,s}\rangle := \sum_{(l,m,s)\in I} \Bigg(\int_0^\infty e(p)|\psi_{l,m,s}(p)|^2 dp \\ -\alpha \frac{Z}{\pi} \int_0^\infty \int_0^\infty \psi_{l,m,s}(p')^* k_{l,s}(p',p)\psi_{l,m,s}(p) dp dp' \Bigg)$$

by performing the calculation in momentum space. Here, $e(p) := (p^2+m^2)^{1/2}$ and the index set I is given by $I := \{(l,m,s) | l \in \mathbb{N}_0, m = -l-1/2, \dots, l + 1/2, s = \pm 1/2, \Omega_{l,m,s} \neq 0\}$. The kernel is obtained to be $k_{l,s} = k_{l,s}^{(0)} + k_{l,s}^{(1)}$ with

$$k_{l,s}^{(n)}(p',p) := \sqrt{1 + \frac{(-1)^n m}{e(p)}}\, Q_{l+2ns}\left(\frac{p}{2p'} + \frac{p'}{2p}\right) \sqrt{1 + \frac{(-1)^n m}{e(p')}}.$$

and $n(p) = [2e(p)(e(p)+m)]^{1/2}$. 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).

We consider in the following mainly the operator restricted to particles with spin 1/2 in the lowest angular momentum channel $l = 0$ and denote it for brevity by $b := b_{0,1/2}$.

Definition 1

$$b\psi(p) := e(p)\psi(p) - \frac{\alpha}{2\pi}\int_0^\infty \psi(p')k_{0,1/2}(p',p)dp =: ([e-\alpha v]\psi)(p) \qquad (2)$$

with domain $D(b) = D(p) = L^2(\mathbb{R}^+, (1+p^2)dp)$ *acting in* $L^2(\mathbb{R}^+)$.

Note that the operator is well defined since $D(p) \subseteq D(v)$ and $e(p) - p \in L^\infty(\mathbb{R}^+)$ and that for simplicity αZ was replaced by α and α_c corresponds to αZ_c in the following.

To consider domain questions it is enough to consider an operator which differs from the operator b by a bounded operator. The next Lemma tells us that this is the case for the operator $b(0)$ where $b(0)$ is the operator b with mass $m = 0$.

Theorem 1 *The operator* $b(m) - b(0)$ *extends to a bounded operator on* $L^2(\mathbb{R}^+)$.

Proof. We will show that $\sup_\psi |\langle\psi, [b(m)-b(0)]\psi\rangle| < \infty$ for $\psi \in L^2(\mathbb{R}^+)$ and $||\psi|| = 1$ by considering the kinetic and potential energy separately. Since $e(p) - p \in L^\infty(\mathbb{R}^+)$ we need to consider only the potential energy

$$\frac{\alpha Z}{2\pi}\int_0^\infty\int_0^\infty \psi(p')^*[\tilde{k}_0(p',p) + \tilde{k}_1(p',p)]\psi(p)dpdp' \qquad (3)$$

with the kernels $\tilde{k}_j$ given by

$$\tilde{k}_j(p',p) := \left(\sqrt{1+\frac{(-1)^j m}{e(p)}}\sqrt{1+\frac{(-1)^j m}{e(p')}} - 1\right) Q_j\left(\frac{p}{2p'} + \frac{p'}{2p}\right)$$

which is well defined on $L^2(\mathbb{R}^+)$ since $Q_j(\cdot/2p' + p'/2\cdot) \in L^2(\mathbb{R}^+)$. We replace all terms by their moduli $\left|\langle\psi, (\tilde{k}_0 + \tilde{k}_1)\psi\rangle\right| \le \langle|\psi|(|\tilde{k}_0| + |\tilde{k}_1|)|\psi|\rangle$ and start to consider the term with the $\tilde{k}_0$ kernel by estimating

$$\sqrt{1+\frac{m}{e(p)}}\sqrt{1+\frac{m}{e(p')}} - 1 \le \frac{m}{2e(p)} + \frac{m}{2e(p)} + \frac{m^2}{4e(p)e(p')}.$$

With $1/[e(p)e(p')] \le 1/e(p) + 1/e(p')$ it remains to prove finiteness of

$$\int |\psi(p')^*| Q_0\left(\frac{p}{2p'} + \frac{p'}{2p}\right)\left(\frac{1}{e(p)} + \frac{1}{e(p')}\right)|\psi(p)|\, dpdp'. \qquad (4)$$

Introducing test functions $h(p) > 0$ and using the Schwarz inequality (see also [3, 18]), the upper bound

$$\int_0^\infty dp|\psi(p)|^2 \int_0^\infty Q_0\left(\frac{p}{2p'} + \frac{p'}{2p}\right)\left(\frac{1}{e(p)} + \frac{1}{e(p')}\right)\frac{h(p')}{h(p)}dp'$$

is obtained. This can be done since the kernel in (4) is symmetric and positive. We choose $h(p) = p^{-\alpha}$ with $0 < \alpha < 1$ and estimate

$$\int_0^\infty Q_0\left(\frac{p}{2p'} + \frac{p'}{2p}\right)\frac{h(p')}{h(p)}\frac{dp'}{e(p')} \leq \int_0^\infty Q_0\left(\frac{1}{2x} + \frac{x}{2}\right)\frac{dx}{x^{1+\alpha}} < \infty$$

since $Q_0(x/2 + 1/2x) = O(1/x)$ for $x \to \infty$ and $Q_0(x/2 + 1/2x) = O(x)$ for $x \to 0$. The remaining term can immediately seen to be finite by scaling.

The term with the $\tilde{k}_1$ kernel can be estimated analogously by noting that $Q_0(t) \geq Q_1(t)$ for $t \geq 1$. $\square$

Since $Q_0(t) \geq Q_1(t) \geq Q_2(t) \ldots$ for $t \geq 1$ the Theorem holds for any operator $b_{l,s}$:

Corrolary 1 *The operators $b_{l,s}(m) - b_{l,s}(0)$ extends to bounded operators on $L^2(\mathbb{R}^+)$.*

3 The massless operator

In this chapter we will consider the operator $b(0)$. To elucidate its structure the unitary Mellin transform M will be helpful (see Appendix A for the definition and some properties). With $b^\# = Mb(0)M^{-1}$ and $\psi^\# = M\psi$ we obtain

$$b^\#\psi^\#(s) = [1 - \alpha V(s + i/2)]\psi^\#(s + i)$$

with $V(z) = [V_0(z) + V_1(z)]/2$ and

$$V_0(z) = \frac{\tanh(\pi z/2)}{z}, \qquad V_1(z) = \frac{1}{1+z^2}\frac{z}{\tanh(\pi z/2)} \tag{5}$$

(see Appendix A) acting in $L^2(\mathbb{R})$. The Mellin transformed domain is characterized by the following

Theorem 2 *The function ψ is in $D(p^\lambda) = L^2(\mathbb{R}^+, (1+p^{2\lambda})dp)$ if and only if there exists a unique function $\Psi^\#$ holomorphic in the strip $S(0,\lambda) = \{z \in \mathbb{C} \,|\, 0 < \Im(z) < \lambda\}$ with*

- $\lim_{y\to 0} \int_{\mathbb{R}} |\Psi^\#(s+iy) - \psi^\#(s)|^2 \, ds = 0$
- $\lim_{y\to\lambda} \int_{\mathbb{R}} |\Psi^\#(s+iy) - \psi^\#(s+i\lambda)|^2 \, ds = 0$
- $\sup_{y\in(0,\lambda)} \int_{\mathbb{R}} |\Psi^\#(s+iy)|^2 \, ds < \infty$

and $\psi^\# \in L^2(\mathbb{R})$ and $Mp^\lambda\psi(s) = \psi^\#(s+i\lambda)$.

Such Paley-Wiener type Theorems can be found in [16]. We will identify $\Psi^\#$ and $\psi^\#$ in the following.

The Theorems concerning the operator $b(0)$ can now more or less be copied from [19]. Note that the difference between the massless Herbst and Brown Ravenhall operator is the different function V arising from the different potential energy. However, their overall behavior (which is important for the proof) is the same.

Theorem 3 *The operator $b^\#$ is closed for $\alpha \in \mathbb{C}$ if and only if $\alpha \notin \Delta_0 := \{V(s+i/2)^{-1} | s \in \mathbb{R}\}$*

Proof. Let $\alpha \in \mathbb{C}\backslash\Delta_0$ and choose a convergent series $\{\psi_n^\#, b^\#\psi_n^\#\} \in \Gamma(b^\#)$, where $\Gamma(b^\#)$ is the graph of $b^\#$ and $\psi_n^\# \to \psi^\#$. Since $V(s+i/2) \to 0$ for $s \to \pm\infty$ which follows from(16), it is $C_1 \leq |1 - \alpha V(s+i/2)|$ with $0 < C_1$. This lower bound implies the convergence of $\psi_n^\#(s+i) = MpM^{-1}\psi_n^\#(s) =: p^\#\psi_n^\#(s)$ from the converges of $b^\#\psi_n^\#$. Since the operator p with domain $D(p)$ is closed we have that $\psi_n^\#(s+i) \to \psi^\#(s+i)$ and because the function $|1 - \alpha V(s+i/2)|$ is bounded we also have $b^\#\psi_n^\# \to b^\#\psi^\#$ which ends the proof.

Now let $\alpha \in \Delta_0$ with $\alpha = V(s_0+i/2)^{-1}$ for some $s_0 \in \mathbb{R}$. Take the series $\psi_n^\#(s) = (s - s_0 - i - i/n)^{-1} \to (s - s_0 - i)^{-1}$ and note that $\psi_n^\# \in D(b^\#)$ but $(s - s_0 - i)^{-1} \notin D(b^\#)$ because of the singularity at $s_0 + i$. Since $[1 - \alpha V(s+i/2)]\psi_n^\#(s+i)$ converges because of the zero of $1 - \alpha V(s+i/2)$ at $s = s_0$, the operator is not closed. $\square$

Considering just real values for the coupling constant α we get the

Corrolary 2 *Let $\alpha \in \mathbb{R}$. Then the operator b is closed if and only if $\alpha \neq \alpha_c' = 3/4$*

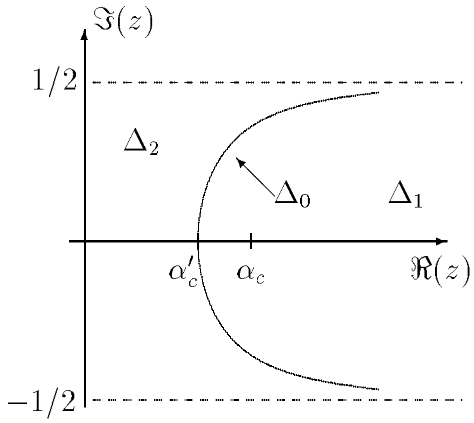

Figure 1: The complex plane divided according to $V(z)^{-1}$

Proof. From (16) we find that $V(s+i/2)$ is real for $s \in \mathbb{R}$ if and only if $s = 0$. From $V(i/2) = 4/3$ follows the claim. $\square$

The next Theorem characterizes the adjoint of b. To state the Theorem the complex plain is divided in three disjoint sets according to the Mellin transformed potential:

Definition 2

$$\begin{aligned}
\Delta_0 &:= \{V(s+i/2)^{-1} | s \in \mathbb{R}\} \\
\Delta_1 &:= \{V(z)^{-1} | \, |\Im(z)| < 1/2\} \\
\Delta_2 &:= \mathbb{C} \backslash (\Delta_0 \cup \Delta_1)
\end{aligned}$$

Theorem 4 *Let $\alpha \in \mathbb{C}$. Then, the adjoint $b^{\#*}$ is an extension of $p^{\#} - \alpha^* v^{\#}$ with*

$$b^{\#*}\psi^{\#}(s) = [1 - \alpha^* V(s+i/2)]\psi^{\#}(s+i)$$

and

$$D(b^{\#*}) = \{\psi^{\#} \in L^2(\mathbb{R}) | [1 - \alpha^* V(s-i/2)]\psi^{\#}(s) \in D(p^{\#}). \tag{6}$$

Moreover,

1. *If $\alpha \in \Delta_0$, then $b^{\#*} = \overline{p^{\#} - \alpha^* v^{\#}}$, the closure of $p^{\#} - \alpha^* v^{\#}$.*

2. *Let $\alpha \in \Delta_1$ and z_0 the solution of $\alpha = V(z_0)^{-1}$ with $|\Im(z_0)| < 1/2$ and let $\psi^\# = \phi^\# + \xi^\#$ with $\phi^\# \in D(p^\#)$. Then*

$$D(b^{\#*}) = \begin{cases} \{\psi^\# \,|\xi^\# \in \mathrm{span}\,[(s-i/2-z_0^*)^{-1}, (s-i/2+z_0^*)^{-1}]\,\} & z_0 \neq 0 \\ \{\psi^\# \,|\xi^\# \in \mathrm{span}\,[(s-i/2)^{-1}, (s-i/2)^{-2}]\,\} & z_0 = 0. \end{cases} \tag{7}$$

3. *If $\alpha \in \Delta_2$, then $b^{\#*} = p^\# - \alpha^* v^\#$.*

Proof. Note that for a bounded operator B and a self-adjoint operator A with domain $D(A)$, $\psi \in D\,[(BA)^*]$ is equivalent to $B^*\psi \in D(A)$, and on $D\,[(BA)^*]$ it is $(BA)^* = AB^*$. Now let $\alpha \in \mathbb{C}$ and take $B\psi^\#(s) := [1-\alpha V(s+i/2)]\psi^\#(s)$ and $A := p^\#$. Then the first part of the Theorem for $\alpha \in \mathbb{C}$ follows immediately if we can show that $b^{\#*}$ is an extension of $p^\# - \alpha^* v^\#$. But since $V(z-i/2)$ is analytic and bounded in the strip $-1/2+\epsilon < \Im(z) < 3/2-\epsilon$ for $\epsilon > 0$ which follows from (16), then $\psi^\# \in D(p^\#)$ implies $[1-\alpha^* V(s-i/2)]\psi^\#(s) \in D(p^\#)$.

Let $\alpha \in \Delta_2$. Then the function $1-\alpha^* V(z)$ has no zero for $\Im(z) \leq 1/2$ and we can find some constant $C_1 > 0$ such that $|1-\alpha^* V(z)| \geq C_1$. Therefore, $|1-\alpha^* V(z)|^{-1}$ is analytic in the strip $\Im(z) < 1/2$ and bounded when $\Im(z) \leq 1/2$ and from $[1-\alpha^* V(s-i/2)]\psi^\#(s) \in D(p^\#)$ follows $\psi^\# \in D(p^\#)$. Since $b^{\#*}$ is an extension of $p^\# - \alpha^* v^\#$ this proofs the claim.

Let $\alpha \in \Delta_1$ and $z_0 \neq 0$. Then the function $1-\alpha^* V(z)$ has exactly two zeros z_0^* and $-z_0^*$ according to Lemma 2. Because of these zeros

$$[1-\alpha^* V(s-i/2)](s-i/2 \pm z_0^*)^{-1} \in D(p^\#)$$

and therefore the domain given in (7) is included in the domain (6). It remains to show the converse inclusion, i.e., for $[1-\alpha^* V(s-i/2)]\psi^\#(s) \in D(p^\#)$ with $\psi^\# \in L^2(\mathbb{R})$ we need to show that

$$\phi^\#(s) := \psi^\#(s) - c_1(s-i/2-z_0^*)^{-1} - c_2(s-i/2+z_0^*)^{-1} \in D(p^\#).$$

Since possible simple poles of $\psi^\#(s)$ are subtracted if $c_1, c_2 \in \mathbb{C}$ are chosen appropriately we have that $\phi^\#(s)$ is holomorphic in $S(0,1)$ and it remains to proof that $\sup_{y\in(0,1)} \int |\phi^\#(s+iy)|^2\, ds < \infty$. Let C_1 be the upper bound for $\phi^\#(z)$ in a closed rectangle $R \subset S(0,1)$ with length X and $\{z_0^*, -z_0^*\} \subset R\backslash\partial R$

and let C_2 be the lower bound off $1-\alpha^* V(z-i/2)$ in $\overline{S(0,1)}\backslash R$. Then the estimate

$$\int |\phi^\#(s+iy)|^2\, ds \le C_2^{-2} \int |[1-\alpha^* V(s-i/2+iy)]\psi^\#(s+iy)|^2\, ds + XC_1^2$$

holds and the supremum of the r.h.s. is finite by the assumption on ψ and therefore $\phi^\# \in D(p^\#)$. The case $z_0 = 0$ can be treated in the same manner.

Finally, let $\alpha \in \Delta_0$. Since $b^{\#*}$ is an extension of $p^\# - \alpha^* v^\#$ and is closed we have the inclusion $D(b^{\#*}) \subseteq D(\overline{p^\# - \alpha^* v^\#})$. So it remains to prove the converse inclusion, i.e., for $\psi^\# \in D(b^{\#*})$ there should exist a sequence $\psi_n^\# \in D(p^\#)$ such that $\psi_n^\# \to \psi^\#$ and $(p^\# - \alpha^* v^\#)\psi_n^\#$ converges. The construction of the series $\psi_n^\#$ can be found in [19, proof of Theorem 2]. □

We are now able to specialize the results to the physical interesting case of a real coupling constant with

Corrolary 3 *Let $\alpha \in \mathbb{R}$. Then $b^\#$ is self-adjoint for $\alpha < \alpha_c'$, essentially self-adjoint for $\alpha = \alpha_c'$, and symmetric with defect indices $(1,1)$ for $\alpha_c' < \alpha \le \alpha_c$.*

Proof. The case $\alpha = \alpha_c' \in \Delta_0$ and $\alpha < \alpha_c'$, i.e., $\alpha \in \Delta_1$, is clear. Let $\alpha_c' < \alpha \le \alpha_c$ which is equivalent with $\alpha \in \Delta_2$. Since the sum of the defect indices $n_\pm = \dim[\mathrm{Ker}(b^\# \pm i)]$ can be expressed as $n_+ + n_- = \dim[D(b^{\#*})/D(b^\#)]$ (see [12, Theorem X.2]) we have $n_+ + n_- = 2$ according to Theorem 2, Part 2). Since $b(0)$ is a real operator, Neumann's Theorem tells us that $n_+ = n_-$. □

For $\alpha_c' < \alpha \le \alpha_c$ the operator $b^\#$ is symmetric and admits a one parametric family of self-adjoint extensions since the self-adjoint extensions are in one-to-one correspondence with the partial isometries of the deficiency subspaces. The Friedrichs extension is considered to be the physical relevant one and will be characterized in the following

Theorem 5 *Let $\alpha_c' < \alpha \le \alpha_c$ and $-1/2 < \beta \le 0$ the solution of $\alpha = V(i\beta)^{-1}$. Then the Friedrichs extension $b_F^\#$ of $b^\#$ is given by $b^{\#*}$ restricted to the domain*

$$D(b_F^\#) = \left\{\phi^\# \,\middle|\, \xi^\# \in \mathrm{span}\left[(s-i/2+i\beta)^{-1}\right]\right\}$$

with $\phi^\# = \psi^\# + \xi^\#$ and $\psi^\# \in D(p^\#)$.

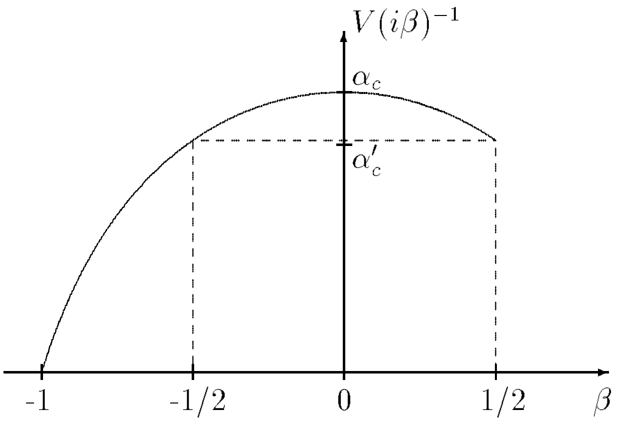

Figure 2: The function $V(i\beta)^{-1}$ over β

Note that the inverse Mellin transform of $(s - i/2 + i\beta)^{-1}$ is given by $i\sqrt{2\pi}\Theta(p-1)p^{-1+\beta}$ according to (17) and the asymptotic behavior of this function for $p \to \infty$ is exactly what is used as a test function in [17] to obtain a lower bound for the ground state energy of b. The function $V(i\beta)^{-1}$ is illustrated in Figure 2. *Proof.* For the proof of the Theorem the characterization $D(b_F^{\#}) = D(b^{\#*}) \cap Q(b^{\#})$ of the domain of the Friedrichs extension will be useful. Here, $Q(b^{\#})$ is the form domain of the closure of the quadratic associated with $b^{\#}$. For $\alpha < \alpha_c$ we have according to [3] that $Q(b_0) = Q(p) = D(p^{1/2})$. From Theorem 4, Part 2), we obtain $D(b^{\#*})$ and note that from $\{(s-i/2+i\beta)^{-1}, (s-i/2-i\beta)^{-1}\}$ the second function is not in $Q(b)$ but the first one is.

Now let $\alpha = \alpha_c$ which corresponds to $\beta = 0$. Since we do not know the domain $Q(b)$ in this case we have to investigate the quadratic form more closely. For $\psi_1^{\#}, \psi_2^{\#} \in D(p^{\#})$ it is

$$\langle \psi_1^{\#}, b^{\#}\psi_2^{\#}\rangle = \int_{\mathbb{R}} \psi_1^{\#}(s)^*(1-\alpha_c V(s+i/2))\psi_2^{\#}(s+i)\,ds.$$

Note that $\psi^{\#}(z^*)^*$ is holomorphic in $S(-1,0)$ and so is the rest of the integrand. Therefore the Cauchy Theorem can be used to shift the integration by $-1/2$ in the lower complex plane. By change of variables

$$\int_{\mathbb{R}} \psi_1^{\#}(s+i/2)^*[1-\alpha_c V(s)]\psi_2^{\#}(s+i/2)\,ds \tag{8}$$

is obtained. Now suppose that from $\psi^\# \in Q(b^\#)$ would follow that

$$(s-i/2)(s-iA)^{-1}\psi^\#(s) \in D(\sqrt{p^\#})$$

with a fixed $A>1$. Note that $\psi^\# \in D(b^{\#*})$ means $\psi^\# = \phi^\# + \xi^\#$ with $\phi^\# \in D(p^\#)$ and $\xi^\# \in \operatorname{span}[(s-i/2)^{-1},(s-i/2)^{-2}]$. If $\xi^\#(s)=(s-i/2)^{-1}$ then $(s-i/2)(s-iA)^{-1}\xi^\#(s) \in D(\sqrt{p^\#})$ but if $\xi^\#(s)=(s-i/2)^{-2}$ this product is not in $D(\sqrt{p^\#})$. Therefore, $b^{\#*}$ restricted on the set

$$\left\{\psi^\# \,\middle|\, \psi^\# = \phi^\# + \xi^\#,\, \phi^\# \in D(p^\#),\, \xi^\# \in \operatorname{span}\left[(s-i/2)^{-1}\right]\right\} \tag{9}$$

is an extension of $b_F^\#$. When we can show that this extension is self-adjoint we know that it is the Friedrichs extension since the Friedrichs extension is the only self-adjoint extension which domain is included in the form domain $Q(b^\#)$. We begin to prove the Lemma which we already used:

Lemma 1 *Let $\alpha=\alpha_c$. Then $\psi^\# \in Q(b^\#)$ implies $(s-i/2)(s-iA)^{-1}\psi^\#(s) \in D(\sqrt{p^\#})$ for $A>1$.*

Proof. Assume $\psi^\# \in Q(b^\#)$, then there exists a sequence $\psi_n^\# \in D(b^\#)$ with $\psi_n^\# \to \psi^\#$ such that $\langle \psi_n^\# - \psi_m^\#, b^\#(\psi_n^\# - \psi_m^\#)\rangle \to 0$ for $n,m\to\infty$. From (8) follows that this is equivalent with the convergence of $[1-\alpha_c V(s)]^{1/2}\psi_n^\#(s+i/2)$. Note that $1-\alpha_c V(s)$ has a double zero at $s=0$ and $V(s)\to 0$ for $s\to\pm\infty$. This implies that the convergence of the previous series is equivalent with the convergence of $s(s+i/2-iA)^{-1}\psi_n^\#(s+i/2)$. Now let $\phi_n^\#(s) := (s-i/2)(s-iA)^{-1}\psi_n^\#(s)$ and note that $\phi_n^\# \in D(b^\#) \subset D(\sqrt{p^\#})$. Then $\sqrt{p^\#}\phi_n^\#$ converges and

$$\int_{\mathbb{R}} |\phi_n^\#(s) - (s-i/2)(s-iA)^{-1}\psi^\#(s)|^2\, ds \to 0.$$

Since the multiplication operator $\sqrt{p}$ is closed, $(s-i/2)(s-iA)^{-1}\psi^\#(s) \in D(\sqrt{p^\#})$. $\square$

Now we are left to prove self-adjointness of $b^{\#*}$ restricted to the set (9). Denote this operator by $b_f^\#$. Then the adjoint of $b_f^\#$ is the operator $b^{\#*}$ with domain (7) and the additional condition that $\langle b_f^\#(\cdot - i/2)^{-1}, \psi^\#\rangle =$

$\langle(\cdot - i/2)^{-1}, b^{\#*}\psi^{\#}\rangle$ for $\psi^{\#} \in D(b^{\#*})$. This is explicitly

$$\int_{\mathbb{R}} \frac{1-\alpha_c V(s-i/2)}{s-i/2}\left(\xi^{\#}(s) + \frac{c_1}{s-i/2} + \frac{c_2}{(s-i/2)^2}\right) ds$$
$$= \int_{\mathbb{R}} \frac{1-\alpha_c V(s+i/2)}{s+i/2}\left(\xi^{\#}(s+i) + \frac{c_1}{s+i/2} + \frac{c_2}{(s+i/2)^2}\right) ds. \quad (10)$$

The right and the left hand side of (10) are the integrals of the function

$$[1-\alpha_c V(z)]\left(\xi^{\#}(z+i/2) + c_1 z^{-1} + c_2 z^{-2}\right) z^{-1}$$

along the lines $\mathcal{L}(s) = s + i/2$ and $\mathcal{L}(s) = s - i/2$, $s \in \mathbb{R}$. Between these two lines the function has a simple pole at $z = 0$ when $c_2 \neq 0$ because of the double zero of $V(z)$ at $z = 0$ and therefore a nonzero residue. If and only if $c_2 = 0$ the integrals are equal and we get $b_f^{\#*} = b_f^{\#}$ and therefore $b_f^{\#} = b_F^{\#}$. $\Box$

Now we will introduce a self-adjoint holomorphic family of operators which shows that, near the critical coupling constant α_c, the operator $b^{\#}$ is not holomorphic in α but in $\sqrt{\alpha_c - \alpha}$. However, since we are not able to "explain" with this Theorem that b is strict positive at $\alpha = \alpha_c$ we will not state the proof here whose analogon for the square root operator can be found in [19]. Let us start to define

Definition 3 *Let $G = \{z \in \mathbb{C} \mid -1/2 \leq \Re(z) < 1/2\} \cup (\Delta_2)^{-1}$ where $(\Delta_2)^{-1}$ is the reciprocal image of Δ_2 by the function $V(i\cdot)^{-1}$ and let for $\beta \in G$*

$$b_\beta \psi^{\#}(s) = \left[1 - \frac{V(s+i/2)}{V(i\beta)}\right]\psi^{\#}(s+i)$$

with

$$D(b_\beta) = \left\{\psi^{\#} \in L^2(\mathbb{R}) \,|\, \frac{s - i/2 + i\beta}{s - iA}\psi^{\#}(s) \in D(b^{\#})\right\}$$

and a fixed $A > 1$.

Note that this definition is suggested by the previous result about the Friedrichs extension. When $\beta \in \mathbb{R}$ and $-1 < \beta \leq 0$, i.e. $\alpha_c' < \alpha \leq \alpha_c$, b_β is just the Friedrichs extension. For $0 < \beta < 1/2$, i.e. $\alpha_c > \alpha > \alpha_c'$, b_β is another extension of b. It turns out that nothing special happens at the critical coupling constant for the operator b_β:

Theorem 6 *The family of operators b_β forms a self-adjoint holomorphic family of operators for $\beta \in G$ (in the sense of Kato).*

The definition of a self-adjoint holomorphic family of operators for unbounded operators can be found in [8, p. 366].

Near α_c the relation $\beta(\alpha)$ behaves like $\sqrt{\alpha_c - \alpha}$, i.e. the operator b (or the Friedrichs extension of b) is holomorphic when considered as an operator depending on $\sqrt{\alpha_c - \alpha}$.

4 The operator B and the essential spectrum for $Z = Z_c$

The analysis carried out in the last Section can be done analogously for any of the operators $b_{l,s}$ with domain $D(p)$:

Theorem 7 *The operators $b_{0,1/2}$ and $b_{1,-1/2}$ are self-adjoint for $\alpha < \alpha'_c$, essentially self-adjoint for $\alpha = \alpha'_c$ and symmetric with defect indices $(1,1)$ for $\alpha'_c < \alpha \leq \alpha_c$. The domain of their Friedrichs extension $b^F_{l,s}$ is given by*

$$\left\{\phi = \psi + \xi \,|\, \psi \in D(p), \xi \in \mathrm{span}[\Theta(p-1)p^{-1-\beta}]\right\} \tag{11}$$

where $0 \leq \beta < 1/2$ is determined by the equation

$$\frac{2}{\alpha} = \frac{\tan(\pi\beta/2)}{\beta} + \frac{\beta}{(1-\beta^2)\tan(\pi\beta/2)}.$$

The operators $b_{l,s}$ with $(l,s) \notin \{(0,1/2),(1,-1/2)\}$ are self-adjoint for $\alpha \leq \alpha_c$.

Proof. Let $b^{\#}_{l,s}\psi^{\#}(s) = [1 - V_{l,s}(s+i/2)]\psi^{\#}(s+i)$ with $V_{l,s}(z) = [V_l(z) + V_{l+2s}(z)]/2$ and $V_l(z)$ given by (16). Since $b_{0,1/2} = b_{1,-1/2}$ in the case $m = 0$ and the domain (11) is just the domain $D(b^{\#}_F)$ in momentum space we only have to check that the corresponding α'_c for the operators $b_{l,s}$ with $(l,s) \notin \{(0,1/2),(1,-1/2)\}$ denoted by $\alpha'_{c,(l,s)}$ is bigger than α_c. From (17) we get that $\alpha'_{c,(l,s)} = V_{l,s}(i/2)^{-1} = 2/[(l+1/2)^{-1} + (l+2s+1/2)^{-1}]$ and this is already for $l = 1$ and $s = 1/2$ bigger than α_c. □

Now we are able to characterize the Friedrichs extension of the operator B by defining it as a direct sum $B = \bigoplus_{(l,m,s)\in I} b_{l,s}$ acting in $\mathfrak{H}$ with domain

$$D(B) = \left\{ \psi \in \mathfrak{H} \,|\, \psi_{l,m,s} \in D(b_{l,s}^F), \sum_{(l,m,s)\in I} ||\psi_{l,m,s}||^2 < \infty \right\} \tag{12}$$

This operator is self-adjoint for $\alpha \leq \alpha_c$. For $\alpha < \alpha_c$ the essential spectrum was already localized in [3] to be $\sigma_{\mathrm{ess}}(B) = [m, \infty)$. We extend the result to the critical case by the

Theorem 8 *$\sigma_{ess}(B) = [m, \infty)$ for $\alpha \leq \alpha_c$.*

Proof. Since the Theorem is known for $\alpha < \alpha_c$ let $\alpha = \alpha_c$ and $B = B_0 - \Lambda_+ W \Lambda_+$ with $W = \alpha_c/|\boldsymbol{x}|$ and $B_0 = \Lambda_+ D_0 \Lambda_+$. We will show that $(B+1)^{-1} - (B_0+1)^{-1}$ is compact and therefore $\sigma_{\mathrm{ess}}(B) = \sigma_{\mathrm{ess}}(B_0)$ [13, Theorem XIII.14]. Since $D(B_0) \subseteq D(B)$ we have for any $\psi \in D(B_0)$

$$(B+1)\psi - (B_0+1)\psi = -\Lambda_+ W \Lambda_+ \psi. \tag{13}$$

Taking $\psi = (B_0+1)^{-1}\phi$ with $\phi \in L^2(\mathbb{R}^3)\otimes\mathbb{C}^4$ and multiplying with $(B+1)^{-1}$ from the left we obtain

$$\begin{aligned}(B+1)^{-1} - (B_0+1)^{-1} &= (B+1)^{-1}\Lambda_+ W \Lambda_+ (B_0+1)^{-1} \\ &= (B+1)^{-1}\Lambda_+ W^t W^{1-t} \Lambda_+ (B_0+1)^{-1}\end{aligned} \tag{14}$$

where we choose $0 < t < 1/2$. Consider the second factor

$$W^{1-t}\Lambda_+(B_0+1)^{-1} = W^{1-t}(B_{00}+1)^{-1}\Lambda_+$$

with $B_{00} = \sqrt{\boldsymbol{p}^2 + m^2}$, which is compact since $W^{1-t}(B_{00})^{-1}$ is compact according to [19, Lemma 4] and Λ_+ is bounded. The first factor can be written as

$$(B+1)^{-1}\Lambda_+ W^t = (B+1)^{-1}(B_{00}+1)^t(B_{00}+1)^{-t}\Lambda_+ W^t$$

and $(B_{00}+1)^{-t}\Lambda_+ W^t = \Lambda_+(B_{00}+1)^{-t}W^t$. Now consider the operator $W^t(B_{00}+1)^{-t}$. Since $D(|\boldsymbol{p}|^t) \subseteq D(|\boldsymbol{x}|^{-t})$ according to [6, Theorem 2.5] it is everywhere defined. The operator W^t is closed and $(\sqrt{\boldsymbol{p}^2+m^2}+1)^{-t}$ is bounded so the closed graph Theorem gives boundedness of this operator.

Then it is easy to see that the densely defined operator $(B_{00}+1)^{-t}W^t$ is bounded. It remains to prove boundedness of $(B+1)^{-1}(B_0+1)^t$. Again we start to consider the operator $(B_{00}+1)^t(B+1)^{-1}$ and note that $D(B) \subseteq D([B_{00}+1]^t) = D(|\boldsymbol{p}|^t)$ for $0 < t < 1/2$ which follows from (12) and Theorem 7. Since $(\sqrt{\boldsymbol{p}^2+m^2}+1)^t$ is closed and $(B+1)^{-1}$ is bounded $(B_{00}+1)^t(B+1)^{-1}$ is bounded and we conclude that the densely defined operator $(B+1)^{-1}(B_{00}+1)^t$ is also bounded. Having shown that the r.h.s. of (14) is the product of a compact and bounded operators this ends the proof. $\square$

Note that the last Theorem allows to extend the remark made in [18] that $\sigma_{\mathrm{disc}}(B)$ has infinitely many elements for $Z < Z_c$ to the critical case.

A The Mellin transform

The Mellin transform M can be defined for $\psi \in L^2(\mathbb{R}^+)$ as

$$\psi^\#(s) := M\psi(s) = \frac{1}{\sqrt{2\pi}}\int_0^\infty dp\, p^{-1/2-is}\psi(p), \qquad s \in \mathbb{R}.$$

The inverse mapping is given by

$$M^{-1}\psi^\#(p) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^\infty ds\, s^{-1/2+ip}\psi^\#(s), \qquad p \in \mathbb{R}^+.$$

The Mellin transform is a unitary mapping from $L^2(\mathbb{R}^+)$ in $L^2(\mathbb{R})$ and is closely connected with the Fourier transform. In fact, it can be viewed as the Fourier transform on the group $(\mathbb{R}^+, \cdot)$ and obeys a convolution Theorem of the form

$$M\psi \star \phi(s) := M\left[\int_0^\infty \frac{dp}{p}\psi(p)\phi\left(\frac{\cdot}{p}\right)\right](s) = \psi^\#(s)\phi^\#(s).$$

To obtain the Mellin transform of the operator $b(0) = p - \alpha v(0)$ note that $2\pi p^{-1/2}v(0)p^{-1/2}\psi = [Q_0(\cdot/2+2/\cdot) + Q_1(\cdot/2+2/\cdot)] \star \psi$ and that the Mellin transforms of the Legendre functions of the second kind with this special argument are given by

$$V_l(z) := \frac{1}{\pi}M\left[Q_l\left(\frac{\cdot}{2}+\frac{2}{\cdot}\right)\right](z) = \frac{1}{2}\frac{\Gamma([l+1-iz]/2)}{\Gamma([l+2-iz]/2)}\frac{\Gamma([l+1+iz]/2)}{\Gamma([l+2+iz]/2)} \tag{15}$$

which can be seen from [10, p. 72, 8.17] or by using the definition of the functions Q_l and writing this as a convolution [19]. Finally, from the identities $\Gamma(z)\Gamma(1-z) = \pi/\sin(\pi z)$ and $\Gamma(z+1) = z\Gamma(z)$ the function $V(z) = [V_0(z) + V_1(z)]/2$ in (5) is obtained.

The partial fraction expansion [11, p. 5]

$$V_l(z) = \frac{2}{\pi}\sum_{j=0}^{\infty} \frac{\Gamma(n+1/2)}{\Gamma(n+1)} \frac{\Gamma(n+l+1)}{\Gamma(n+l+3/2)} \frac{2n+l+1}{(2n+l+1)^2+z^2} \tag{16}$$

will be useful to explore properties of $V(z)$ and to prove the

Lemma 2 *$V(z)$ is holomorphic in the strip $S(-1,1) = \{z \in \mathbb{C}| -1 < \Im(z) < 1\}$ and for $\alpha \in \Delta_1$ the equation $V(z)^{-1} = \alpha$ has exactly two solutions $z_0, -z_0 \in S(-1/2, 1/2)$.*

Proof. Consider the closed path $-X + i/2 \to X + i/2 \to X - i/2 \to -X - i/2 \to -X + i/2$. The image of this path under $V(z)$ is a closed curve which is covered twice according to (16). The images of the points inside the path are inside the closed curve. Therefore there are just two zeros and the second one is $-z_0$ since the function V is quadratic in z. $\square$

Finally, we remark that the Mellin transform of the function $\mu^{-is}/(s-ia)$ is given by

$$M^{-1}\frac{\mu^{-i\cdot}}{\cdot - ia}(p) = \begin{cases} i\sqrt{2\pi}\,\Theta(p-\mu)\,p^{-1/2-a}, & \Re(a) > 0 \\ -i\sqrt{2\pi}\,\Theta(\mu-p)\,p^{-1/2-a}, & \Re(a) < 0 \end{cases} \tag{17}$$

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