THE SPECTRUM OF RELATIVISTIC ATOMS ACCORDING TO BETHE AND SALPETER AND BEYOND

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Abstract. We review Evans' contributions to the spectral theory of operators describing relativistic particle systems. We will concentrate on no-pair operators and recent extensions of that work.

1. William Desmond Evans' Papers on Relativistic Quantum Mechanics

William Desmond Evans contributed to the spectral theory of operators describing relativistic particle systems as follows:

(1) W. D. Evans. A problem in relativistic quantum mechanics. *Quart. J. Math. Oxford Ser. (2)*, 17:345–358, 1966.
(2) W. D. Evans. Eigenfunction expansions associated with the Dirac relativistic equations. *Quart. J. Math. Oxford Ser. (2)*, 17:211–233, 1966.
(3) W. D. Evans. Eigenfunction expansions associated with the Dirac relativistic equations. II. *Quart. J. Math. Oxford Ser. (2)*, 18:239–262, 1967.
(4) W. D. Evans. The Dirac equations with a spherically symmetrical scalar potential. *Quart. J. Math. Oxford Ser. (2)*, 21:89–99, 1970.
(5) W. D. Evans. On the decomposition method and the spectrum of the Dirac operator. *Proc. London Math. Soc. (3)*, 21:651–673, 1970.
(6) W. D. Evans. On the unique self-adjoint extension of the Dirac operator and the existence of the Green matrix. *Proc. London Math. Soc. (3)*, 20:537–557, 1970.
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(17) A. A. Balinsky and W. D. Evans. On the spectral properties of the Brown-Ravenhall operator. *J. Comput. Appl. Math., 148(1):239–255, 2002. On the occasion of the 65th birthday of Professor Michael Eastham.*
(18) A. A. Balinsky and W. D. Evans. On the zero modes of Weyl-Dirac operators and their multiplicity. *Bull. London Math. Soc.*, 34(2):236–242, 2002.
(19) A. A. Balinsky and W. D. Evans. Zero modes of Pauli and Weyl-Dirac operators. In *Advances in differential equations and mathematical physics (Birmingham, AL, 2002)*, volume 327 of *Contemp. Math.*, pages 1–9. Amer. Math. Soc., Providence, RI, 2003.

2. The Energy According to Bethe and Salpeter

2.1. **The Brown-Ravenhall Operator.** The Coulomb-Dirac operator is

$$D_g := \boldsymbol{\alpha} \cdot \mathfrak{p} + m\beta - g|\cdot|^{-1}, \tag{1}$$

where $\mathfrak{p} := -\mathrm{i}\nabla$, m is the electron rest mass, $g = Z\alpha$, $\alpha \approx 1/137$ (Sommerfeld fine structure constant), and Z is the atomic number. The four 4×4 Dirac matrices $\boldsymbol{\alpha}$ and *beta* are given through the three Pauli matrices $\boldsymbol{\sigma}$ as

$$\alpha_\nu := \begin{pmatrix} 0 & \sigma_\nu \\ \sigma_\nu & 0 \end{pmatrix}$$

for $\nu = 1, 2, 3$ and

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

The Pauli matrices in turn are defined as

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

The operator D_g is well-defined on $\mathcal{S}(\mathbb{R}^3)\otimes\mathbb{C}^4 \subset \mathfrak{H} := L^2(\mathbb{R}^3)\otimes\mathbb{C}^4$ and essentially self-adjoint for $g \in (-\sqrt{3}/2, \sqrt{3}/2)$ (Landgren and Rejto [20] and Landgren et al. [21]).

We define $\Lambda_g := \chi_{(0,\infty)}(D_g)$, $\mathcal{F}_g := \Lambda_g(\mathcal{S}(\mathbb{R}^3) \otimes \mathbb{C}^4)$, $\mathfrak{H}_g := \Lambda_g(\mathfrak{H})$.

Brown and Ravenhall [4] – see also Bethe and Salpeter [3] – introduce the operator B_g. It is the unique self-adjoint operator generated by

$$\mathcal{E}_g : \mathcal{F}_0 \to \mathbb{R} \tag{2}$$

$$\psi \mapsto (\psi, D_g\psi). \tag{3}$$

The basic fact allowing for this claim is

Theorem 1 (Evans et al. [8])**.** *If $0 \le g \le g_c^B := 2/(\pi/2 + 2/\pi)$, then $\mathcal{E}_g$ is bounded from below. If $g > g_c^B$, then $\mathcal{E}$ is unbounded from below.*

This allows us to define the Brown-Ravenhall operator

$$B_g = \Lambda_0 D_g \Lambda_0 \tag{4}$$

in the Hilbert space $\mathfrak{H}_0$ by form methods.

Physically speaking, the negative energy states constitute the Dirac sea of forbidden electron states.

We remark that the value g_c^B of the coupling constant corresponds to atomic numbers Z up to 124.

We mention some additional facts about the operator B_g and generalizations beyond the one-center one-electron Coulomb potential.

Evans et al. [8]**:** $\sigma_{\text{ess}}(B_g) = [m, \infty)$.
Evans et al. [8]**:** $\sigma_{\text{s.c.}}(B_g) = \emptyset$.
Tix [29, 30] **and Burenkov and Evans** [6]**:** Positivity of B_g.
Griesemer et al. [10]**:** The n-th eigenvalue of B_g is less than or equal to the n-th eigenvalue of D_g.
Balinsky and Evans [1]**:** Many center case with one electron.
Hoever and Siedentop [11]**:** Stability of matter beyond $2/\pi$.
Jakubaßa-Amundsen [16] **and Morozov and Vugalter** [22]**:** The location of the essential spectrum for the atomic and ionic Brown-Ravenhall operator (HWZ theorem).
Morozov and Vugalter [22]**:** Conditions on the finiteness of the discrete spectrum.

2.2. **Reducing to Two Components.** Spinors $\psi \in \mathfrak{H}_0$ (4 components) in the positive spectral subspace of the free Dirac operator can be parameterized by 2-component spinors u:

$$\psi = \begin{pmatrix} \frac{E(\mathfrak{p})+m}{\sqrt{2E(\mathfrak{p})(E(\mathfrak{p})+m)}} u \\ \frac{\boldsymbol{\sigma}\cdot\mathfrak{p}}{\sqrt{2E(\mathfrak{p})(E(\mathfrak{p})+m)}} u \end{pmatrix} \tag{5}$$

with $E(\mathfrak{p}) := \sqrt{m^2 + \mathfrak{p}^2}$, and $N(\mathfrak{p}) = \sqrt{2E(\mathfrak{p})(E(\mathfrak{p}) + m)}$.

The energy functional $\mathcal{E}_g$ – viewed as a function of 2-spinors – becomes

$$\mathcal{B}_g(u) := (u, b_g u) \tag{6}$$

where

$$b_g := E(\mathfrak{p}) - g\frac{E(\mathfrak{p}) + m}{N(\mathfrak{p})}\frac{1}{|\cdot|}\frac{E(\mathfrak{p}) + m}{N(\mathfrak{p})} - g\frac{\boldsymbol{\sigma}\cdot\mathfrak{p}}{N(\mathfrak{p})}\frac{1}{|\cdot|}\frac{\sigma\cdot\mathfrak{p}}{N(\mathfrak{p})} \tag{7}$$

is unitarily equivalent to B_g (Evans et al. [8]).

2.3. **A Different View of the Brown-Ravenhall Operator.** We can take a slightly different perspective using the Foldy-Wouthuysen transform (Foldy and Wouthuysen [9])

$$U_{\text{FW}}(\mathfrak{p}) = \frac{D_0 + E(\mathfrak{p})\beta}{N(\mathfrak{p})}. \tag{8}$$

It block diagonalizes the free Dirac operator

$$U_{\text{FW}}(\mathfrak{p})D_0U_{\text{FW}}(\mathfrak{p})^* = \begin{pmatrix} E(\mathfrak{p}) & 0 & 0 & 0 \\ 0 & E(\mathfrak{p}) & 0 & 0 \\ 0 & 0 & -E(\mathfrak{p}) & 0 \\ 0 & 0 & 0 & -E(\mathfrak{p}) \end{pmatrix}. \tag{9}$$

Then the Brown-Ravenhall operator is the projection of the Foldy-Wouthuysen transformed Dirac operator onto the upper two components, i.e.,

$$B_g = \beta_+ U_{\text{FW}}(\mathfrak{p})D_gU_{\text{FW}}(\mathfrak{p})^*\beta_+, \tag{10}$$

where $\beta_\pm := (1 \pm \beta)/2$ is projection onto the upper, respectively lower, two components.

3. Beyond Bethe and Salpeter

Physically the eigenvalues of the Dirac operator describe one-particle systems well. The eigenvalues of the Brown-Ravenhall operator are too low.

The idea to improve the situation is to replace U_{FW} by a unitary transform U block-diagonalizing D_g (Douglas and Kroll [7], Jansen and Heß [17]) and to approximate U in powers of g.

3.1. **The Jansen-Heß Operator.** Douglas and Kroll [7], corrected later by Jansen and Heß [17], derived an operator that takes further relativistic corrections into account. Formally, the Jansen-Heß operator is given as

$$J_g := B_g + g^2 \tilde{K} \tag{11}$$

with

$$\tilde{K} = -\frac{1}{2}(W \circ P + P \circ W), \tag{12}$$

$$P = \frac{\boldsymbol{\sigma}\cdot\mathfrak{p}}{N(\mathfrak{p})} \circ \frac{1}{|\mathfrak{x}|} \circ \frac{E(\mathfrak{p})+m}{N(\mathfrak{p})} - \frac{E(\mathfrak{p})+m}{N(\mathfrak{p})} \circ \frac{1}{|\mathfrak{x}|} \circ \frac{\boldsymbol{\sigma}\cdot\mathfrak{p}}{N(\mathfrak{p})}, \tag{13}$$

and

$$W := \int_0^\infty \mathrm{d}t e^{-tE(\mathfrak{p})} P e^{-tE(\mathfrak{p})}, \tag{14}$$

i.e.,

$$\tilde{K} = \int_0^\infty e^{-tE(\mathfrak{p})} P e^{-tE(\mathfrak{p})} P + P e^{-tE(\mathfrak{p})} P e^{-tE(\mathfrak{p})} \mathrm{d}t. \tag{15}$$

The energy corresponding to this symmetric operator is

$$\mathcal{J}_g(u) := (u, J_g u) = \mathcal{B}_g(u) + g^2 (u, \tilde{K} u). \tag{16}$$

We introduce the constants

$$g_c := 4\pi \frac{\pi^2 + 4 - \sqrt{-\pi^4 + 24\pi^2 - 16}}{(\pi^2-4)^2} \tag{17}$$

and

$$d_g := 1 - g - 4\sqrt{2}(3+\sqrt{2})g^2. \tag{18}$$

Then, for the form $\mathcal{J}_g : \mathcal{S}(\mathbb{R}^3) \otimes \mathbb{C}^4 \to \mathbb{R}$, $\mathcal{J}_g(\psi) := (\psi, J_g \psi)$ and the corresponding self-adjoint operator – also denoted by J_g – we have

Theorem 2 (Brummelhuis et al. [5])**.**

1. *If $g \in [0, g_c]$, then $\mathcal{J}_g$ is bounded from below.*
2. *If $g > g_c$, then $\mathcal{J}_g$ is unbounded from below.*
3. *If $g \in [0, g_c^B]$, then $\mathcal{J}_g(u) \geq d_g m \|u\|^2$.*

Note:

- The critical coupling constant is $g_c \approx 1.006077340$.
- The theorem covers all known elements up 137.
- The energy is even bounded below for g slightly bigger than 1.

Additional facts on J_g and its extension to the multi-particle case have been obtained by Jakubaßa-Amundsen [13, 15, 14] and Iantchenko and Jakubaßa-Amundsen [12], e.g.,

- $\sigma_{\mathrm{ess}}(\mathcal{J}_g) = [m, \infty)$.
- $\sigma_{\mathrm{s.c.}}(\mathcal{J}_g) = \emptyset$.

3.2. **Systematic Block-Diagonalization.** The idea which we are going to pursue is the following: expose the electronic (positive) energies of D_g by a unitary transform $\tilde{U}(g)$ block-diagonalizing

$$H_g = \tilde{U}(g) D_g \tilde{U}(g)^{-1} = \begin{pmatrix} h_+ & 0 \\ 0 & h_- \end{pmatrix} \tag{19}$$

where the operators $h_\pm$ act on two-component spinors, $h_+ > 0$, $h_- < 0$.

Douglas-Kroll-Heß [7] proposed a block-diagonalization method (see also Barysz and Sadlej [2], Jansen and Hess [17], Kutzelnigg [19], Wolf et al [31], Reiher and Wolf [25, 26]) in order to approximate the operator h_+ as a polynomial in g. The hope is, that these polynomials approximate the energy better as their degree grows. This, however, is not clear a priori, not even speaking of convergence properties as the degree increases to infinity. The following will address this question based on work of Siedentop and Stockmeyer [27, 28].

We write the Dirac operator as

$$D_g = \Lambda_g D_g \Lambda_g + \Lambda_g^\perp D_g \Lambda_g^\perp \tag{20}$$

and find a unitary transform $\tilde{U}(g)$ such that

$$\tilde{U}(g) \Lambda_g \tilde{U}(g)^{-1} = \beta_+. \tag{21}$$

Writing $\tilde{U} = U(g) \circ U_{\mathrm{FW}}$ Kato's choice [18] of $U(g)$ is

$$U(g) = [1 + (\Lambda_0 - \Lambda_0^\perp)(\Lambda_g - \Lambda_0)](1 - (\Lambda_g - \Lambda_0)^2)^{-1/2}. \tag{22}$$

We will adopt it but emphasize that it is – by no means – the only possible choice. The operators $U(g)$ will turn out to be a well defined family of unitary operators. In fact, we will be able to show that $U(g)$ is analytic in g and fulfills

$$U(g) \Lambda_g U^{-1}(g) = \Lambda_0. \tag{23}$$

This can be shown for a wide variety of potentials. In particular, for point nuclei it is valid across the periodic table from hydrogen up to at least neptunium, i.e., up to atomic numbers $Z = 93$.

This result has two important consequences:

(1) We get the block diagonal operator

$$H_g := \beta_+ U_{\mathrm{FW}} U(g) D_g U^{-1}(g) U_{\mathrm{FW}}^{-1} \beta_+ + \beta_- U_{\mathrm{FW}} U(g) D_g U^{-1}(g) U_{\mathrm{FW}}^{-1} \beta_-. \tag{24}$$

(2) Analyticity of $U(g)$ allows controlled approximations.

3.3. **Convergence of the Douglas-Kroll-Heß Method.** We decompose the Hamiltonian as

$$H_g = H_g^N + R_g^N \tag{25}$$

where H_g^N is the Taylor polynomial of order N and R_g^N is the remainder. We call H_g^N the generalized Douglas-Kroll-Heß Hamiltonian of order N.

We assume on $D_g = D_0 + gV$ and $\tilde{U}(g)$: There exists a constant g_c such that for all $g \in (0, g_c)$ the following holds:

(1) The operator $D_0 + gV$ has a distinguished self-adjoint extension in the sense of Nenciu [23].
(2) $0 \notin \sigma(D_g)$.
(3) The operator $D_0^{-1} - D_g^{-1}$ is compact.
(4) The potential V is relative operator bounded with respect to D_0.
(5) The operator family $|D_0|^{1/2} \tilde{U}(g) |D_0|^{-1/2}$ is bounded for each g and is analytic in g.

Conditions (1), (2), (3), and (4) are fulfilled for all reasonable "physical" potentials, in particular screened or unscreened electric potentials of point or extended nuclei with atomic number less than 137.

The Condition (5) is also of general nature. For our choice (22) of the unitary transform U and choosing $V(\mathfrak{x}) = -1/|\mathfrak{x}|$ we can guarantee it presently up to $g_c = 0.3775$, i.e., $Z < 52$ (tellurium).

Under these conditions we obtain the following convergence result on the Douglas-Kroll-Heß Approximations.

Theorem 3. *The following holds for all $g \in (0, g_c)$ under the above hypotheses:*

1. *Pick $\lambda \in (-m, m)$ but λ not in the spectrum of H_g. Then, for large enough N, λ is not in the spectrum of H_g^N and $1/(\lambda - H_g^N) \to 1/(\lambda - H_g)$ in norm.*
2. *Pick the coupling constant $g \in (0, g_c)$ and pick any two energies $a, b \in (-m, m)$, $a < b$, which are not eigenvalues of D_g. Then the spectral projection onto (a, b) of H_g^N converges in norm to the spectral projection onto the same interval of H_g, i.e.,*

$$\lim_{N\to\infty} \|\chi_{(a,b)}(H_g^N) - \chi_{(a,b)}(H_g)\| = 0 \tag{26}$$

3. $\sigma_{\mathrm{ess}}(D_g) = \sigma_{\mathrm{ess}}(H_g) = (-\infty, -m] \cup [m, \infty)$.
4. *Pick $a, b \in (-m, m)$, $a < b$. Then, for large enough N, the only possible spectral points of H_g^N in the interval (a, b) are finitely many eigenvalues (counting multiplicity).*
5. *Pick again $a, b \in (-m, m)$, $a < b$, and suppose that D_g has N eigenvalues – counting multiplicity – in (a, b). Then, for large enough N, the approximating operators H_g^N have also exactly N eigenvalues in (a, b).*

Proof of Claims 1 and 2: Firstly, we address the self-adjointness. Condition 4 implies that $|D_0|^{-1/2} V |D_0|^{-1/2}$ is bounded. Thus $|D_0|^{-1/2} H_g |D_0|^{-1/2}$ is analytic, since $|D_0|^{1/2} \tilde{U}(g) |D_0|^{-1/2}$ is analytic by Condition 5. This means that the rest R_g^N is small, i.e.,

$$\lim_{N\to\infty} \||D_0|^{-1/2} R_g^N |D_0|^{-1/2}\| = 0. \tag{27}$$

The convergence of the spectra of operators is then a consequence of norm resolvent convergence of the approximating sequence H_g^N of operators.

Secondly, we address the convergence of $1/H_g^N$: it is enough to show that

$$\lim_{N-\infty} \|(\tilde{U}(g)^{-1} H_g^N \tilde{U}(g) + \mathrm{i})^{-1} - (D_g + \mathrm{i})^{-1}\| = 0. \tag{28}$$

To prove (28) we write $\tilde{U}(g)^{-1} H_g^N \tilde{U}(g) = D_g - \hat{R}_g^N$ where $\hat{R}_g^N = \tilde{U}(g)^{-1} R_g^N \tilde{U}(g)$ and we note that

$$\frac{1}{\tilde{U}_g^{-1} H_g^N \tilde{U}(g) + \mathrm{i}} = \frac{|D_g|^{1/2}}{D_g + \mathrm{i}} \left(1 + |D_g|^{-1/2} \hat{R}_g^N |D_g|^{-1/2} \frac{|D_g|}{D_g + \mathrm{i}}\right)^{-1} |D_g|^{-1/2}. \tag{29}$$

Now, $|D_0|^{\frac{1}{2}} |D_g|^{-\frac{1}{2}}$ is bounded because of Condition 4. Thus, $|D_g|^{-\frac{1}{2}} \hat{R}_g^N |D_g|^{-\frac{1}{2}}$ tends to zero in norm for large N. Because of (29), this implies (28) which in turn implies the Claims 1 and 2 (Reed and Simon [24, Theorem VIII.23]).

Proof of Claim 3: It follows immediately from Weyl's theorem on the invariance of the essential spectra of operators under compact perturbations.

Proof of Claim 4: By possibly slightly enlarging the interval (a, b) we can always assume $a, b \notin \sigma(D_g)$, since $(-m, m) \cap \sigma_{\mathrm{ess}}(D_g) = \emptyset$. This allows us to make use of the first claim.

Now assume that there exists $\lambda \in (a, b)$ such that no matter how big we choose N_0 there is always an $N \geq N_0$ such $\lambda \in \sigma_{\mathrm{ess}}(H_g^N)$. Because of Claim 1, λ must be

different from 0. Then, according to Weyl, we can find for each N an orthonormal sequence of vectors ψ_m^N, $m = 1, 2, ...$ such that

$$\lim_{m\to\infty} \|(1/H_g^N - 1/\lambda)\psi_m^N\| = 0. \tag{30}$$

But

$$\|(1/H_g^N - 1/\lambda)\psi_m^N\| \geq \|(1/H_g - 1/\lambda)\psi_m^N\| - \|(1/H_g^N - 1/H_g)\psi_m^N\|. \tag{31}$$

Since $\lambda \notin \sigma_{\rm ess}(H_g)$ we can find an $\epsilon > 0$ and a subsequence ψ_{m_μ} such that $\|(1/H_g - 1/\lambda)\psi_{m_\mu}^N\| \geq \epsilon$ for all μ. Pick N so big that $\|1/H_g - 1/H_g\| < \epsilon/2$. Thus the right hand side of (31) is bigger than $\epsilon/2$ which is definitely positive, contradicting (30). Thus, for large N, $\sigma_{\rm ess}(H_g^N) \cap (a, b) = \emptyset$.

Proof of Claim 5: By possibly slightly shrinking the interval (a, b) we can assume that $a, b \notin \sigma(D_g)$ since it is discrete in $(-m, m)$. Now, let us suppose the claim were not true. Then it would be possible to find a subsequence of operators such that the dimensions of the ranges of the two projections, $d_n := \dim P_n(\mathfrak{H})$ and $d := \dim P(\mathfrak{H})$, differ by at least one.(For brevity, we introduced $P_n := \chi_{(a,b)}(H_g^n)$ and $P := \chi_{(a,b)}(H_g)$. Let us first suppose that $d_n > d$. Then $P_n P(\mathfrak{H})$ is a proper linear subspace of $P(\mathfrak{H})$. Thus there exists a normalized $\psi \in P_n(\mathfrak{H})$ such that $\psi \perp P_N P(\mathfrak{H})$. Then

$$\|P_n - P\| \geq \|((P_n - P)\psi\| = \|\psi\| = 1. \tag{32}$$

But the same inequality would also hold, if $d_n < d$. Thus $\|P_n - P\|$ cannot converge to zero contradicting (26) utterly. This concludes the proof of all of our assertions.

We remark:

Block-Diagonalization: The block-diagonalization of the Hamiltonian can be done up to any order in the coupling constant g and is correct up to the order of the approximation degree N.

Identical Main Terms: The first two terms reproduce the Brown-Ravenhall operator and the Jansen-Heß operator, i.e., $H_g^1 = B_g$, $H_g^2 = J_g$.

3.4. **Open Questions.** We close this overview with a list of open problems for the models described above.

Brown-Ravenhall Operator:

- Is stability of matter up to $\alpha Z = 2/(\pi/2 + 2/\pi)$ and $\alpha \approx 1/137$ true?
- Prove the HWZ theorem for all particle numbers. (Note added in proof: This question has recently been answered by Jakubaßa-Amundsen [16] and Morozov and Vugalter [22].)
- Determine the structure of the essential spectrum.
- Prove any bound on the excess charge.
- Find the Scott correction.
- Find criteria for no-binding for positive ions.

Jansen-Heß Operator:

- Is J_g positive up to g_c?
- Find any range of α and Z such that stability of matter holds.
- Answer all the above questions in the Brown-Ravenhall context (appropriately modified to the Jansen-Heß context).

Generalized Douglas-Kroll-Heß Operator:

- Find optimal ranges (α and Z) for the validity of the convergence.
- Show compactness of resolvent differences for all H_g^N.
- Show for even N the ground state energy is overestimated and for odd N underestimated.
- Extend the procedure to self-consistent fields.

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