A MINIMAX PRINCIPLE FOR THE EIGENVALUES IN SPECTRAL GAPS

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Abstract

A minimax principle is derived for the eigenvalues in the spectral gap of a possibly non-semibounded self-adjoint operator. It allows the nth eigenvalue of the Dirac operator with Coulomb potential from below to be bound by the nth eigenvalue of a semibounded Hamiltonian which is of interest in the context of stability of matter. As a second application it is shown that the Dirac operator with suitable non-positive potential has at least as many discrete eigenvalues as the Schrödinger operator with the same potential.

1. *Introduction*

The minimax principle provides a variational characterization of all eigenvalues below (or above) the essential spectrum of a self-adjoint operator that is bounded below (above) (see, for example, Courant and Hilbert [**2**, Chapter VI, §1.4] or Reed and Simon [**14**, Chapter XIII.1]). It allows one to estimate, say, the nth eigenvalue without *a priori* knowledge on the spectrum or eigenfunctions, which might be the main reason why it is one of the most used and most powerful tools in the investigation of the spectrum.

Clearly it would be desirable to have a similar variational characterization of eigenvalues in gaps of the essential spectrum and for operators which are not semibounded. There are important systems to which such a characterization would be applicable. We mention periodic Schrödinger operators with localized perturbation (they occur in the description of crystals with impurities) and Dirac operators. In this paper we are mainly concerned with Dirac operators.

Minimax principles for the lowest eigenvalue of the Dirac operator are in fact discussed in the quantum chemistry literature (see, for example, Rosenberg and Spruch [**15**], Drake and Goldman [**5**], Kutzelnigg [**9**], Talman [**18**] and Datta and Deviah [**3**]). According to Talman, and Datta and Deviah,

$$\min_g \left[\max_f \frac{(\psi, H\psi)}{(\psi, \psi)} \right] \tag{1}$$

should be the first positive eigenvalue of the Dirac operator H. (As a matter of fact Datta and Deviah not only do not refer to Talman, but also those articles that refer to these two papers according to the Science Citation Index of January 1997 always ignore the corresponding other author(s).) Here ψ is a Dirac spinor whose upper and lower two components are denoted by g and f respectively. The arguments given for (1) are not stringent but they were still convincing enough to be the motivation for the present work on such minimax principles.

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Our main result is a minimax principle for discrete eigenvalues in a gap of the essential spectrum of a possibly non-semibounded self-adjoint operator. It generalizes the standard minimax principle and allows us to prove that (1), with the correction $g \neq 0$, is indeed the lowest discrete eigenvalue of the Dirac operator for suitable potentials. As a second application of this new minimax principle we show that the nth eigenvalue of the Dirac operator with Coulomb potential is an upper bound for the nth eigenvalue of an operator due to Brown and Ravenhall [**1**]. Hamiltonians of this kind (also called no-pair Hamiltonians) are of interest for the description of heavy atoms and molecules (Sucher [**17**]) and are used in quantum chemistry (Ishikawa and Koc [**7**]). They have also been discussed in the context of stability of relativistic matter (Lieb *et al.* [**12**, **13**]). Thirdly, we show that the Dirac operator with suitable non-positive potential has at least as many discrete eigenvalues as the Schrödinger operator, more precisely the Pauli operator, with the same potential. This generalizes to operators including a magnetic field. All these results are new to our knowledge. Moreover, it seems hard to prove them without the minimax principle. To conclude we would like to mention that a minimax principle for the eigenvalues of Dirac operators has also been announced by Dolbeault *et al.* [**4**].

This work is organized as follows. In Section 2 we formulate and prove the new minimax principle in an abstract form. Section 3 contains two applications of the main result, the second being the comparison of the discrete eigenvalues of Dirac and Brown–Ravenhall operators. In Section 4 we re-cover the minimax principle of Talman and Datta and Deviah (Subsection 4.1) and finally prove the above-mentioned lower bound on the number of eigenvalues of the Dirac operator (Subsection 4.2).

2. *The minimax principle*

In this section we state and prove our main result, Theorem 3, a minimax principle for discrete eigenvalues of a possibly non-semibounded self-adjoint operator A. Although bounded operators are covered by this result, we state and prove it for bounded A separately (Theorem 1), since in this case the statement is less technical and the proof is short and simple.

We begin with a few notations. Suppose that A is a self-adjoint operator in a Hilbert space $\mathfrak{h}$. Then $\mathfrak{D}(A)$ denotes the domain and $\mathfrak{Q}(A)$ the form-domain of A. The operator $P_{(a,b)}(A)$ is the spectral projection of A for the interval (a, b). If A is bounded from below then

$$\mu_n(A) := \inf_{\substack{M \subset \mathfrak{D}(A) \\ \dim(M)=n}} \sup_{\substack{\varphi \in M \\ \|\varphi\|=1}} \langle \varphi, A\varphi \rangle$$

is the nth eigenvalue (counted from below and counting multiplicity) of A or, if A has less then n eigenvalues below the essential spectrum, the bottom of the essential spectrum [**14**]. As usual $\sigma(A)$ denotes the spectrum of A and $\rho(A) := \mathbb{C} \backslash \sigma(A)$. Finally $\mathbf{B}(\mathfrak{h})$ stands for the set of bounded linear operators on the Hilbert space $\mathfrak{h}$.

THEOREM 1. *Let* $A = A^* \in \mathbf{B}(\mathfrak{h})$ *and* $\mathfrak{h} = \mathfrak{h}_+ \oplus \mathfrak{h}_-$ *where* $\mathfrak{h}_+ \perp \mathfrak{h}_-$. *Let* $P_+ = P_{(0,\infty)}(A)$ *and*

$$\lambda_n(A) := \inf_{\substack{M_+ \subset \mathfrak{h}_+ \\ \dim(M_+)=n}} \sup_{\substack{\varphi \in M_+ \oplus \mathfrak{h}_- \\ \|\varphi\|=1}} \langle \varphi, A\varphi \rangle, \quad n \leqslant \dim \mathfrak{h}_+.$$

(i) *If* $\langle \varphi, A\varphi \rangle \leqslant 0$ *for all* $\varphi \in \mathfrak{h}_-$, *then*

$$\lambda_n(A) \leqslant \mu_n(A \upharpoonright P_+ \mathfrak{h}).$$

(ii) *If* $\langle\varphi, A\varphi\rangle > 0$ *for all non-zero* $\varphi \in \mathfrak{h}_+$, *then*

$$\lambda_n(A) \geqslant \mu_n(A \restriction P_+ \mathfrak{h}).$$

REMARK 2. (i) For $\mathfrak{h}_+ = P_+ \mathfrak{h}$ one can drop $\mathfrak{h}_-$ in the definition of $\lambda_n(A)$, that is, the theorem is trivial in this case. (ii) The theorem says that $\mathfrak{h}_\pm$ need only be approximate spectral subspaces in the above sense in order that $\lambda_n(A) = \mu_n(A \restriction P_+ \mathfrak{h})$.

Proof of Theorem 1. Set $\lambda_n := \lambda_n(A)$ and $\mu_n := \mu_n(A \restriction P_+ \mathfrak{h})$, and let Λ_+ and Λ_- be the orthogonal projection onto $\mathfrak{h}_+$ and $\mathfrak{h}_-$ respectively.

(i) First note that $\Lambda_+ : P_+ \mathfrak{h} \longrightarrow \mathfrak{h}_+$ is one-to-one. If not, there would exist a $\varphi \in \mathfrak{h}_- \cap P_+ \mathfrak{h}$ with $\varphi \neq 0$ so that

$$0 \geqslant \langle\varphi, A\varphi\rangle = \langle P_+ \varphi, A P_+ \varphi\rangle > 0.$$

Now pick $\varepsilon > 0$ and let $M := P_{(0, \mu_n + \varepsilon)}(A)\mathfrak{h}$. Then $\dim(M) \geqslant n$ and hence $\dim(\Lambda_+ M) \geqslant n$. Therefore

$$\lambda_n \leqslant \sup_{\substack{\varphi \in \Lambda_+ M \oplus \mathfrak{h}_- \\ \|\varphi\| = 1}} \langle\varphi, A\varphi\rangle = \sup_{\substack{\varphi \in M + \mathfrak{h}_- \\ \|\varphi\| = 1}} \langle\varphi, A\varphi\rangle,$$

where $\Lambda_+ M \oplus \mathfrak{h}_- = M + \mathfrak{h}_-$ was used. To estimate this from above we first decompose $\varphi \in M + \mathfrak{h}_-$ as $\varphi = \varphi_1 + \varphi_2$, where $\varphi_1 \in M$ and $\varphi_2 \in M^\perp \cap (M + \mathfrak{h}_-)$, and then φ_2 as $\varphi_2 = \varphi_3 + \varphi_-$ where $\varphi_3 \in M$ and $\varphi_- \in \mathfrak{h}_-$. Since $A\varphi_3 \in M$ and $\varphi_3 + \varphi_- \in M^\perp$ we have $\langle A\varphi_3, \varphi_-\rangle = -\langle A\varphi_3, \varphi_3\rangle$. Using this, $\langle A\varphi_3, \varphi_3\rangle \geqslant 0$, and $\langle\varphi_-, A\varphi_-\rangle \leqslant 0$ we find

$$\begin{aligned}\langle\varphi, A\varphi\rangle &= \langle\varphi_1, A\varphi_1\rangle + \langle\varphi_2, A\varphi_2\rangle \\ &= \langle\varphi_1, A\varphi_1\rangle - \langle\varphi_3, A\varphi_3\rangle + \langle\varphi_-, A\varphi_-\rangle \leqslant \langle\varphi_1, A\varphi_1\rangle \leqslant (\mu_n + \varepsilon)\langle\varphi, \varphi\rangle.\end{aligned}$$

(ii) Now $\Lambda_+ P_+ \mathfrak{h}$ is dense in $\mathfrak{h}_+$ because otherwise there exists a $\varphi \in \mathfrak{h}_+ \cap (\Lambda_+ P_+ \mathfrak{h})^\perp = \mathfrak{h}_+ \cap P_- \mathfrak{h}$ with $\varphi \neq 0$ and thus

$$0 < \langle\varphi, A\varphi\rangle = \langle P_- \varphi, A P_- \varphi\rangle \leqslant 0.$$

Since A is bounded it follows that

$$\lambda_n(A) = \inf_{\substack{M_+ \subset \Lambda_+ P_+ \mathfrak{h} \\ \dim(M_+) = n}} \sup_{\substack{\varphi \in M_+ \oplus \mathfrak{h}_- \\ \|\varphi\| = 1}} \langle\varphi, A\varphi\rangle \geqslant \inf_{\substack{M \subset P_+ \mathfrak{h} \\ \dim(M) = n}} \sup_{\substack{\varphi \in M \\ \|\varphi\| = 1}} \langle\varphi, A\varphi\rangle = \mu_n(A \restriction P_+ \mathfrak{h}).$$

To prove the inequality use each M_+ is of the form $M_+ = \Lambda_+ M$ for some $M \subset P_+ \mathfrak{h}$ with $\dim(M) = n$, and $\Lambda_+ M \oplus \mathfrak{h}_- \supset M$. □

Notice that in the proof of Theorem 1(ii) the assumption is only used to show that $\Lambda_+ P_+ \mathfrak{h}$ is dense in $\mathfrak{h}_+$, while in the proof of Theorem 1(i) the assumption is used in the estimate. This is the reason for the asymmetry in the set of states on which these assumptions are imposed in the following unbounded case.

THEOREM 3. *Suppose that A is a self-adjoint operator in a Hilbert space* $\mathfrak{h} = \mathfrak{h}_+ \oplus \mathfrak{h}_-$ *where* $\mathfrak{h}_+ \perp \mathfrak{h}_-$. *Let* $\Lambda_\pm$ *be the orthogonal projections onto* $\mathfrak{h}_\pm$ *and let* $\mathfrak{Q}$ *be a subspace with* $\mathfrak{D}(A) \subset \mathfrak{Q} \subset \mathfrak{Q}(A)$ *and* $\Lambda_\pm \mathfrak{D}(A) \subset \mathfrak{Q}$. *Let* $P_+ := P_{(0,\infty)}(A)$, $P_- := P_{(-\infty, 0]}(A)$, $\mathfrak{Q}_\pm := \mathfrak{Q} \cap \mathfrak{h}_\pm$, *and*

$$\lambda_n(A) := \inf_{\substack{M_+ \subset \mathfrak{Q}_+ \\ \dim(M_+) = n}} \sup_{\substack{\varphi \in M_+ \oplus \mathfrak{Q}_- \\ \|\varphi\| = 1}} \langle\varphi, A\varphi\rangle.$$

(i) *If* $\langle\varphi, A\varphi\rangle \leqslant 0$ *for all* $\varphi \in \mathfrak{Q}_-$, *then*

$$\lambda_n(A) \leqslant \mu_n(A \restriction P_+ \mathfrak{h}).$$

(ii) *If* $\langle \varphi, A\varphi \rangle > 0$ *for all* $\varphi \in \mathfrak{Q}(A) \cap \mathfrak{h}_+$ *and* $(|A|+1)^{1/2} P_- \Lambda_+ \in \mathbf{B}(\mathfrak{h})$*, then*

$$\lambda_n(A) \geqslant \mu_n(A \restriction P_+ \mathfrak{h}).$$

REMARK 4. Notice that $(|A|+1)^{1/2} P_-$ is bounded, if A is bounded from below.

Proof of Theorem 3. (i) The proof of (i) is essentially the same as that for bounded A.

(ii) Pick $a > \mu_n(A \restriction P_+ \mathfrak{h})$, set $f(x) := \min\{x, a\}$, let $\tilde{A} := f(A)$, and let us assume that

$$\inf_{\substack{M_+ \subset \mathfrak{Q}_+ \\ \dim(M_+)=n}} \sup_{\substack{\varphi \in M_+ \oplus \mathfrak{Q}_- \\ \|\varphi\|=1}} \langle \varphi, \tilde{A}\varphi \rangle = \inf_{\substack{M_+ \subset \Lambda_+ P_+ \mathfrak{D}(A) \\ \dim(M_+)=n}} \sup_{\substack{\varphi \in M_+ \oplus \mathfrak{Q}_- \\ \|\varphi\|=1}} \langle \varphi, \tilde{A}\varphi \rangle, \tag{2}$$

where $\mathfrak{Q}_+$ on the left-hand side is replaced by $\Lambda_+ P_+ \mathfrak{D}(A)$ on the right-hand side. Since $A \geqslant \tilde{A}$ the left-hand side is bounded from above by $\lambda_n(A)$ while the right-hand side is bounded from below by $\mu_n(\tilde{A} \restriction P_+ \mathfrak{h})$. The latter is proved in the same way as in the bounded case. Since $\tilde{A}$ and A have the same spectrum in $(-\infty, a)$ it follows that

$$\lambda_n(A) \geqslant \mu_n(\tilde{A} \restriction P_+ \mathfrak{h}) = \mu_n(A \restriction P_+ \mathfrak{h}). \tag{3}$$

To prove (2) we first show that $\Lambda_+ P_+ \mathfrak{D}(A)$ is dense in $\mathfrak{Q}_+$. If this were wrong, then there would be a $\varphi_+ \in \mathfrak{h}_+ \cap (\Lambda_+ P_+ \mathfrak{h})^\perp = \Lambda_+ \mathfrak{h} \cap P_- \mathfrak{h}$ with $\varphi_+ \neq 0$, so that $\varphi_+ = (|A|+1)^{-1/2} (|A|+1)^{1/2} P_- \Lambda_+ \varphi_+ \in \mathfrak{Q}(A)$ and we would arrive at the contradiction $0 < \langle \varphi_+, A\varphi_+ \rangle = \langle P_- \varphi_+, AP_- \varphi_+ \rangle \leqslant 0$.

Now, pick $M_+ \subset \mathfrak{Q}_+$, $\dim(M_+) = n$, and $\varepsilon > 0$. Since $\Lambda_+ P_+ \mathfrak{D}(A)$ is dense in $\mathfrak{Q}_+$, we can find a subspace $M_+^\varepsilon \subset \Lambda_+ P_+ \mathfrak{D}(A)$ with $\dim(M_+^\varepsilon) = n$ such that for each $\varphi_+^\varepsilon \in M_+^\varepsilon$, $\|\varphi_+^\varepsilon\| \leqslant 1$, there is a $\varphi_+ \in M_+$ with

$$\|\varphi_+ - \varphi_+^\varepsilon\| \leqslant \varepsilon \quad \text{and} \quad \|\varphi_+\| = \|\varphi_+^\varepsilon\|. \tag{4}$$

(To prove the existence of M_+^ε approximate the vectors of a given basis of M_+ with vectors of $\Lambda_+ P_+ \mathfrak{D}(A)$.) Now, equation (2) follows if

$$\sup_{\substack{\varphi \in M_+ \oplus \mathfrak{Q}_- \\ \|\varphi\|=1}} \langle \varphi, \tilde{A}\varphi \rangle \geqslant \liminf_{\varepsilon \to \infty} \sup_{\substack{\varphi^\varepsilon \in M_+^\varepsilon \oplus \mathfrak{Q}_- \\ \|\varphi^\varepsilon\|=1}} \langle \varphi^\varepsilon, \tilde{A}\varphi^\varepsilon \rangle. \tag{5}$$

Since, by (3), the supremum on the right-hand side is not smaller than $\mu_n(A \restriction P_+ \mathfrak{h})$ which is non-negative, we can restrict it to vectors φ^ε with $\langle \varphi^\varepsilon, \tilde{A}\varphi^\varepsilon \rangle \geqslant -1$. To prove (5) it therefore suffices, if for any given $\varphi^\varepsilon \in M_+^\varepsilon \oplus \mathfrak{Q}_-$ with $\|\varphi^\varepsilon\| = 1$ and $\langle \varphi^\varepsilon, \tilde{A}\varphi^\varepsilon \rangle \geqslant -1$ there exists a $\varphi \in M_+ \oplus \mathfrak{Q}_-$ (which will depend on φ^ε) with $\|\varphi\| = 1$ such that

$$\langle \varphi^\varepsilon, \tilde{A}\varphi^\varepsilon \rangle - \langle \varphi, \tilde{A}\varphi \rangle \to 0 \quad (\varepsilon \to 0) \tag{6}$$

uniformly in φ^ε. Pick such a φ^ε and let $\varphi_\pm^\varepsilon := \Lambda_\pm \varphi^\varepsilon$. We define $\varphi := \varphi_+ + \varphi_-^\varepsilon$ where $\varphi_+ \in M_+$ obeys (4), so that $\|\varphi\| = \|\varphi^\varepsilon\|$, and we define a semi-norm $|||\cdot|||$ on $\mathfrak{Q}(A)$ by $|||\psi|||^2 := \langle \psi, (a - \tilde{A})\psi \rangle$ with $a \in \mathbb{R}$ as in the definition of $\tilde{A}$. Then

$$\left| \langle \varphi^\varepsilon, \tilde{A}\varphi^\varepsilon \rangle - \langle \varphi, \tilde{A}\varphi \rangle \right| = \left| |||\varphi^\varepsilon|||^2 - |||\varphi|||^2 \right| \leqslant |||\varphi^\varepsilon - \varphi||| \, (2|||\varphi^\varepsilon||| + |||\varphi^\varepsilon - \varphi|||).$$

Here $|||\varphi^\varepsilon|||^2 \leqslant a + 1$ because $\langle \varphi^\varepsilon, \tilde{A}\varphi^\varepsilon \rangle \geqslant -1$, and

$$\begin{aligned} |||\varphi^\varepsilon - \varphi|||^2 &= |||\varphi_+^\varepsilon - \varphi_+|||^2 \\ &\leqslant -\langle (\varphi_+^\varepsilon - \varphi_+), AP_-(\varphi_+^\varepsilon - \varphi_+) \rangle + a\|\varphi_+^\varepsilon - \varphi_+\|^2 \\ &\leqslant \text{const}\, \|\varphi_+^\varepsilon - \varphi_+\|^2 \leqslant \text{const}\, \varepsilon^2, \end{aligned}$$

because $(|A|+1)^{1/2} P_- \Lambda_+$ is a bounded operator. This proves (6) and thus the theorem. □

3. *Applications*

In this section we give two applications of Theorem 3. The first exhibits its perturbative character and is of abstract nature. It assumes that $A = A_0 + A_1$ where A_0 has a gap (a, b) in the spectrum while A may have discrete eigenvalues in this gap. These eigenvalues are provided by the minimax principle for the decomposition $\mathfrak{h} = P_{(a,\infty)}(A_0)\,\mathfrak{h} \oplus P_{(-\infty,a]}(A_0)\,\mathfrak{h}$. The operator A_0 could be, for example, a periodic Schrödinger operator or the free Dirac operator. As a second application we show that the nth eigenvalue of the Coulomb–Dirac operator is an upper bound for the nth eigenvalue of the so-called Brown–Ravenhall operator. (See the introduction.)

3.1. *The case of relatively compact perturbations of self-adjoint operators with spectral gap*

THEOREM 5. *Let $A = A_0 + A_1$ be the sum of the self-adjoint operators A_0 and $A_1 \in \mathbf{B}(\mathfrak{h})$ in the Hilbert space $\mathfrak{h}$. Suppose there are real numbers $a < b$ such that*

(i) $\sigma(A_0) \cap (a, b) = \emptyset$;

(ii) $0 \geqslant A_1 > -|b-a|$;

(iii) $A_1(A_0+i)^{-1}$ *is compact;*

and let $\Lambda_+ = P_{(a,\infty)}(A_0)$ and $\Lambda_- = 1 - \Lambda_+$. Then

$$\mu_n(A \upharpoonright P_{(a,\infty)}(A)\,\mathfrak{h}) = \inf_{\substack{M_+ \subset \Lambda_+ \mathfrak{D}(A_0) \\ \dim(M_+) = n}} \; \sup_{\substack{\varphi \in M_+ \oplus \Lambda_- \mathfrak{D}(A_0) \\ \|\varphi\| = 1}} \langle \varphi, A\varphi \rangle.$$

Proof. We apply Theorem 3 to $A - a$, $\mathfrak{h}_\pm = \Lambda_\pm \mathfrak{h}$ and $\mathfrak{Q} = \mathfrak{D}(A) = \mathfrak{D}(A_0)$. Then $\mathfrak{Q}_\pm = \Lambda_\pm \mathfrak{D}(A_0)$ so that the right-hand side is exactly $\lambda_n(A)$. By definition of $\Lambda_\pm$ and by hypothesis (ii) we have $\langle \varphi, (A-a)\,\varphi \rangle \leqslant 0$ for $\varphi \in \Lambda_- \mathfrak{D}(A_0)$ and $\langle \varphi, (A-a)\,\varphi \rangle > 0$ for $\varphi \in \Lambda_+ \mathfrak{D}(A_0)$. Thus

$$\mu_n(A \upharpoonright P_{(a,\infty)}(A)\,\mathfrak{h}) \geqslant \lambda_n(A) \geqslant a$$

by Theorem 3 and the definition of $\lambda_n(A)$. If eigenvalues of A accumulate from above at a then $\mu_n(A \upharpoonright P_{(a,\infty)}(A)\,\mathfrak{h}) = a$ for all n and the theorem is proved. It remains to show that $(|A|+1)^{1/2} P_- \Lambda_+$ is bounded in the case where $(a, a+\varepsilon)$ contains no eigenvalues for some $\varepsilon > 0$.

From condition (iii) on A_1 it follows that $\sigma_{\text{ess}}(A) = \sigma_{\text{ess}}(A_0) \subset \mathbb{R} \backslash (a, b)$ and hence $(a, a+\varepsilon) \subset (\rho(A) \cap \rho(A_0))$. In particular the path $\gamma : \mathbb{R} \longrightarrow \mathbb{C}$ with $\gamma(t) = a + \varepsilon/2 - it$ is contained in $\rho(A) \cap \rho(A_0)$. Therefore

$$P_+ = \frac{1}{2} + \frac{1}{2\pi i} \int_\gamma dz (z-A)^{-1}$$

and similarly for Λ_+ and A_0 (Kato [**8**, p. 359]) which leads us to

$$(|A|+1)^{1/2} (\Lambda_+ - P_+) = \frac{1}{2\pi i} \int_\gamma dz (|A|+1)^{1/2} (z-A)^{-1} (-A_1) (z-A_0)^{-1}.$$

Since A_1 is bounded and $\|(A+1)^{1/2} (z-A)^{-1} A_1 (z-A_0)^{-1}\| \leqslant \text{const}(1+|t|)^{-3/2}$ the integral converges absolutely which implies that $\text{Ran}(\Lambda_+ - P_+) \subset \mathfrak{Q}(A)$ and that $(|A|+1)^{1/2} (\Lambda_+ - P_+)$ is bounded. Hence $(|A|+1)^{1/2} P_- \Lambda_+ = P_-(|A|+1)^{1/2} (\Lambda_+ - P_+)$ is bounded as well. □

3.2. *Relation between the spectra of Dirac and no-pair Hamiltonians*

Let $\mathfrak{h} = L^2(\mathbb{R}^3; \mathbb{C}^4)$ and let $\alpha_1, \alpha_2, \alpha_3$ and β denote the usual Dirac matrices

$$\alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

σ_i being the Pauli matrices. Let $H_0 = -i\boldsymbol{\alpha}\cdot\nabla + \beta m$ with $\mathfrak{D}(H_0) = H^1(\mathbb{R}^3, \mathbb{C}^4)$ and let H denote the closure of the operator $H_0 + V$ where

$$0 \geqslant V(x) \geqslant -\frac{\kappa}{|x|}, \quad \kappa < \frac{\sqrt{3}}{2}.$$

Then H is self-adjoint [**16**] and $\mathfrak{D}(H) = \mathfrak{D}(H_0)$ (Landgren and Rejto [**10**] and Landgren *et al.* [**11**]). Let $\Lambda_+ := P_{(0,\infty)}(H_0)$, and consider the quadratic form

$$\varphi \longmapsto \langle \varphi, H\varphi \rangle, \quad \varphi \in \Lambda_+ \mathfrak{D}(H_0).$$

It is bounded from below (in fact even positive [**20**]) and closable as recently shown by Evans *et al.* [**6**]. The closure defines a unique self-adjoint operator which we denote by B.

THEOREM 6. *With the above notations we have for all n*

$$\mu_n(B) \leqslant \mu_n(H \upharpoonright P_{(-m,\infty)}(H)\,\mathfrak{h}).$$

Proof. Apply Theorem 3 to $A = H + m$, $\mathfrak{h}_\pm = \Lambda_\pm \mathfrak{h}$ and $\mathfrak{Q} = \mathfrak{D}(H_0) = \mathfrak{D}(H)$. Then $\mathfrak{Q}_\pm = \Lambda_\pm \mathfrak{D}(H_0)$, and for all $\varphi \in \Lambda_- \mathfrak{D}(H_0)$ we have $\langle \varphi, (H+m)\varphi \rangle \leqslant \langle \varphi, (H_0 + m)\varphi \rangle \leqslant 0$. Hence $\mu_n(H \upharpoonright P_{(-m,\infty)}(H)\,\mathfrak{h}) \geqslant \lambda_n(H)$ by Theorem 3(i). On the other hand we get by dropping $\mathfrak{Q}_- = \Lambda_- \mathfrak{D}(H_0)$ in the definition of $\lambda_n(H)$

$$\lambda_n(H) \geqslant \inf_{\substack{M_+ \subset \Lambda_+ \mathfrak{D}(H_0) \\ \dim(M_+) = n}} \sup_{\substack{\varphi \in M_+ \\ \|\varphi\| = 1}} \langle \varphi, H\varphi \rangle = \mu_n(B). \qquad \square$$

4. *Perturbed supersymmetric Dirac operators*

In this section we derive the minimax principle for the Dirac operator and the decomposition of a Dirac spinor into upper and lower (large and small) components. (Note that Theorem 3 cannot be applied to this case, because the boundedness assumption is not satisfied.) In particular we prove formula (1) of Talman [**18**], and Datta and Deviah [**3**], for certain bounded potentials. Moreover, we show that the Dirac operator with suitable non-positive potential has at least as many discrete eigenvalues as the Schrödinger operator with the same potential. These results generalize to systems including a magnetic field.

4.1. *The minimax principle of Talman and Datta and Deviah*

To compensate for the boundedness of $(|A|+1)^{1/2} P_- \Lambda_+$ in the proof of our minimax principle it suffices that the considered operator has the form $Q + \beta m + V$ where $Q + \beta m$ is a so-called Dirac operator with supersymmetry and V is a bounded perturbation. It is therefore natural to work with the class of such generalized Dirac operators, which in particular includes Dirac operators with magnetic and (bounded) electric potential.

DEFINITION 7. Let Q be a self-adjoint operator in a Hilbert space $\mathfrak{h}$ and let $m \in \mathbb{R}_+$. Furthermore let $\beta = \beta^* \in \mathbf{B}(\mathfrak{h})$ with $\sigma(\beta) = \{\pm 1\}$. If $\beta\mathfrak{D}(Q) \subset \mathfrak{D}(Q)$ and

$$\beta Q + Q\beta = 0 \quad \text{on } \mathfrak{D}(Q)$$

then $Q + \beta m$ is called a *Dirac operator with supersymmetry*.

REMARK 8. A consequence of the anticommutativity $\beta Q + Q\beta = 0$ is that $(Q+\beta m)^2 = Q^2 + m^2 \geqslant m^2$ which means that the spectrum of $Q + \beta m$ has the gap $(-m, m)$.

A typical example of a Dirac operator with supersymmetry is the Dirac operator $\boldsymbol{\alpha} \cdot (-i\nabla + \mathbf{A}) + \beta m$ with magnetic field $\nabla \times \mathbf{A}(x)$. For many other examples we refer to Thaller [**19**]. In the following we will use the notations $\beta_\pm := 1/2(1 \pm \beta)$, $\mathfrak{h}_\pm = \beta_\pm \mathfrak{h}$ and $V_{\pm\pm} := \beta_\pm V \beta_\pm \restriction \mathfrak{h}_\pm$ if $V \in \mathbf{B}(\mathfrak{h})$.

THEOREM 9. *Let $H_0 = Q + \beta m$ be a Dirac operator with supersymmetry in the Hilbert space $\mathfrak{h}$ and let $V \in \mathbf{B}(\mathfrak{h})$ with $V^* = V$. Let $H := H_0 + V$, $P_+ := P_{(0,\infty)}(H)$ and*

$$\lambda_n(H) := \inf_{\substack{M_+ \subset \beta_+ \mathfrak{D}(H) \\ \dim(M_+) = n}} \sup_{\substack{\varphi \in M_+ \oplus \beta_- \mathfrak{D}(H) \\ \|\varphi\| = 1}} \langle \varphi, H\varphi \rangle.$$

(i) *If $V_{--} \leqslant m$, then*

$$\lambda_n(H) \leqslant \mu_n(H \restriction P_+ \mathfrak{h}).$$

(ii) If $V_{++} > -m$ *and $(V-a) H_0^{-1}$ is compact for some $a \in \mathbb{R}$ with $-m < a \leqslant m$, then*

$$\lambda_n(H) \geqslant \mu_n(H \restriction P_+ \mathfrak{h}).$$

The theorem applies in particular to the usual Dirac operator where $Q = -i\boldsymbol{\alpha} \cdot \nabla$ and V is multiplication with a real-valued function.

COROLLARY 10. *Let $H = -i\boldsymbol{\alpha} \cdot \nabla + \beta m + V$ where $V \in L^\infty(\mathbb{R}^3)$. Suppose that $V(x) \to 0$ as $|x| \to \infty$ and $-2m < V(x) \leqslant 0$ almost everywhere. Then for all n*

$$\mu_n(H \restriction P_{(-m,\infty)}(H)\, \mathfrak{h}) = \inf_{\substack{M_+ \subset \beta_+ \mathfrak{D}(H) \\ \dim(M_+) = n}} \sup_{\substack{\varphi \in M_+ \oplus \beta_- \mathfrak{D}(H) \\ \|\varphi\| = 1}} \langle \varphi, H\varphi \rangle. \tag{7}$$

REMARK 11. Specializing our assertion to $n = 1$ proves that (1) with the correction $g \neq 0$ is indeed the lowest discrete eigenvalue of H. Note, however, that the requirement $g \neq 0$ cannot be dropped. Already in the case of a diagonal matrix with eigenvalues 1 and -1 one can easily prove the corresponding assertion without this additional condition false.

Proof of Theorem 9. Assertion (i) follows from Theorem 3(i) for $(A, \Lambda_\pm) = (H, \beta_\pm)$ because $\langle \varphi, H\varphi \rangle = \langle \varphi, (-m+V)\varphi \rangle \leqslant 0$ for all $\varphi \in \mathfrak{h}_-$.

(ii) Since $(V-a) H_0^{-1}$ is compact, $\sigma_{\text{ess}}(H) \cap (-m+a, m+a) = \varnothing$, and in particular $\sigma_{\text{ess}}(H) \cap (0, \varepsilon) = \varnothing$ for some $\varepsilon > 0$ by assumption on a. If the eigenvalues of H accumulate from above at 0, then the assertion is trivial, because then $\mu_n(H \restriction P_+ \mathfrak{h}) =$

0 for all n, while $\lambda_n(H) \geqslant 0$ as a consequence of $\langle \varphi, H\varphi\rangle = \langle \varphi, (m+V_+)\varphi\rangle \geqslant 0$ on $\beta_+ \mathfrak{D}(Q)$. We may therefore assume that $(0,\varepsilon) \subset \rho(H)$ for some $\varepsilon > 0$ ($\varepsilon \leqslant m$). It now suffices to show that

$$\lambda_n(H) = \inf_{\substack{M_+ \subset \beta_+ P_+ \mathfrak{D}(H) \\ \dim(M_+) = n}} \sup_{\substack{\varphi \in M_+ \oplus \beta_- \mathfrak{D}(H) \\ \|\varphi\| = 1}} \langle \varphi, H\varphi\rangle \tag{8}$$

because (ii) then follows in the same way as Theorem 3(ii) followed from (2). To prove (8) we show that $\beta_+ P_+ \mathfrak{D}(H)$ is dense in $\beta_+ \mathfrak{D}(H)$ with respect to the form-norm of H_0. We do this in three steps, step (1) and step (2) being prerequisites for step (3).

Step 1. Let $P_+^0 := P_{(0,\infty)}(H_0)$. Then $|H_0|^{1/2}(P_+ - P_+^0)$ is a bounded operator.

For the proof of this assertion see the proof of Theorem 5 and recall that $(0,\varepsilon) \subset \rho(H)$.

Step 2. Let $P_- = 1 - P_+$. Then $P_- \mathfrak{h} \cap \mathfrak{h}_+ \subset \mathfrak{Q}(H_0)$.

Let $P_-^0 = 1 - P_+^0$ and pick $\varphi \in P_- \mathfrak{h} \cap \mathfrak{h}_+$. Then $\varphi = P_- \varphi = (P_- - P_-^0)\varphi + P_-^0 \varphi$ and $\beta_- \varphi = 0$. Therefore

$$\beta_- P_-^0 \varphi = \beta_-(P_+ - P_+^0)\varphi.$$

Since β_- commutes with $|H_0|^{1/2}$ the right-hand side belongs to $\mathfrak{Q}(H_0)$ by step (1). Hence $\mathfrak{Q}(H_0) \ni \beta_- P_-^0 \varphi = \beta_- P_-^0 \beta_+ \varphi$. Using $P_-^0 = 1/2(1 - |H_0|^{-1} H_0)$ and $Q\beta_+ \mathfrak{D}(Q) \subset \mathfrak{h}_-$ we get $-Q|H_0|^{-1}\varphi \in \mathfrak{Q}(H_0)$ which implies that

$$\infty > \|Q|H_0|^{-1/2}\varphi\|^2 + \|m|H_0|^{-1/2}\varphi\|^2 = \langle \varphi, (Q^2+m^2)|H_0|^{-1}\varphi\rangle = \langle \varphi, |H_0|\varphi\rangle.$$

This proves step (2).

Step 3. The set $\beta_+ P_+ \mathfrak{D}(Q) \subset \beta_+ \mathfrak{D}(Q)$ is dense with respect to the norm $\varphi \longmapsto \| |H_0|^{1/2}\varphi\|$.

To see this claim, note that it is equivalent to

$$\overline{\beta_+ |H_0|^{1/2} P_+ \mathfrak{D}(Q)}^{\mathfrak{h}} = \mathfrak{h}_+$$

because $|H_0|^{1/2}$ commutes with β_+. Let us assume that this is wrong. Then there exists a $\varphi_+ \in \mathfrak{h}_+$ with $\varphi_+ \neq 0$ and

$$\langle \varphi_+, |H_0|^{1/2} P_+ \varphi\rangle = 0 \quad \forall \varphi \in \mathfrak{D}(Q). \tag{9}$$

Writing now $P_+ = P_+ - P_+^0 + P_+^0$ and $\varphi = |H_0|^{-1/2}\psi$ with $\psi \in \mathfrak{Q}(H_0)$ one finds

$$|H_0|^{-1/2} B^* \varphi_+ + P_+^0 \varphi_+ = 0 \tag{10}$$

where $B = |H_0|^{1/2}(P_+ - P_+^0) \in \mathbf{B}(\mathfrak{h})$ by step 1. Thus $P_+^0 \varphi_+ \in \mathfrak{Q}(H_0)$ and hence $\mathfrak{Q}(H_0) \ni 2\beta_+ P_+^0 \varphi_+ = \beta_+(1 - |H_0|^{-1} H_0)\varphi_+ = (1 + m|H_0|^{-1})\varphi_+$, that is, $\varphi_+ \in \mathfrak{Q}(H_0)$. Now (9) and step 2 mean that $\psi_+ = |H_0|^{1/2}\varphi_+ \in P_- \mathfrak{h} \cap \mathfrak{h}_+ \subset \mathfrak{Q}(H_0)$, which leads to the contradiction

$$0 < \langle \psi_+, (m+V)\psi_+\rangle = \langle \psi_+, H\psi_+\rangle = \langle P_- \psi_+, HP_- \psi_+\rangle \leqslant 0.$$

This proves the theorem. □

4.2. *Comparing discrete eigenvalues of Dirac and Schrödinger operators*

As an application of Theorem 9 we now compare the number of eigenvalues in $(-m, m)$ of the Dirac operator with the number of negative eigenvalues of the Schrödinger operator with the same potential.

THEOREM 12. *Let $H_0 = Q + \beta m$ be a Dirac operator with supersymmetry in the Hilbert space $\mathfrak{h}$ and suppose that $V = V^* \in \mathbf{B}(\mathfrak{h})$ commutes with β and VH_0^{-1} is compact. Let $H = H_0 + V$. If $0 \geqslant V_{--}$ and $V_{++} > -2m$, then*

$$\dim P_{(-m,\,m)}(H)\,\mathfrak{h} \geqslant \dim P_{(-\infty,\,0)}(Q^2/(2m) + V)\,\mathfrak{h}_+.$$

REMARK 13. By Weyl's theorem the spectrum of $H_0 + V$ in $(-m, m)$ is discrete because $\sigma(H_0) \cap (-m, m) = \emptyset$ and VH_0^{-1} is compact. Similarly the spectrum of $Q^2/2m + V$ in $(-\infty, 0)$ is discrete because $\sigma(Q^2/2m) \subset [0, \infty)$ and $V(Q^2 + m^2)^{-1} = VH_0^{-1}H_0^{-1}$ is compact.

Let us again specialize to the case where $Q = -i\boldsymbol{\alpha} \cdot \boldsymbol{\nabla}$ and V is multiplication with a real-valued function.

COROLLARY 14. *Suppose that $V \in L^\infty(\mathbb{R}^3)$, $V(x) \to 0$ as $|x| \to \infty$ and $-2m < V(x) \leqslant 0$ almost everywhere. Then, counting multiplicity, the operator $-i\boldsymbol{\alpha} \cdot \boldsymbol{\nabla} + \beta m + V$ has at least as many discrete eigenvalues as $-\Delta/(2m) + V$ on $L^2(R^3, \mathbb{C}^2)$.*

This can be understood as an expression of the fact that the non-relativistic kinetic energy of an electron is at least as large as the relativistic one: $p^2/(2m) + m \geqslant \sqrt{p^2 + m^2}$. The proof of Theorem 12 is based on the minimax principle Theorem 9 and the following lemma, where $D = Q \restriction \beta_+ \mathfrak{D}(Q)$. Note that Q has the form

$$Q = \begin{pmatrix} 0 & D^* \\ D & 0 \end{pmatrix} \tag{11}$$

with respect to the decomposition $\mathfrak{h} = \mathfrak{h}_+ \oplus \mathfrak{h}_-$ (Thaller [**19**]).

LEMMA 15. *Assume the hypotheses of Theorem* 12. *Define*

$$E(\varphi_+) = \sup_{\varphi_- \in \beta_- \mathfrak{D}(Q)} \left. \frac{\langle \varphi, H\varphi \rangle}{\langle \varphi, \varphi \rangle} \right|_{\varphi = \varphi_+ + \varphi_-}$$

for $\varphi_+ \in \beta_+ \mathfrak{D}(Q) \backslash \{0\}$. If $\mathrm{E}(\varphi_+) > 0$ *then*

$$E(\varphi_+) = \langle \varphi_+, [D^*(m + E(\varphi_+) - V_{--})^{-1} D + m + V_{++}]\,\varphi_+ \rangle \langle \varphi_+, \varphi_+ \rangle^{-1}.$$

Proof. By the special form of Q given in (11) and because $V \in \mathbf{B}(\mathfrak{h})$, the map $\varphi_- \longmapsto \langle \varphi, H\varphi \rangle$ is continuous. Therefore

$$E(\varphi_+) = \sup_{\varphi_- \in \mathfrak{h}_-} \left. \frac{\langle \varphi, H\varphi \rangle}{\langle \varphi, \varphi \rangle} \right|_{\varphi = \varphi_+ + \varphi_-}. \tag{12}$$

If there exists a maximizer $\varphi_- \in \mathfrak{h}_-$ of (12) then it obeys the corresponding Euler–Lagrange equation $\varphi_- = (m + E(\varphi_+) - V_{--})^{-1} D\varphi_+$. Substitute this for φ_- on the right-hand side of

$$E(\varphi_+) \langle \varphi_+, \varphi_+ \rangle = \langle \varphi, H\varphi \rangle - E(\varphi_+) \langle \varphi_-, \varphi_- \rangle$$

to get the claimed equation. It remains to prove the existence of a maximizer.

Choose a sequence $\varphi^n = \varphi_+ + \varphi_-^n$ for which

$$\lim_{n \to \infty} \frac{\langle \varphi^n, H\varphi^n \rangle}{\langle \varphi^n, \varphi^n \rangle} = E(\varphi_+).$$

Since $E(\varphi_+) > 0$ also $\langle \varphi^n, H\varphi^n \rangle > 0$ for large n and

$$0 < \langle \varphi^n, H\varphi^n \rangle = \langle \varphi_+, (m+V_{++})\,\varphi_+ \rangle + 2\mathrm{Re}\,\langle D\varphi_+, \varphi_-^n \rangle + \langle \varphi_-^n, (-m+V_{--})\,\varphi_-^n \rangle$$
$$\leqslant \mathrm{const} + 2\|D\varphi_+\|\,\|\varphi_-^n\| - m\langle \varphi_-^n, \varphi_-^n \rangle.$$

This implies that $\sup_n \|\varphi_-^n\| < \infty$. Hence there exists a $\varphi_-^* \in \mathfrak{h}_-$ and a weakly convergent subsequence, call it φ_-^n again, with $\varphi_-^n \rightharpoonup \varphi_-^*$ as $n \to \infty$. Since $-m+V_{--} < 0$ the map $\varphi_- \longmapsto \langle \varphi, H\varphi \rangle$ is weakly upper semicontinuous. The map $\varphi_- \longmapsto \langle \varphi, \varphi \rangle$ is weakly lower semicontinuous. Thus

$$E(\varphi_+) = \lim_{n\to\infty} \frac{\langle \varphi^n, H\varphi^n \rangle}{\langle \varphi^n, \varphi^n \rangle} \leqslant \limsup_{n\to\infty} \langle \varphi^n, H\varphi^n \rangle \limsup_{n\to\infty} \frac{1}{\langle \varphi^n, \varphi^n \rangle}$$
$$\leqslant \frac{\langle \varphi^*, H\varphi^* \rangle}{\langle \varphi^*, \varphi^* \rangle} \leqslant E(\varphi_+)$$

where $\varphi^* = \varphi_+ + \varphi_-^*$. Therefore φ_-^* is a maximizer. □

Proof of Theorem 12. Since $P_{(-\infty,0)}((1/2m)\,Q^2 + V)\,\mathfrak{h}_+ = P_{(-\infty,0)}((1/2m)\,D^*D + V_{++})\,\mathfrak{h}_+$, it suffices to show that

$$\mu_n(H \restriction P_{(-m,\infty)}(H)\,\mathfrak{h}) \geqslant m \qquad \Longrightarrow \qquad \mu_n\left(\frac{1}{2m} D^*D + V_{++}\right) \geqslant 0. \tag{13}$$

By Theorem 9(ii) applied to $V+m$ and $a = m$

$$\lambda_n(H) \geqslant \mu_n(H \restriction P_{(-m,\infty)}(H)\,\mathfrak{h}) \geqslant m. \tag{14}$$

Here we can add the condition $\beta_+\varphi \neq 0$ in the definition of $\lambda_n(H)$, because $\langle \varphi, H\varphi \rangle \leqslant 0$, if $\beta_+\varphi = 0$. It then follows from (14) and Lemma 15 that for every subspace $M_+ \subset \beta_+\mathfrak{D}(Q)$ with $\dim(M_+) = n$

$$m \leqslant \sup_{\substack{\varphi \in M_+ \oplus \beta_- \mathfrak{D}(H) \\ \|\varphi\|=1}} \langle \varphi, H\varphi \rangle = \sup_{\substack{\varphi_+ \in M_+ \\ \|\varphi_+\|=1}} E(\varphi_+)$$
$$= \sup_{\substack{\varphi_+ \in M_+ \\ \|\varphi_+\|=1}} \langle \varphi_+, [D^*(m+E(\varphi_+)-V_{--})^{-1} D + m + V_{++}]\,\varphi_+ \rangle \langle \varphi_+, \varphi_+ \rangle^{-1}. \tag{15}$$

Obviously the second and third supremum may be restricted to $\varphi_+ \in M_+$ with $E(\varphi_+) \geqslant m(1-2\varepsilon)$ and $\varepsilon > 0$ small. Then $(m+E(\varphi_+)-V_{--})^{-1} \leqslant (2m(1-\varepsilon))^{-1}$ and thus (15) implies that

$$0 \leqslant \mu_n\left(\frac{1}{2m(1-\varepsilon)} D^*D + V_{++}\right) \qquad 0 < \varepsilon < 1.$$

To see that this proves (13) multiply both sides by $(1-\varepsilon)$ and use that V_{++} is bounded. □

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