A Minimax Principle for Eigenvalues in Spectral Gaps: Dirac Operators with Coulomb Potentials [1]

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Abstract. We prove the minimax principle for eigenvalues in spectral gaps introduced in [5] based on an alternative set of hypotheses. In the case of the Dirac operator these new assumptions allow for potentials with Coulomb singularites.

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1 Introduction

Recently Dolbeault, Esteban, and Séré [4, 3, 2] have found a minimax principle for Dirac operators with Coulomb potentials. Independently, Griesemer and Siedentop [5] have found a minimax principle characterizing the eigenvalues of self-adjoint operators in their spectral gaps, which is flexible enough to adapt to various situations. In particular it can also be applied to Dirac operators. Such a minimax principle is of particular interest for applications, e.g., in solid state physics and relativistic quantum chemistry where differential operators having gaps in their spectra naturally arise. Apart from the computational point of view (see, e.g., Kutzelnigg [7]) it can serve as a tool to obtain non-asymptotic eigenvalue estimates, e.g., comparing the number of eigenvalues of

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the Dirac operator in the gap with the number of negative eigenvalues of a corresponding Schrödinger operator (see [5]).
Comparing [3, 2] and [5] shows, that although the hypotheses for the validity of the minimax principle overlap, the methods of proof are quite different. On the other hand, with these different hypotheses different classes of operators can be treated: Dolbeault, Esteban, and Séré's result allows for Dirac operators with singular potentials of Coulomb type. Griesemer and Siedentop's result allows for a flexible formulation of the minimax principle adaptable to various situations, e.g., an earlier minimax principle for the first positive eigenvalue of the Dirac operator considered by Talman [9] and Datta and Deviah [1] can be proved.
This difference in hypotheses indicates that the optimal assumption for the abstract minimax principle is yet to be found. The present paper is a step in this direction.
In Section 2 we prove the abstract minimax principle under assumptions alternative to those in [5]. In Section 3 we show that these hypotheses allow for Dirac operators with Coulomb potentials. Applications to other self-adjoint operators with eigenvalues in spectral gaps like perturbed periodic Schrödinger operators are also conceivable.

2 THE MINIMAX PRINCIPLE

In this section we formulate and prove the abstract minimax principle. Suppose A and A_0 are self-adjoint operators in a Hilbert space $\mathfrak{H}$ and assume that their form domains are equal

$$\mathfrak{Q}(A) = \mathfrak{Q}(A_0) = \mathfrak{Q}. \tag{1}$$

Let $\mathfrak{D}(A)$ and $\mathfrak{D}(A_0)$ denote the domains of A and A_0 respectively and let $P_I(A)$ be the spectral projection of A corresponding to the interval $I \subset \mathbb{R}$. Define

$$\begin{aligned} \Lambda_+ &= P_{(0,\infty)}(A_0), & \Lambda_- &= 1 - \Lambda_+, \\ P_+ &= P_{(0,\infty)}(A), & P_- &= 1 - P_+. \end{aligned} \tag{2}$$

We set $\mathfrak{H}_\pm := \Lambda_\pm \mathfrak{H}$ and $\mathfrak{Q}_\pm := \Lambda_\pm \mathfrak{Q}$. Then $\mathfrak{H} = \mathfrak{H}_+ \oplus \mathfrak{H}_-$ and, by assumption (1), $\mathfrak{Q}_\pm \subset \mathfrak{Q}$. The minimax values in which we are interested are given by

$$\lambda_n(A) := \inf_{\substack{\mathfrak{M}_+ \subset \mathfrak{Q}_+ \\ \dim(\mathfrak{M}_+) = n}} \sup_{\substack{\psi \in \mathfrak{M}_+ \oplus \mathfrak{Q}_- \\ \|\psi\| = 1}} (\psi, A\psi), \tag{3}$$

and have been introduced in [5]. These minimax values are to be compared with the standard (Courant) minimax values

$$\mu_n(B) := \inf_{\substack{\mathfrak{M} \subset \mathfrak{Q}(B) \\ \dim(\mathfrak{M}) = n}} \sup_{\substack{\psi \in \mathfrak{M} \\ \|\psi\| = 1}} (\psi, B\psi)$$

for the eigenvalues of a self-adjoint operator B which is bounded from below. The value $\mu_n(B)$ is the n-th eigenvalue of B counting from below (see, e.g., Reed and Simon [8]).

THEOREM 1. *Suppose A and A_0 are self-adjoint operators in $\mathfrak{H}$ with the same form domain $\mathfrak{Q}$ and define $\Lambda_\pm$, $P_\pm$, $\mathfrak{Q}_\pm$, $\lambda_n(A)$ and $\mu_n(\cdot)$ as above. If $(\psi, A\psi) \le 0$ for all $\psi \in \mathfrak{Q}_-$ and if*

$$\|(|A_0|+1)^{1/2}\Lambda_+ P_-(|A_0|+1)^{-1/2}\| < 1 \tag{4}$$

then $\lambda_n(A) = \mu_n(A\restriction P_+\mathfrak{H})$ for all $n \le \dim \mathfrak{H}_+$.

We remark that $|A_0|+1$ can be replaced by $|A_0|$ in (4), if we assume that 0 is in the resolvent set of A_0. This will be obvious from the proof.

Proof. We prove the theorem in two steps. Although these are partly contained in [5] we do not omit the similar parts in order to be self-contained: First, we show that it suffices to prove that $\Lambda_+ : P_+\mathfrak{Q} \to \mathfrak{Q}_+$ is a bijection. Secondly, we verify this property using assumption (4) and the negativity of $(\psi, A\psi)$ on $\mathfrak{Q}_-$.

Step 1. If $\Lambda_+ P_+ \mathfrak{Q} = \mathfrak{Q}_+$, then we have

$$\lambda_n(A) = \inf_{\substack{\mathfrak{M}_+ \subset \Lambda_+ P_+ \mathfrak{Q} \\ \dim(\mathfrak{M}_+)=n}} \sup_{\substack{\psi \in \mathfrak{M}_+ \oplus \mathfrak{Q}_- \\ \|\psi\|=1}} (\psi, A\psi) \tag{5}$$

using the defining Equation (3). Since for each $\mathfrak{M}_+ \subset \Lambda_+ P_+ \mathfrak{Q}$ with $\dim(\mathfrak{M}_+) = n$, we can find a subspace $\mathfrak{M} \subset P_+\mathfrak{Q}$ with $\dim(\mathfrak{M}) = n$ such that $\mathfrak{M}_+ = \Lambda_+\mathfrak{M}$ and since $\Lambda_+\mathfrak{M} \oplus \mathfrak{Q}_- \supset \mathfrak{M}$, we get from (5)

$$\begin{aligned}
\lambda_n(A) &= \inf_{\substack{\mathfrak{M}_+ \subset \Lambda_+ P_+ \mathfrak{Q} \\ \dim(\mathfrak{M}_+)=n}} \sup_{\substack{\psi \in \mathfrak{M}_+ \oplus \mathfrak{Q}_- \\ \|\psi\|=1}} (\psi, A\psi) \\
&\ge \inf_{\substack{\mathfrak{M} \subset P_+ \mathfrak{Q} \\ \dim(\mathfrak{M})=n}} \sup_{\substack{\psi \in \mathfrak{M} \\ \|\psi\|=1}} (\psi, A\psi) = \mu_n(A\restriction P_+\mathfrak{H}).
\end{aligned}$$

To prove the converse inequality we proceed as in [5]: pick $\epsilon > 0$ and let $\mathfrak{M} := P_{(0,\mu_n+\epsilon)}(A)\mathfrak{Q}$. Then $\dim(\mathfrak{M}) \ge n$ and hence $\dim(\Lambda_+\mathfrak{M}) \ge n$ by the remark above. Therefore

$$\lambda_n \le \sup_{\substack{\psi \in \Lambda_+\mathfrak{M} \oplus \mathfrak{Q}_- \\ \|\psi\|=1}} (\psi, A\psi) = \sup_{\substack{\psi \in \mathfrak{M} + \mathfrak{Q}_- \\ \|\psi\|=1}} (\psi, A\psi),$$

where $\Lambda_+\mathfrak{M} \oplus \mathfrak{Q}_- = \mathfrak{M} + \mathfrak{Q}_-$ was used. To estimate this from above we first decompose $\psi \in \mathfrak{M} + \mathfrak{Q}_-$ as $\psi = \psi_1 + \psi_2$, where $\psi_1 \in \mathfrak{M}$ and $\psi_2 \in \mathfrak{M}^\perp \cap (\mathfrak{M} + \mathfrak{Q}_-)$, and then ψ_2 as $\psi_2 = \psi_3 + \psi_-$ where $\psi_3 \in \mathfrak{M}$ and $\psi_- \in \mathfrak{Q}_-$.

Since $A\psi_3 \in \mathfrak{M}$ and $\psi_3 + \psi_- \in \mathfrak{M}^\perp$ we have $(A\psi_3, \psi_-) = -(A\psi_3, \psi_3)$. Using this, $(A\psi_3, \psi_3) \geq 0$, and $(\psi_-, A\psi_-) \leq 0$ we find

$$\begin{aligned}(\psi, A\psi) &= (\psi_1, A\psi_1) + (\psi_2, A\psi_2)\\ &= (\psi_1, A\psi_1) - (\psi_3, A\psi_3) + (\psi_-, A\psi_-) \leq (\psi_1, A\psi_1) \leq (\mu_n + \epsilon)(\psi, \psi)\end{aligned}$$

which implies $\lambda_n \leq \mu_n$.
Step 2. Surjectivity: Since $\Lambda_+ P_+ \mathfrak{Q} \subset \mathfrak{Q}_+$ it suffices that $\Lambda_+ P_+ \mathfrak{Q}_+ = \mathfrak{Q}_+$, which is equivalent to $(|A_0|+1)^{1/2}\Lambda_+ P_+ (|A_0|+1)^{-1/2}\mathfrak{H}_+ = \mathfrak{H}_+$. Now $\Lambda_+ P_+ = 1 - \Lambda_+ P_-$ on $\mathfrak{H}_+$ so that

$$(|A_0| + 1)^{1/2}\Lambda_+ P_+ (|A_0| + 1)^{-1/2} = 1 - (|A_0| + 1)^{1/2}\Lambda_+ P_- (|A_0| + 1)^{-1/2}$$

on $\mathfrak{H}_+$. By assumption (4) the latter is an isomorphism from $\mathfrak{H}_+$ to $\mathfrak{H}_+$.
Injectivity: Suppose $\Lambda_+ : P_+\mathfrak{Q} \to \mathfrak{Q}_+$ would not be one-to-one. Then there would exist a non-zero $\psi \in \mathfrak{H}_- \cap P_+\mathfrak{Q}$ such that

$$0 \geq (\psi, A\psi) = (P_+\psi, AP_+\psi) > 0.$$

$\square$

3 Application to the Dirac Operator

The hypothesis (4) of Theorem 1 contains the a priori unknown operator P_-, i.e., it is not straightforward to check. In this section we will show how to verify it for given operators nevertheless. To be specific we restrict ourselves to the Dirac operator D_γ with a screened Coulomb potential, i.e., $D_\gamma := (1/i)\nabla \cdot \boldsymbol{\alpha} + m\beta - \gamma\varphi$ in $\mathfrak{H} := L^2(\mathbb{R}^3)^4$, where $\varphi(x) = y(x)/|x|$ with measurable y and $y(\mathbb{R}^3) \subset [0, 1]$. By Hardy's inequality we have that D_γ is an operator perturbation of D_0 for $\gamma \in (-1/2, 1/2)$. We will assume this restriction on γ henceforth. In particular, perturbation theory for $|D_0| = (-\Delta + m^2)^{1/2}$ implies by Hardy's and Kato's inequality

$$\forall_{\gamma\in[0,1/2)} \quad \mathfrak{D}(D_\gamma) = H^1(\mathbb{R}^3) \otimes \mathbb{C}^4 =: \mathfrak{D}, \tag{6}$$

$$\forall_{\gamma\in[0,2/\pi)} \quad \mathfrak{Q}(D_\gamma) = H^{1/2}(\mathbb{R}^3) \otimes \mathbb{C}^4 =: \mathfrak{Q} \tag{7}$$

for the operator and form domain of D_γ, respectively. To make connections with Section 2 we pick $A_0 := D_0$ and $A := D_\gamma$. The notation (2) is used correspondingly here.
By γ_0 we denote the real solution of $2\gamma_0^3 - 3\gamma_0^2 + 4\gamma_0 = 1$. Note that $0.305 < \gamma_0 < 0.306$ holds.

THEOREM 2. *For* $\gamma \in [0, \gamma_0)$

$$\inf_{\substack{\mathfrak{M}_+\subset\mathfrak{Q}_+\\ \dim\mathfrak{M}_+=n}} \sup_{\substack{\psi\in\mathfrak{M}_+\oplus\mathfrak{Q}_-\\ \|\psi\|=1}} (\psi, D_\gamma\psi) \tag{8}$$

is equal to the n*-th positive eigenvalue – counting multiplicity – of the Dirac operator* D_γ *or equals the mass* m.

Our strategy is to roll the proof back to a verification of the hypotheses of Theorem 1. The main step is the verification of (4) which we break up into several steps:

LEMMA 1. *For all $f \in \mathfrak{H}$*

$$\begin{aligned} \Lambda_+ P_- f = & -\tfrac{\gamma}{2\pi}\Lambda_+ \textstyle\int_{-\infty}^{\infty}(D_0 - iz)^{-1}\varphi(D_\gamma - iz)^{-1}dzf \\ = & -\tfrac{\gamma}{\pi}\Lambda_+ \textstyle\int_0^{\infty}\left[(D_0^2+z^2)^{-1}(D_0\varphi D_\gamma - z^2\varphi)(D_\gamma^2+z^2)^{-1}\right]dzf. \end{aligned} \tag{9}$$

Proof. Since for $\gamma \in [0, 2/\pi)$, zero is in the resolvent set of D_γ, we have that

$$P_\pm = \frac{1}{2} \pm \frac{1}{2\pi}\int_{-\infty}^{\infty}(D_\gamma - iz)^{-1}dz = \frac{1}{2} \pm \frac{1}{\pi}\int_0^\infty D_\gamma(D_\gamma^2 + z^2)^{-1}dz \tag{10}$$

(Kato [6], Chapter VI.5, Lemma 5.6); $\Lambda_\pm$ is obtained from (10) by setting $\gamma = 0$. Therefore, by (10), and the second resolvent identity

$$P_- = \Lambda_- - \frac{\gamma}{2\pi}\int_{-\infty}^{\infty}(D_0 - iz)^{-1}\varphi(D_\gamma - iz)^{-1}dz$$

from which we may conclude that the first part of (9) holds.
We can simplify

$$\begin{aligned} & \int_{-\infty}^{\infty}(D_0 - iz)^{-1}\varphi(D_\gamma - iz)^{-1}dzf \\ = & \int_0^\infty \left[(D_0 - iz)^{-1}\varphi(D_\gamma - iz)^{-1} + (D_0 + iz)^{-1}\varphi(D_\gamma + iz)^{-1}\right]dzf \\ = & \int_0^\infty \left[\frac{D_0 + iz}{D_0^2 + z^2}\varphi\frac{D_\gamma + iz}{D_\gamma^2 + z^2} + \frac{D_0 - iz}{D_0^2 + z^2}\varphi\frac{D_\gamma - iz}{D_\gamma^2 + z^2}\right]dzf \\ = & \; 2\int_0^\infty \left[(D_0^2 + z^2)^{-1}(D_0\varphi D_\gamma - z^2\varphi)(D_\gamma^2 + z^2)^{-1}\right]dzf \end{aligned}$$

which implies that the second part of (9) holds. □

LEMMA 2. *For $\gamma \in \mathbb{R}_+$ we have $(1/2 - \gamma)^2\varphi^2 \le |D_\gamma|^2 \le (1 + 2\gamma)^2|D_0|^2$.*

Proof. For all $\psi \in \mathfrak{D}(D_0)$ we have $\|D_\gamma\psi\| \ge \|D_0\psi\| - \gamma\|\varphi\psi\| \ge (1/2 - \gamma)\|\varphi\psi\|$, where we first use the triangle inequality and then Hardy's inequality. This implies the first stated operator inequality. The second one follows from $\|D_\gamma\psi\| \le \|D_0\psi\| + \gamma\|\varphi\psi\| \le (1 + 2\gamma)\|D_0\psi\|$. □

LEMMA 3. *For all $\gamma \in (0, \frac{1}{2})$ and $f \in \mathfrak{H}$ we have*

$$\begin{aligned} & \left\||D_0|^{1/2}\int_0^\infty (D_0^2 + z^2)^{-1}(D_0\varphi D_\gamma - z^2\varphi)(D_\gamma^2 + z^2)^{-1}dz|D_0|^{-1/2}f\right\| \\ & \qquad \le \pi\frac{\sqrt{1 + 2\gamma}}{1 - 2\gamma}\|f\|. \end{aligned} \tag{11}$$

Proof. Using the fact that

$$\|h\| = \sup_{\|g\|=1} |(g,h)|, \quad h \in \mathfrak{H}$$

and setting $f' := |D_0|^{-1/2} f$ we see that the norm on the left hand side of (11) can be approximated by finding an upper bound for

$$|(g, |D_0|^{1/2} \int_0^\infty \left[(D_0^2+z^2)^{-1}(D_0\varphi D_\gamma - z^2\varphi)(D_\gamma^2+z^2)^{-1}\right] dz f')|, \quad \|g\| = 1. \tag{12}$$

First, consider the term

$$\begin{aligned} &|(g, |D_0|^{1/2} \int_0^\infty \left[(D_0^2+z^2)^{-1}(D_0\varphi D_\gamma)(D_\gamma^2+z^2)^{-1}\right] dz f')| \\ &\leq \left[\int_0^\infty \|D_0(D_0^2+z^2)^{-1}|D_0|^{1/2}g\|^2 dz\right]^{\frac{1}{2}} \left[\int_0^\infty \|\varphi D_\gamma(D_\gamma^2+z^2)^{-1}f'\|^2 dz\right]^{\frac{1}{2}}. \end{aligned} \tag{13}$$

Note that

$$\int_0^\infty \frac{dz}{(1+z^2)^2} = \int_0^\infty \frac{z^2 dz}{(1+z^2)^2} = \frac{\pi}{4}. \tag{14}$$

Thus, the first factor yields

$$\int_0^\infty \|D_0(D_0^2+z^2)^{-1}|D_0|^{1/2}g\|^2 dz = \int_0^\infty (g, \frac{|D_0|^3}{(D_0^2+z^2)^2} g) dz = \frac{\pi}{4}(g,g). \tag{15}$$

In a similar manner we show for $\gamma \in (0, 1/2)$

$$\int_0^\infty \|\varphi D_\gamma(D_\gamma^2+z^2)^{-1}f'\|^2 dz \tag{16}$$

$$= \int_0^\infty (f', (D_\gamma^2+z^2)^{-1}D_\gamma\varphi^2 D_\gamma(D_\gamma^2+z^2)^{-1}f')dz \tag{17}$$

$$\leq \frac{1}{(1/2-\gamma)^2}\int_0^\infty (f', (D_\gamma^2+z^2)^{-1}|D_\gamma|^4(D_\gamma^2+z^2)^{-1}f')dz \tag{18}$$

$$= \frac{\pi}{(1-2\gamma)^2}(f', |D_\gamma|f') \leq \frac{\pi(1+2\gamma)}{(1-2\gamma)^2}(f', |D_0|f') \leq \frac{\pi(1+2\gamma)}{(1-2\gamma)^2}(f,f) \tag{19}$$

where we have used the first inequality of Lemma 2 to go from (17) to (18) and the second inequality of that Lemma in (19).
Thus we have for the product

$$|(g, |D_0|^{1/2} \int_0^\infty \left[(D_0^2+z^2)^{-1}(D_0\varphi D_\gamma)(D_\gamma^2+z^2)^{-1}\right] dz f')| \leq \frac{\pi}{2}\frac{\sqrt{1+2\gamma}}{1-2\gamma}\|f\|.$$

Likewise, we estimate the second term in (12)

$$
\begin{aligned}
&|(g, |D_0|^{1/2}\int_0^\infty (D_0^2+z^2)^{-1}z^2\varphi(D_\gamma^2+z^2)^{-1}dz|D_0|^{-1/2}f)| \\
&\qquad = |\int_0^\infty (z(D_0^2+z^2)^{-1}|D_0|^{1/2}g, z\varphi(D_\gamma^2+z^2)^{-1}f')dz| \\
&\leq \left[\int_0^\infty \|z(D_0^2+z^2)^{-1}|D_0|^{1/2}g\|^2dz\right]^{\frac12}\left[\int_0^\infty \|z\varphi(D_\gamma^2+z^2)^{-1}f'\|^2dz\right]^{\frac12}. \quad (20)
\end{aligned}
$$

By scaling and (14) we get for the first factor

$$\int_0^\infty \|z|D_0|^{1/2}(D_0^2+z^2)^{-1}g\|^2dz = \frac{\pi}{4}. \quad (21)$$

The second factor yields using Lemma 2 twice

$$
\begin{aligned}
&\int_0^\infty \|z\varphi(D_\gamma^2+z^2)^{-1}f'\|^2dz = (f', \int_0^\infty (D_\gamma^2+z^2)^{-1}\varphi^2z^2(D_\gamma^2+z^2)^{-1}dzf') \\
\leq& \frac{1}{(1/2-\gamma)^2}(f', \int_0^\infty (D_\gamma^2+z^2)^{-1}|D_\gamma|^2z^2(D_\gamma^2+z^2)^{-1}dzf') \\
=& \frac{\pi}{4(1/2-\gamma)^2}(f', D_\gamma f') \leq \pi\frac{1+2\gamma}{(1-2\gamma)^2}(f', D_0f').
\end{aligned}
$$

Thus we get

$$|(g, |D_0|^{1/2}\int_0^\infty (D_0^2+z^2)^{-1}z^2\varphi(D_\gamma^2+z^2)^{-1}dzf')| \leq \frac{\pi}{2}\frac{\sqrt{1+2\gamma}}{1-2\gamma}\|f\|, \quad (22)$$

i.e., the same upper bound as for the first term. By (11), (12), and the calculations above, we have the upper bound

$$
\begin{aligned}
&\||D_0|^{1/2}\int_0^\infty \left[(D_0^2+z^2)^{-1}(D_0\varphi D_\gamma - z^2\varphi)(D_\gamma^2+z^2)^{-1}\right]dz|D_0|^{-1/2}f\| \\
&\qquad\qquad \leq \pi\frac{\sqrt{1+2\gamma}}{1-2\gamma}\|f\|
\end{aligned}
$$

for $\gamma \in [0, 1/2)$ which we claimed. □

From Lemmata 1 and 3 we have the immediate

Corollary 1. *For all* $\gamma \in (0, \frac12)$

$$\||D_0|^{1/2}\Lambda_+P_-|D_0|^{-1/2}\| \leq \gamma\frac{\sqrt{1+2\gamma}}{1-2\gamma}.$$

We remark that an argument similar to the proofs of Lemmata 1 and 3 shows that $\|\Lambda_+P_-\| = O(\gamma)$ as $\gamma \to 0$ which implies that $\Lambda_+P_+\mathfrak{H} = \mathfrak{H}_+$ and $\mathfrak{H}_+ \cap P_-\mathfrak{H} = \{0\}$ for small enough positive γ.
We turn now to the proof of Theorem 2.

Proof. First, we reiterate our remark (7) that for $\gamma \in [0, 2/\pi)$ the form domain of $\mathfrak{Q} := \mathfrak{Q}(D_\gamma) = H^{1/2}(\mathbb{R}^3) \otimes \mathbb{C}^4$. In particular, it is independent of γ. This also means that $P_\pm$ and $\Lambda_\pm$ leave $\mathfrak{Q}$ invariant. Moreover, $\Lambda_- D_\gamma \Lambda_-$ is certainly non-positive. Finally, Corollary 1 implies that (4) holds true for $\gamma \in [0, \gamma_0)$ which completes the proof. □

Finally, we remark, that the construction of this Section is easily generalized to other types of potentials, as long as one can prove an analogue of Lemma 3.

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