On the eigenvalues of operators with gaps. Application to Dirac operators.

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Abstract. This paper is devoted to a general min-max characterization of the eigenvalues in a gap of the essential spectrum of a self-adjoint unbounded operator. We prove an abstract theorem, then we apply it to the case of Dirac operators with a Coulomb-like potential. The result is optimal for the Coulomb potential.

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I. Introduction.

The aim of this paper is to prove a very general result on the variational characterization of the eigenvalues of operators with gaps in the essential spectrum.

More precisely, let $\mathcal{H}$ be a Hilbert space with scalar product $(\cdot,\cdot)$, and $A : D(A) \subset \mathcal{H} \to \mathcal{H}$ a self-adjoint operator. We denote by $\mathcal{F}(A)$ the form-domain of A. Let $\mathcal{H}_+$, $\mathcal{H}_-$ be two orthogonal Hilbert subspaces of $\mathcal{H}$ such that $\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_-$.

We denote Λ_+, Λ_- the projectors on $\mathcal{H}_+$, $\mathcal{H}_-$. We assume the existence of a core F (i.e. a subspace of $D(A)$ which is dense for the norm $\|.\|_{D(A)}$), such that :

(i) $F_+ = \Lambda_+ F$ and $F_- = \Lambda_- F$ are two subspaces of $\mathcal{F}(A)$.

(ii) $a = \sup_{x_- \in F_- \setminus \{0\}} \frac{(x_-, Ax_-)}{\|x_-\|^2_{\mathcal{H}}} < +\infty$.

We consider the sequence of min-max levels

$$\lambda_k = \inf_{\substack{V \text{ subspace of } F_+ \\ \dim V = k}} \ \sup_{x \in (V \oplus F_-) \setminus \{0\}} \frac{(x, Ax)}{||x||^2_{\mathcal{H}}} , \qquad k \geq 1. \tag{1}$$

Our last assumption is

(iii) $\qquad \lambda_1 > a$.

Now, let $b = \inf\, (\sigma_{\text{ess}}(A) \cap (a, +\infty)) \in [a, +\infty]$. For $k \geq 1$, we denote by μ_k the k^{th} eigenvalue of A in the interval (a, b), counted with multiplicity, *if this eigenvalue exists*. If there is no k^{th} eigenvalue, we take $\mu_k = b$. The main result of this note is

Theorem 1 . *With the above notations, and under assumptions $(i)-(ii)-(iii)$,*

$$\lambda_k \ = \ \mu_k \ , \quad \forall k \geq 1 \ .$$

As a consequence, $b = \lim_{k\to\infty} \lambda_k = \sup_k \lambda_k \ > \ a$.

Such a min-max approach was first proposed by Talman [13] and Datta-Deviah [2] in the particular case of Dirac operators with a potential, to compute numerically their first positive eigenvalue. In that case, the decomposition of $\mathcal{H}$ was very convenient for practical purposes: each 4-spinor was decomposed in its upper and lower parts. Note that in the Physics litterature, other min-max approaches were proposed, for the study of the eigenvalues of Dirac operators with a potential (see for instance [4], [8]).

A rigorous min-max procedure was then considered by Esteban and Séré in [5] for Dirac operators $H_0 + V$, V being a Coulomb-like potential. This time, $\mathcal{H}_+$ and $\mathcal{H}_-$ were the positive and negative spectral spaces of the free Dirac operator H_0.

To our knowledge, the first abstract theorem on the variational principle (1) is due to Griesemer and Siedentop [6]. These authors proved an analogue of Theorem 1, under conditions (i), (ii), and two additional hypotheses instead of (iii): they assumed that $(Ax, x) > a\|x\|^2$ for all $x \in F_+ \setminus \{0\}$, and they required the operator $(|A|+1)^{1/2} P_- \Lambda_+$ to be bounded. Here, Λ_+ is the orthogonal projection of $\mathcal{H}$ on $\mathcal{H}_+$ and P_- is the spectral projection of A for the interval $(-\infty, a]$, *i.e.* $P_- = \chi_{(-\infty,a]}(A)$.

Then, Griesemer and Siedentop applied their abstract result to the Dirac operator with potential. They proved that the min-max procedure proposed by Talman and Datta-Deviah was mathematically correct for a particular class of bounded potentials. In this case, the restrictions on the potentials were necessary in order to fulfill to the requirement $(Ax, x) > a\|x\|^2$ $\forall x \in F_+ \setminus \{0\}$. Such a hypothesis excludes the Coulomb potentials which appear in atomic models. Griesemer and Siedentop also applied their theorem to the min-max of [5], but the boundedness of $(|A|+1)^{1/2} P_- \Lambda_+$ seems difficult to check in the case of Coulomb potentials.

In [3], we extended the result of [5] to a larger class of Coulomb-like potentials and introduced a minimization approach to define the first positive eigenvalue of $H_0 + V$.

The present work is motivated by the abstract result of Griesemer and Siedentop [6]. Our Theorem 1 contains, as particular cases, the results on the min-max principle for the Dirac operator of [5], [6], [3]. It also applies to the Talman and Datta-Deviah procedure for atomic Coulomb potentials, under optimal conditions. However, Griesemer-Siedentop's abstract result is not a consequence of Theorem 1. Indeed, their hypothesis $(Ax_+, x_+) > a\|x_+\|^2$ $\forall x_+ \in F_+ \setminus \{0\}$ does not imply (iii).

In Section II of this paper we prove Theorem 1. The arguments are based on an abstract version of those in [3] (§4: the minimization procedure).

In the third section, we use Theorem 1 to justify Talman's and Datta-Deviah's min-max procedure for Dirac operators $H_0 + V$, for a large class of potentials V including Coulomb potentials. To check the optimality of our result, we consider the particular case of potentials behaving like Coulomb potentials $-Z\alpha/|x|$ and show that this very convenient and simple min-max which does not involve the use of complicated projector operators, yields all the eigenvalues of H_0+V in the gap under the only assumption that the first eigenvalue in the gap is positive, i.e. as long as $Z\alpha < 1$. This condition is optimal since it is well known that when the first eigenvalue of $H_0 - Z\alpha/|x|$ approaches 0 (for $Z\alpha \to 1^-$), the first eigenfunction "disappears".

II. Proof of Theorem 1.

The inequality $\lambda_k \leq \mu_k$ is an easy consequence of conditions (i) and (ii) (see [6] for the proof in a similar situation). It remains to prove that $\lambda_k \geq \mu_k$ for all k, under the additional assumption (iii). Replacing A by $A-a$ (if necessary), we may assume, without restricting the generality, that $\sup_{x_-\in F_-\setminus\{0\}} \frac{(x_-,Ax_-)}{||x||^2_{\mathcal{H}}} = 0$.

For $E>0$ and $x_+ \in F_+$, let us define

$$\begin{aligned} \varphi_{E,x_+} : \quad & F_- \to \mathbb{R} \\ & y_- \mapsto \varphi_{E,x_+}(y_-) = \Big((x_+ + y_-), A(x_+ + y_-)\Big) - E||x_+ + y_-||^2_{\mathcal{H}}. \end{aligned}$$

From assumptions $(i)-(ii)$, $N(y_-) = \sqrt{||y_-||^2_{\mathcal{H}} - (y_-, Ay_-)}$ is a norm on F_-. Let $\overline{F}^N_-$ be the completion of F_- for this norm. Since $||.||_{\mathcal{H}} \leq N$ on F_-, we have $\overline{F}^N_- \subset \mathcal{H}_-$. For all $x_+ \in F_+$, there is an $x \in F$ such that $\Lambda_+ x = x_+$. If we consider the new variable $z_- = y_- - \Lambda_- x$, we can define

$$\psi_{E,x}(z_-) := \varphi_{E,\Lambda_+ x}(z_- + \Lambda_- x) = (A(x+z_-), x+z_-) - E(x+z_-, x+z_-)\,.$$

Since F is a subspace of $D(A)$, $\psi_{E,x}$ (hence φ_{E,x_+}) is well-defined and continuous for N, uniformly on bounded sets. So, φ_{E,x_+} has a unique continuous extension $\overline{\varphi}_{E,x_+}$ on $\overline{F}^N_-$, which is continuous for the extended norm $\overline{N}$. It is well-known (see e.g. [10]) that there is a unique self-adjoint operator $B : D(B) \subset \mathcal{H}_- \to \mathcal{H}_-$ such that $D(B)$ is a subspace of $\overline{F}^N_-$, and

$$\overline{N}(x_-)^2 \;=\; ||x_-||^2_{\mathcal{H}} + (x_-, Bx_-)\;, \quad \forall x_- \in D(B)\;.$$

Now, $\overline{\varphi}_{E,x_+}$ is of class C^2 on $\overline{F}^N_-$ and

$$\begin{aligned} D^2\overline{\varphi}_{E,x_+}(x_-)\cdot(y_-,y_-) &= -2(y_-, By_-) - 2E||y_-||^2_{\mathcal{H}} \\ &\leq -2\min(1,E)\,\overline{N}(y_-)^2\;. \end{aligned} \tag{2}$$

So $\overline{\varphi}_{E,x_+}$ has a unique maximum, at the point $y_- = L_E(x_+)$. The Euler-Lagrange equations associated to this maximization problem are :

$$\Lambda_- A x_+ - (B+E)y_- = 0\,. \tag{3}$$

In the sequel of this note, we shall use the notation $\mathcal{X}'$ for the dual of a Hilbert space $\mathcal{X}$. Note that $(B+E)^{-1}$ is well-defined and bounded from $(\overline{F_-}^N)'$ to $\overline{F_-}^N$ since $(y_-, By_-) \geq 0$, $\forall y_- \in D(B)$. Moreover, $x_+ \in F_+ = \Lambda_+ F$ is of the form $x_+ = \Lambda_+ x = x - \Lambda_- x$ for some $x \in F \subset D(A)$. By assumption (i), $\Lambda_- x \in \mathcal{F}(A) \cap (\overline{F_-}^N)$, and finally $\Lambda_- A(x_+) = \Lambda_- Ax - \Lambda_- A \Lambda_- x \in (\overline{F_-}^N)'$. So the expression $(B+E)^{-1}\Lambda_- x_+$ is meaningful, and we have

$$L_E = (B+E)^{-1}\ \Lambda_- A\ . \tag{4}$$

Remark 2 *The unique maximizer of* $\overline{\psi}_{E,x} := \overline{\varphi}_{E,\Lambda_+ x}(\cdot + \Lambda_- x)$ *is the vector* $z_- = M_E x := L_E \Lambda_+ x - \Lambda_- x$ *and one has the following equation for* $M_E x$*:*

$$M_E x = (B+E)^{-1}\Lambda_-(A-E)x\,. \tag{5}$$

This expression is well-defined, since $x \in D(A)$.

The above arguments allow us, for any $E > 0$, to define a map

$$\begin{aligned} Q_E :\ \ & F_+ \to\ \ \mathbb{R} \\ & x_+ \mapsto\ \ Q_E(x_+) = \sup_{x_- \in F_-}\ \varphi_{E,x_+}(x_-) = \overline{\varphi}_{E,x_+}(L_E x_+) \\ & \qquad\qquad = (x_+, (A-E)x_+) + \Big(\Lambda_- A x_+, (B+E)^{-1}\Lambda_- A x_+\Big)\ . \end{aligned} \tag{6}$$

Note that for any $x \in F$,

$$\begin{aligned} Q_E(\Lambda_+ x) = (x, Ax)\ \ & +\ 2\,\mathrm{Re}\ (Ax, M_E x) \\ & -\ (M_E x, BM_E x) - E\|x + M_E x\|^2\ . \end{aligned} \tag{7}$$

It is easy to see that Q_E is a quadratic form with domain $F_+ \subset \mathcal{H}_+$.

We may also, for $E > 0$ given, define the norm $n_E(x_+) = ||x_+ + L_E x_+||_{\mathcal{H}}$. The following lemma gives some useful inequalities involving n_E and Q_E:

Lemma 3 . *If* $0 < E < E'$, *then*

$$\|\cdot\|_{\mathcal{H}} \leq n_{E'} \leq n_E \leq \frac{E'}{E} n_{E'}\,, \tag{8}$$

$$(E'-E)n_{E'}^2 \leq Q_E - Q_{E'} \leq (E'-E)n_E^2\,. \tag{9}$$

Moreover, $Q_{\lambda_1} \geq 0$.

Proof. Inequality (8) follows immediately from

$$n_E(x_+)^2 = ||x_+||^2_{\mathcal{H}} + ||(B+E)^{-1}\Lambda_- A x_+||^2_{\mathcal{H}} \, .$$

On the other hand, (9) is a consequence of

$$Q_{E'}(x_+) \geq \overline{\varphi}_{E',x_+}(L_E(x_+)) \, , \text{ for all } \; E, E' > 0 \, .$$

Finally, the definition of λ_1 implies that $Q_E(x_+) > 0$ for all $x_+ \in F_+ \setminus \{0\}$ and $0 < E < \lambda_1$. But (8) and (9) imply that

$$Q_{\lambda_1}(x_+) \geq Q_E(x_+) + (E - \lambda_1)\frac{\lambda_1}{E} n_{\lambda_1}(x_+) \, .$$

Passing to the limit $E \to \lambda_1$, we obtain $Q_{\lambda_1}(x_+) \geq 0$. □

We are now going to give a new definition of the numbers λ_k, equivalent to formula (1). First of all, let us recall the standard definitions and results on Rayleigh-Ritz quotients (see e.g. [11]).

Let T be a self-adjoint operator on a Hilbert space X, with domain $D(T)$ and form-domain $\mathcal{F}(T)$. If T is bounded from below, we may define a sequence of min-max levels,

$$\ell_k(T) \;=\; \inf_{\substack{Y \text{ subspace of } \mathcal{F}(T) \\ \dim Y = k}} \; \sup_{x \in Y \setminus \{0\}} \frac{(x, Tx)}{||x||^2_X}.$$

To each k we also associate the (possibly infinite) multiplicity number

$$n_k(T) \;=\; \operatorname{card}\Big\{k' \geq 1 \;,\; \ell_{k'}(T) = \ell_k(T)\Big\} \;\geq\; 1 \;.$$

Then $\ell_k(T) \leq \inf \sigma_{\rm ess}(T)$. In the case $\ell_k(T) < \inf \sigma_{\rm ess}(T)$, ℓ_k is an eigenvalue of T with multiplicity $n_k(T)$.

As a consequence, if $\mathcal{C} \subset \mathcal{F}(T)$ is a form-core for T (i.e. a dense subspace of $\mathcal{F}(T)$ for $||.||_{\mathcal{F}(T)}$), then there is a sequence (Z_n) of subspaces of $\mathcal{C}$, with dim $(Z_n) = n_k(T)$ and

$$\sup_{\substack{z \in Z_n \\ ||z||_X = 1}} \; ||Tz - \ell_k(T)z||_{(\mathcal{F}(T))'} \quad \underset{n \to \infty}{\longrightarrow} \quad 0 \; .$$

Coming back to our situation, we consider the completion X of F_+ for the norm n_E. By (8), X does not depend on $E > 0$. We denote by $\overline{n}_E$ the extended norm, and by $< \cdot, , \cdot >_E$ its polar form:

$$< x_+, x_+ >_E = (\overline{n}_E(x_+))^2 \, , \; \forall x_+ \in X \, .$$

Since $n_E(x_+) \geq ||x_+||_{\mathcal{H}}$, X is a subspace of $\mathcal{H}_+$. Also, we may define another norm on F_+ by

$$\mathcal{N}_E(x_+) = \sqrt{Q_E(x_+) + (K_E+1)(n_E(x_+))^2}$$

with $K_E = \max(0, \frac{E^2(E-\lambda_1)}{\lambda_1^2})$.

From (8) and (9), $\mathcal{N}_E$ is well-defined and satisfies $\mathcal{N}_E \geq n_E$. Indeed, in the case $0 < E \leq \lambda_1$, Lemma 3 implies $Q_E(x_+) \geq 0$ for all $x_+ \in F_+$. When $E \geq \lambda_1$, again from Lemma 3, we have

$$Q_E \geq Q_{\lambda_1} + (\lambda_1 - E)\, n_{\lambda_1}^2 \geq -K_E n_E^2 \,. \tag{10}$$

Note that for any $0 < E < E'$, Lemma 3 implies the existence of a constant $C_{E,E'} > 1$ such that

$$\mathcal{N}_{E'} \leq \mathcal{N}_E \leq C_{E,E'}\, \mathcal{N}_{E'} \,. \tag{11}$$

Let us consider the completion G of F_+ for the norm $\mathcal{N}_E$. Since $\mathcal{N}_E \geq n_E$, G is a subspace of X, dense for the extended norm $\bar{n}_E$. From (11), G does not depend on E. The extension $\bar{Q}_E$ of Q_E to G is a closed quadratic form with form-domain G. So (see e.g. [10]) there is a unique self-adjoint operator $T_E \,:\, D(T_E) \subset X \to X$ with form-domain $\mathcal{F}(T_E) = G$, such that $\bar{Q}_E(x_+) =< x_+, T_E x_+ >_E$, for any $x_+ \in D(T_E)$. Then F_+ is a form-core of T_E. The min-max levels $\ell_k(T_E)$ are given by

$$\ell_k(T_E) \;=\; \inf_{\substack{V \text{ subspace of } G \\ \dim Y = k}} \; \sup_{x_+ \in V \setminus \{0\}} \frac{\bar{Q}_E(x_+)}{(\bar{n}_E(x_+))^2} \,. \tag{12}$$

The next lemma explains the relashionship between $\ell_k(T_E)$ and the min-max principle (1) for A.

Lemma 4 .

(a) *For any $x_+ \in F_+ \setminus \{0\}$, the positive number*

$$\lambda(x_+) = \sup_{x \in (Span(x_+) \oplus F_-) \setminus \{0\}} \frac{(x, Ax)}{||x||_{\mathcal{H}}^2}$$

is the unique solution of the nonlinear equation

$$Q_\lambda(x_+) = 0 \,. \tag{13}$$

This equation may be written

$$\lambda \|x_+\|^2 = (x_+, Ax_+) + (\Lambda_- Ax_+, (B+\lambda)^{-1}\Lambda_- Ax_+) \ . \tag{14}$$

(b) *The min-max principle (1) is equivalent to*

$$\lambda_k = \inf_{\substack{V \text{ subspace of } F_+ \\ \dim V = k}} \ \sup_{x_+ \in V\setminus\{0\}} \lambda(x_+) \ , \qquad k \geq 1. \tag{15}$$

(c) *For any $k \geq 1$, the level λ_k defined by (1) is the unique solution of the nonlinear equation*

$$\ell_k \left(T_\lambda\right) \ = \ 0 \ . \tag{16}$$

In other words, 0 is the k^{th} min-max level for the Rayleigh-Ritz quotients of T_{λ_k}, and this determines λ_k in a unique way. Moreover, for $\lambda \neq \lambda_k$, the signs of $\lambda_k - \lambda$ and $\ell_k \left(T_\lambda\right)$ are the same.

Proof.

(a) From Lemma 3, $Q_\lambda(x_+)$ is a decreasing continuous function of λ, and $Q_{\lambda_1}(x_+) \geq 0$, $\lim_{\lambda\to+\infty} Q_\lambda(x_+) = -\infty$. So, the equation $Q_\lambda(x_+) = 0$ has a unique solution $\tilde{\lambda}(x_+)$, which lies in the interval $[\lambda_1, +\infty)$. Equation (14) is equivalent to (13) by elementary calculations. Now, if $\lambda < \tilde{\lambda}(x_+)$, then $Q_\lambda(x_+) > 0$, hence $\lambda(x_+) = \sup_{x\in(Span(x_+)\oplus F_-)\setminus\{0\}} \dfrac{(x, Ax)}{||x||^2_{\mathcal{H}}} > \lambda$. Similarly, $\lambda > \tilde{\lambda}(x_+)$ implies $\lambda(x_+) < \lambda$. So we get

$$\tilde{\lambda}(x_+) = \lambda(x_+) \ .$$

(b) Since $\lambda(x_+) = \sup_{x\in(Span(x_+)\oplus F_-)\setminus\{0\}} \dfrac{(x, Ax)}{||x||^2_{\mathcal{H}}}$, (1) is obviously equivalent to (15).

(c) We follow the same arguments as in the proof of (a). From Lemma 3, the map $\lambda \to \ell_k(T_\lambda)$ is continuous, and $\ell_k(T_{\lambda_1}) \geq 0$, $\lim_{\lambda\to+\infty} \ell_k(T_\lambda) = -\infty$. So the equation $\ell_k(T_\lambda) = 0$ has at least one solution $\tilde{\lambda}_k$, which lies in the interval $[\lambda_1, +\infty)$. Now, if $\lambda < \tilde{\lambda}_k$, then it follows from Lemma 3 that $\ell_k(T_\lambda) > 0$, hence $\sup_{x\in(V\oplus F_-)\setminus\{0\}} \dfrac{(x, Ax)}{||x||^2_{\mathcal{H}}} > \lambda$ for any k-dimensional subspace V of F_+. Similarly, $\lambda > \tilde{\lambda}_k$ implies $\sup_{x\in(V\oplus F_-)\setminus\{0\}} \dfrac{(x, Ax)}{||x||^2_{\mathcal{H}}} < \lambda$ for some k-dimensional subspace V of F_+. So, we get $\tilde{\lambda}_k = \lambda_k$.

$\square$

As already mentioned, F_+ is a form-core of T_E and G is its form-domain. So, from Lemma 4 (c), if $m_k = \text{card}\,\{k' \geq 1\ ;\ \lambda_k = \lambda_{k'}\}$, there is a sequence (Z_n) of subspaces of F_+, of dimension m_k, such that

$$\sup_{\substack{x_+ \in Z_n \\ ||x_+||^2_{\mathcal{H}} + ||L_{\lambda_k} x_+||^2_{\mathcal{H}} = 1}} \left\| T_{\lambda_k} x_+ \right\|_{G'} \underset{n\to\infty}{\longrightarrow} 0$$

Using the explicit expressions of Q_E and L_E on F_+ (see (4),(7)), we obtain

$$(17) \quad \sup_{\substack{\tilde{x} \in (\mathbb{1}+\mathrm{L}_{\lambda_k})(\mathrm{Z_n}) \\ ||\tilde{\mathrm{x}}||_{\mathcal{H}} = 1}} \ \sup_{\substack{\tilde{y} \in (\mathbb{1}+\mathrm{L}_{\lambda_k})(\mathrm{F}_+) \\ \tilde{\mathrm{y}} \neq 0}} \frac{|\mathcal{A}(\tilde{x},\tilde{y}) - \lambda_k (\tilde{x},\tilde{y})_{\mathcal{H}}|}{\Big((K_{\lambda_k}+1)\ ||\tilde{y}||^2_{\mathcal{H}} + Q_{\lambda_k}(\Lambda_+ \tilde{y})\Big)^{1/2}} \underset{n\to\infty}{\longrightarrow} 0\ ,$$

where $\mathcal{A}(\tilde{x},\tilde{y}) := (x, Ay) + (Ax, M_{\lambda_k} y) + (M_{\lambda_k} x, Ay) - (BM_{\lambda_k} x, M_{\lambda_k} y)$, with $x, y \in F \subset D(A)$ such that $\Lambda_+ x = \Lambda_+ \tilde{x}$, $\Lambda_+ y = \Lambda_+ \tilde{y}$ and $M_{\lambda_k} x = L_{\lambda_k} \Lambda_+ x - \Lambda_- x$. Note that the value of $\mathcal{A}(\tilde{x},\tilde{y})$ does not depend on the choice of x and y. Indeed, $\mathcal{A}$ is the polar form of the quadratic form $\tilde{y} \mapsto \overline{Q}_{\lambda_k}(\Lambda_+ \tilde{y}) + \lambda_k ||\tilde{y}||^2_{\mathcal{H}}$.

Denote $\tilde{Z}_n = (\mathbb{1} + \mathrm{L}_{\lambda_k})(\mathrm{Z_n})$. Take $y \in F$, and let $\tilde{y} = (\mathbb{1} + \mathrm{L}_{\lambda_k})(\Lambda_+ \mathrm{y})$. There is a constant $C(\lambda_k)$ such that

$$(18) \qquad (K_{\lambda_k}+1)\ ||\tilde{y}||^2_{\mathcal{H}} + Q_{\lambda_k}(\Lambda_+ y) \leq C(\lambda_k)\ ||y||^2_{D(A)}\ .$$

Indeed, by Remark 2,

$$Q_{\lambda_k}(\Lambda_+ y) \leq ||y||_{D(A)} \left(||y||_{\mathcal{H}} + 2||M_{\lambda_k} y||_{\mathcal{H}}\right) - \lambda_k ||M_{\lambda_k} y||^2_{\mathcal{H}} \leq (1+1/\lambda_k) ||y||^2_{D(A)}\ .$$

Moreover, for any $x \in F_+$, and any $z_- \in \mathcal{F}(B)$, by (5) we have : $((Ax - BM_{\lambda_k} x) - \lambda_k (x + M_{\lambda_k} x), z_-) = 0$. As a consequence, (17) is equivalent to

$$\sup_{\substack{\tilde{x} \in \tilde{Z}_n \\ ||\tilde{x}||_{\mathcal{H}} = 1}} \ \sup_{y \in F \setminus \{0\}} \frac{|(\tilde{x}, Ay - \lambda_k y)|}{||y||_{D(A)}} \underset{n\to\infty}{\longrightarrow} 0\ .$$

So, by the standard spectral theory of self-adjoint operators, we obtain an alternative: either $\lambda_k \in \sigma_{\text{ess}}(A) \cap (0,\infty)$, or λ_k is a positive eigenvalue of A with multiplicity greater than or equal to m_k.

We have thus proved the inequality $\lambda_k \geq \mu_k$, $\forall k \geq 1$. This ends the proof of Theorem 1. $\square$

III. Applications and remarks : Dirac operators.

With the notations of the preceding section, let us define $\mathcal{H} = L^2(\mathbb{R}^3, \mathbb{C}^4)$,

$$\mathcal{H}_+ = L^2(\mathbb{R}^3, \mathbb{C}^2) \otimes \left\{ \begin{pmatrix} 0 \\ 0 \end{pmatrix} \right\}, \ \mathcal{H}_- = \left\{ \begin{pmatrix} 0 \\ 0 \end{pmatrix} \right\} \otimes L^2(\mathbb{R}^3, \mathbb{C}^2) \,,$$

so that for any $\psi = \binom{\varphi}{\chi} \in L^2(\mathbb{R}^3, \mathbb{C}^4)$,

$$\Lambda_+\psi = \begin{pmatrix} \varphi \\ 0 \end{pmatrix}, \ \Lambda_-\psi = \begin{pmatrix} 0 \\ \chi \end{pmatrix}.$$

Let $F = C_0^\infty(\mathbb{R}^3, \mathbb{C}^4)$ be the space of smooth, compactly supported functions from $\mathbb{R}^3$ to $\mathbb{C}^4$.

The free Dirac operator is $H_0 = -i\alpha \cdot \nabla + \beta$, with

$$\alpha_1, \alpha_2, \alpha_3, \beta \in \mathcal{M}_{4\times 4}(\mathbb{C}), \ \beta = \begin{pmatrix} \mathbb{I} & 0 \\ 0 & -\mathbb{I} \end{pmatrix}, \ \alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix},$$

σ_i being the Pauli matrices

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

Let V be a scalar potential satisfying

$$V(x) \underset{|x| \to +\infty}{\longrightarrow} 0\,, \tag{19}$$

$$-\frac{\nu}{|x|} - c_1 \le V \le c_2 = \sup(V)\,, \tag{20}$$

with $\nu \in (0,1)$, $c_1, c_2 \in \mathbb{R}$.

Under the above assumptions, $H_0 + V$ has a distinguished self-adjoint extension A with domain $\mathcal{D}(A)$ such that

$$H^1(\mathbb{R}^3, \mathbb{C}^4) \subset \mathcal{D}(A) \subset H^{1/2}(\mathbb{R}^3, \mathbb{C}^4)\,,$$

$$\sigma_{\text{ess}}(A) \ = \ (-\infty, -1] \cup [1, +\infty)\ ,$$

and F is a core for A, with $F_\pm := \Lambda_\pm F \subset F \subset \mathcal{D}(A)$ (see [14], [12],[9], [7]). In the sequel, we shall denote this extension indifferently by A or $H_0 + V$.

The min-max procedure proposed by Talman and Datta-Deviah, for the first eigenvalue of $H_0 + V$ in the gap $(-1, 1)$, is

$$\inf_{\varphi \neq 0} \sup_{\chi} \frac{(\psi, (H_0 + V)\psi)}{(\psi, \psi)}\,. \tag{21}$$

With the choices of $\mathcal{H}$, $\mathcal{H}_\pm$, F and A made above, (21) coincides with the variational principle (1) of Section I, for $k = 1$. So, in order to show that (21) is correct, we just have to check the hypotheses of Theorem 1.

It is clear that assumptions (i) and (ii) of Theorem 1 are satisfied, with

$$a = \sup_{x_-\in F_-\setminus\{0\}} \frac{(x_-, Ax_-)}{\|x_-\|^2_{\mathcal{H}}} = c_2 - 1 \ .$$

In the sequel, we shall denote $\mu_k(V)$ the k-th eigenvalue of $H_0 + V$ in the gap $(a, 1)$, with the understanding that $\mu_k(V) = 1$ whenever $H_0 + V$ has less than k eigenvalues in $(a, 1)$ (this corresponds to the notation $\mu_k(A)$ of Section 1, for $A = H_0 + V$). Similarly, $\lambda_k(V)$ will denote the min-max $\lambda_k(H_0 + V)$ given by formula (1). To check (iii), we will need an additional condition on V :

$$c_1, c_2 \geq 0, \ \ c_1 + c_2 - 1 < \mu_1(-\frac{\nu}{|x|})\,. \tag{22}$$

Here, according to our conventions, $\mu_1(-\frac{\nu}{|x|})$ denotes the smallest eigenvalue of $H_0 - \frac{\nu}{|x|}$ in the interval $(-1, 1)$. It turns out that $\mu_1(H_0 - \frac{\nu}{|x|}) = \sqrt{1-\nu^2}$ for all $\nu \in (0, 1)$.

The main result of this section is

Theorem 5 *Let V a scalar potential satisfying (19)-(20)-(22). Then, for all $k \geq 1$,*

$$\lambda_k(V) = \mu_k(V)\,. \tag{23}$$

Moreover, $\lambda_k(V) = \mu_k(V)$ is given by

$$\lambda_k(V) = \inf_{\substack{Y \text{ subspace of } C_o^\infty(\mathbb{R}^3,\mathbb{C}^2) \\ \dim Y = k}} \ \sup_{\varphi\in Y\setminus\{0\}} \lambda^V(\varphi)\,, \tag{24}$$

where $\lambda^V(\varphi)$ is the unique number in $(a, +\infty)$ such that

$$\lambda^V(\varphi)\int_{\mathbb{R}^3}|\varphi|^2 dx \ = \ \int_{\mathbb{R}^3}\Big(\frac{|L\varphi|^2}{1-V+\lambda^V(\varphi)} + (1+V)|\varphi|^2\Big)dx\ . \tag{25}$$

with $L := i\,\sigma\cdot\nabla$.

Remark 6 *In the case $k = 1$, formula (24) reduces to*

$$\lambda_1(V) = \inf_{\varphi\in C_o^\infty(\mathbb{R}^3,\mathbb{C}^2)\setminus\{0\}} \lambda^V(\varphi)\ ,$$

where $\lambda_1(\varphi)$ is given by equation (25). This is exactly the minimization principle of [3], §4, formula (4.16).

The key point, to prove Theorem 5, is to check that condition (iii) of Theorem 1 is fulfilled by H_0+V. In view of Remark 6, this was already done in [3]. But the arguments can be made simpler and clearer, thanks to the formalism of Section II. First of all, we give, in the present framework, some direct consequences of the results in Section II.

For $E > a = c_2 - 1$, let Q_E^V be the quadratic form given by formula (6), for $A = H_0 + V$. For all $\varphi \in C_o^\infty(\mathbb{R}^3, \mathbb{C}^2)$, we have

$$(26) \qquad Q_E^V(\varphi) \;=\; \int_{\mathbb{R}^3} \Big(\frac{|L\varphi|^2}{1-V+E} + (1+V-E)|\varphi|^2 \Big)\, dx\ .$$

The relashionship between the min-max level λ_1^V and Q_E^V is the following.

Lemma 7 *Let V be a scalar potential satisfying (19)-(20). Then for any $E > a = c_2 - 1$,*

$$(27) \qquad \lambda_1(V) = E \quad \textit{if and only if} \quad \inf_{n_{c_2}(\varphi)=1} Q_E^V(\varphi) = 0\,.$$

Moreover, if $E \neq \lambda_1(V)$ then $\lambda_1(V) - E$ and $\inf_{n_{c_2}(\varphi)=1} Q_E^V(\varphi)$ have the same sign.

Proof. This lemma follows immediately from Lemma 3 and Lemma 4 (c). □

The next lemma explains formulas (24) and (25).

Lemma 8 . *Let V be a scalar potential satisfying (19)-(20)-(22) and assume that $\lambda_1(V) > c_2 - 1 = a$. Then, for any $\varphi \in C_0^\infty(\mathbb{R}^3, \mathbb{C}^2)$, $\varphi \neq 0$,*

$$(28) \qquad \lambda^V(\varphi) := \sup_{\substack{\psi = \binom{\varphi}{\chi} \\ \chi \in C_0^\infty(\mathbb{R}^3, \mathbb{C}^2)}} \frac{((H_0+V)\psi, \psi)}{(\psi, \psi)}$$

is the unique number above $c_2 - 1$ such that

$$(29) \quad \lambda^V(\varphi) \int_{\mathbb{R}^3} |\varphi|^2 dx \;=\; \int_{\mathbb{R}^3} \Big(\frac{|L\varphi|^2}{1-V+\lambda^V(\varphi)} + (1+V)|\varphi|^2 \Big)\, dx\ ,$$

and (24) holds true. Moreover, the maximizer of (28) in $\mathcal{H}^-$ is

$$(30) \qquad \chi(\varphi) = \frac{L\varphi}{1-V+\lambda^V(\varphi)}\,.$$

Proof. This lemma is an immediate consequence of Lemma 4 and formula (4). $\square$

In the sequel, we show that condition (iii) of Theorem 1 holds true for all potentials satisfying (19)-(20)-(22). In particular, this result covers the case of Coulomb-like potentials with singularities $-\nu/|x|$, for all $\nu \in (0,1)$. The proof relies on a continuation argument, based on two facts:

1. For all $\nu \in (0,1)$, $\mu_1(-\frac{\nu}{|x|}) = \sqrt{1-\nu^2} > 0$.
2. The following homogeneous Hardy-type inequality holds:

$$(31) \qquad \int_{\mathbb{R}^3} \frac{|\varphi|^2}{|x|} \leq \int_{\mathbb{R}^3} |x|\,|L\varphi|^2 \;, \quad \forall \varphi \in H^{1/2}(\mathbb{R}^3, \mathbb{C}^2) \;,$$

with $L := i\,\sigma\cdot\nabla$. Taking $\phi = \frac{\varphi}{|x|^{1/2}}$, this inequality is a direct consequence of the standard Hardy inequality

$$\int_{\mathbb{R}^3} \frac{|\phi|^2}{|x|^2} \leq 4 \int_{\mathbb{R}^3} |\nabla\phi|^2 = 4 \int_{\mathbb{R}^3} |L\phi|^2 \;.$$

For potentials V satisfying (19)-(20)-(22), with $c_2 = 0$, let us introduce a very useful auxiliary quantity:

$$(32) \qquad f(\tau,\gamma) := \inf_{\varphi \in F_+ \setminus \{0\}} \frac{\displaystyle\int_{\mathbb{R}^3} \left(\frac{|L\varphi|^2}{\tau|V|+\gamma} + |\varphi|^2 \right) dx}{\displaystyle\int_{\mathbb{R}^3} \tau|V||\varphi|^2 dx} \;.$$

Then we can prove:

Lemma 9 *Let V be a potential satisfying (19)-(20), with $c_2 = 0$. Then, the function $(\tau,\gamma) \mapsto f(\tau,\gamma)$ (resp. $\tau \mapsto I(\tau V)$) is continuous in $\mathbb{R}^+ \times \mathbb{R}^+$ (resp. in $\mathbb{R}^+$).*

Proof.

$$(33)\, g(\tau,\gamma,\varphi) := \frac{\displaystyle\int_{\mathbb{R}^3} \left(\frac{|L\varphi|^2}{\tau|V|+\gamma} + |\varphi|^2 \right) dx}{\displaystyle\int_{\mathbb{R}^3} \tau|V||\varphi|^2 dx} = \frac{\displaystyle\int_{\mathbb{R}^3} \left(\frac{|L\varphi|^2}{\tau^2|V|+\tau\gamma} + \frac{|\varphi|^2}{\tau} \right) dx}{\displaystyle\int_{\mathbb{R}^3} |V||\varphi|^2 dx} .$$

Hence, by straightforward computations, for all $\varphi \in F_+$, $\tau, \tau', \gamma, \gamma' > 0$,

$$g(\tau',\gamma',\varphi) \leq \left(1 + \frac{|\tau^2 - \tau'^2|}{\tau'^2} + \frac{|\tau-\tau'|}{\tau\tau'} + \frac{|\tau'\gamma' - \tau\gamma|}{\tau'\gamma'} \right) g(\tau,\gamma,\varphi) \,.$$

Therefore, for all $\tau, \tau', \gamma, \gamma' > 0$,

$$f(\tau', \gamma') \leq \left(1 + \frac{|\tau^2 - \tau'^2|}{\tau'^2} + \frac{|\tau - \tau'|}{\tau\tau'} + \frac{|\tau'\gamma' - \tau\gamma|}{\tau'\gamma'}\right) f(\tau, \gamma)\,,$$

which proves the lemma. $\square$

The next lemma relates the positivity of λ_1 to the inhomogeneous Hardy-type inequality $f(1,1) > 1$. The proof uses the homogeneous inequality (31), and the assumption $\nu \in (0,1)$ made in (20) plays a crucial role.

Lemma 10 *Assume that V satisfies (19), (20), with $c_2 = 0$. Then $I(V) := f(1,1) > 1$ if and only if $\lambda_1(V) > 0$.*

Proof. Let $I(V) = f(1,1) = 1 + 2\delta > 1$. By Lemma 9, there exists $\gamma > 1$ such that $f(1, \gamma) = 1 + \delta > 1$. By its definition, we already know that $\lambda_1(V) \geq 0$. Moreover, for any $\varphi \in F_+$, $\varphi \neq 0$, such that $\lambda^V(\varphi) < \gamma - 1$, $f(1, \gamma) = 1 + \delta > 1$ implies

$$(34)\quad \lambda^V(\varphi) = \frac{\displaystyle\int_{\mathbb{R}^3} \Big(\frac{|L\varphi|^2}{|V| + 1 + \lambda^V(\varphi)} + |\varphi|^2 - |V||\varphi|^2\Big) dx}{\displaystyle\int_{\mathbb{R}^3} |\varphi|^2 dx} \geq \frac{\delta}{1+\delta} > 0.$$

Hence, $\lambda_1(V) > 0$.

On the other hand, $I(V) < 1$ trivially implies $\lambda_1(V) < 0$.

Finally, assume that $I(V) = 1$. By Lemma 8, $\lambda_1(V) \geq 0$. Let us prove that $\lambda_1(V) = 0$. If $\{\varphi_n\}_n$ is a minimizing sequence for $I(V)$ such that

$$(35)\qquad \int_{\mathbb{R}^3} |V||\varphi_n|^2 dx = 1\ ;\quad \int_{\mathbb{R}^3} \Big(\frac{|L\varphi_n|^2}{|V| + 1} + |\varphi_n|^2\Big) dx = 1 + \frac{1}{n}\,.$$

Then, by (29),

$$(36)\qquad \lambda^V(\varphi_n) \leq \frac{1}{n \displaystyle\int_{\mathbb{R}^3} |\varphi_n|^2 dx}.$$

Therefore, if $\int_{\mathbb{R}^3} |\varphi_n|^2 dx$ is uniformly bounded away from 0, the proof is finished. Assume, by contradiction, that there is a subsequence, still denoted by $\{\varphi_n\}_n$, such that

$$\int_{\mathbb{R}^3} |\varphi_n|^2\, dx \quad \underset{n\to+\infty}{\longrightarrow} \quad 0\,.$$

We then define a new sequence $\tilde\varphi_n = \varphi_n\, g$ by choosing $g \in C_o^\infty(\mathbb{R}^3)$ such that

(37) $$\text{supp}\, g \subset B_\delta,\ g \equiv 1 \text{ in } B_{\delta/2}\ ,\ 0 \le g \le 1\ .$$

let us choose δ small enough so that in $B_{2\delta}$, $|V|+1 \le \frac{\nu'}{|x|}$ for some $\nu' \in (\nu, 1)$. This can be done thanks to assumptions (19)-(20). Then, there exists $\varepsilon_n \to 0$ as $n \to +\infty$ such that

(38) $$\int_{\mathbb{R}^3} |x|\ |L\tilde\varphi_n|^2\, dx \le \nu' \int_{\mathbb{R}^3} \frac{|L\tilde\varphi_n|^2}{|V|+1}\, dx \le \nu'(1+\varepsilon_n)\,,$$

(39) $$\nu' \int_{\mathbb{R}^3} \frac{|\tilde\varphi_n|^2}{|x|}\, dx \ge \int_{\mathbb{R}^3} |V||\tilde\varphi_n|^2\, dx \ge 1-\varepsilon_n\ .$$

Hence,

(40) $$\int_{\mathbb{R}^3} \frac{|\tilde\varphi_n|^2}{|x|}\, dx \ge \frac{1-\varepsilon_n}{\nu'^2(1+\varepsilon_n)}(\nu'(1+\varepsilon_n)) \ge \frac{1-\varepsilon_n}{\nu'^2(1+\varepsilon_n)} \int_{\mathbb{R}^3} |x|\ |L\tilde\varphi_n|^2\, dx,$$

which contradicts the Hardy-type inequality (31). □

Now we will consider the particular case of Coulomb-like potentials $V = -\nu/|x|$, $\nu \in (0,1)$.

Lemma 11 *For $\nu > 0$ small enough, $\lambda_1(-\nu/|x|) > 0$.*

Proof. By Lemma 7, we only have to prove that for ν small enough, there exists some $\varepsilon > 0$ such that

(41) $$\int_{\mathbb{R}^3} \left(\frac{|L\varphi|^2}{1+\frac{\nu}{|x|}} + \left(1 - \frac{\nu}{|x|}\right) |\varphi|^2 \right) dx \ge \varepsilon \int_{\mathbb{R}^3} \left(\frac{|L\varphi|^2}{\left(1+\frac{\nu}{|x|}\right)^2} + |\varphi|^2 \right) dx\ .$$

We remark that a simple localization procedure and (31) imply that for some $C > 0$, we have

(42) $$\int_{\mathbb{R}^3} \frac{|\varphi|^2}{|x|}\, dx \le C \int_{\mathbb{R}^3} \left(|\varphi|^2 + \frac{|L\varphi|^2}{1+\frac{1}{|x|}} \right) dx\,.$$

This, and the fact that for all $\nu > 0$ and all $x \ne 0$, $(1+(\nu/|x|)) \le (1+(\nu/|x|))^2$, prove (41). □

Proof of Theorem 5. First, we notice that if the theorem is proved for the Coulomb-potential $-\nu/|x|$, then, by a simple comparison argument, the theorem follows for all potentials satisfying (19)-(20)-(22). Indeed, let us define the operator $A = H_0 + V$. A satisfies the assumptions (i) and (ii) of Theorem 1. Moreover, by (20) and the definition of $\lambda_1(V)$,

$$\lambda_1(V) \geq \lambda_1(-\frac{\nu}{|x|} - c_1) = \mu_1(-\frac{\nu}{|x|}) - c_1 \, .$$

Hence, by (22),

$$\lambda_1(V) > c_2 - 1 = a \, .$$

Therefore, by Theorem 1, (23) holds true. Moreover, (24) and (25) follow from Lemma 8.

Let us prove the theorem in the particular case $V = -\nu/|x|$, $0 < \nu < 1$. By Theorem 1 and Lemmas 8, 11, the result holds true for ν small enough. We define $\nu_* = \sup\{\nu \in (0,1)\,;\ \lambda_1(-\nu/|x|) > 0\}$. If $\nu_* = 1$, the proof is finished. Assume then that $\nu_* < 1$. For all $\nu \in (0, \nu_*)$, we have $\lambda_1(-\nu/|x|) = \mu_1(-\nu/|x|) \geq \mu_1(-\nu_*/|x|) = \sqrt{1-\nu_*^2}$. So Lemma 7 implies that

$$\int_{\mathbb{R}^3} \left(\frac{|L\varphi|^2}{1+\frac{\nu}{|x|}} + \left(1 - \frac{\nu}{|x|}\right) |\varphi|^2 \right) dx \geq \sqrt{1-\nu_*^2} \int_{\mathbb{R}^3} \left(\frac{|L\varphi|^2}{\left(1+\frac{\nu}{|x|}\right)^2} + |\varphi|^2 \right) dx \, .$$

(43)

Passing to the limit $\nu \to \nu_*$, and using Lemma 7 again, we obtain the inequality $\lambda_1(-\nu_*/|x|) > 0$. Finally, by Lemmas 9 and 10, $I(-\nu/|x|) > 1$ for $\nu > \nu_*$, with $\nu - \nu_*$ small enough. But then, by Lemma 10, $\lambda_1(-\nu/|x|) > 0$, which contradicts the definition of ν_*. Hence, ν_* must be equal to 1 and the proof of Theorem 5 is finished. □

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