# DISTINGUISHED SELF-ADJOINT EXTENSION AND EIGENVALUES OF OPERATORS WITH GAPS. APPLICATION TO DIRAC-COULOMB OPERATORS

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ABSTRACT. We consider a linear symmetric operator in a Hilbert space that is neither bounded from above nor from below, admits a block decomposition corresponding to an orthogonal splitting of the Hilbert space and has a variational gap property associated with the block decomposition. A typical example is the minimal Dirac-Coulomb operator defined on $C_c^\infty(\mathbb{R}^3\setminus\{0\},\mathbb{C}^4)$. In this paper we define a distinguished self-adjoint extension with a spectral gap and characterize its eigenvalues in that gap by a variational min-max principle. This has been done in the past under technical conditions. Here we use a different, geometric strategy, to achieve that by making only minimal assumptions. Our result applied to the Dirac-Coulomb-like Hamitonians covers sign-changing potentials as well as molecules with an arbitrary number of nuclei having atomic numbers less than or equal to 137.

## 1. INTRODUCTION AND MAIN RESULT

The three-dimensional *Dirac-Coulomb operator* is $\mathscr{D}_V = \mathscr{D} + V$ where $\mathscr{D} = -i\,\alpha\cdot\nabla+\beta$ is the linear Dirac operator (see [22] for more detail), and $V$ is the Coulomb operator $-\frac{\nu}{|x|}$ ($\nu>0$) or, more generally, the convolution of $-\frac{1}{|x|}$ with an extended charge density. Usually, one first defines $\mathscr{D}_{-\nu/|x|}$ on the so-called minimal domain $C_c^\infty(\mathbb{R}^3\setminus\{0\},\mathbb{C}^4)$. The resulting minimal operator is symmetric but not closed in the Hilbert space $L^2(\mathbb{R}^3,\mathbb{C}^4)$. It is essentially self-adjoint when $\nu$ lies in the interval $(0,\sqrt{3}/2]$, in other words it has a unique self-adjoint extension, that turns out to be its closure. For larger constants $\nu$, one must define a distinguished, physically relevant, self-adjoint extension and this can be done when $\nu\le 1$. The essential spectrum of this extension is $\mathbb{R}\setminus(-1,1)$, which is neither bounded from above nor from below. In atomic physics, its eigenvalues in the gap $(-1,1)$ are interpreted as discrete electronic energy levels.

Important contributions to the construction of distinguished self-adjoint realisations of minimal Dirac-Coulomb operators were made in the 1970's, see *e.g.* [20, 26, 27, 28, 16, 17, 12, 11]. In these papers, general classes of potentials $V$ are considered, but in the case $V=-\nu/|x|$ one always assumes that $\nu$ is smaller than 1.

Reliable computations of the discrete electronic energy levels in the spectral gap $(-1,1)$ are a central issue in Relativistic Quantum Chemistry. For this purpose, Talman [21] and Datta-Devaiah [1] proposed a min-max principle involving Rayleigh quotients and the

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decomposition of 4-spinors into their so-called large and small 2-components. An abstract version of this min-max principle is concerned with a self-adjoint operator $A$ defined in a Hilbert space $\mathscr{H}$ and satisfying a *variational gap* condition, to be specified later, related to a block decomposition under an orthogonal splitting

$$\mathscr{H} = \mathscr{H}^+ \oplus \mathscr{H}^- . \tag{1}$$

Such an abstract principle was proved for the first time in [10], but its hypotheses were rather restrictive and the application to the distinguished self-adjoint realization of $\mathscr{D}_V$ only gave Talman's principle for bounded electric potentials. In [2], thanks to another approach, this limitation was overcome and the unbounded potential $-\nu/|x|$ was dealt with for $\nu \in (0, \sqrt{3}/2]$. The articles [3, 4, 5, 14, 15, 6, 19, 7] followed and the full range $\nu \in (0,1]$ is now covered.

Using some of the tools of [2], Esteban and Loss [8, 9] proposed a new strategy to build a distinguished, Friedrichs-like, self-adjoint extension of an abstract *symmetric* operator with variational gap and applied it to the minimal Dirac-Coulomb operator, with $\nu \in (0,1]$. In [6, 7], connections were established between this new approach and the earlier constructions, for Dirac-Coulomb operators with general electric potentials $V$.

Some important closability and domain invariance issues had been overlooked in the arguments of [2] and [8, 9]. In [19] these issues are clarified and the self-adjoint extension problem considered in [8, 9] is connected to the min-max principle for eigenvalues of self-adjoint operators studied in [2]. The abstract results in [19] have many important applications, but some examples are not covered yet, due to an essential self-adjointness assumption made on one of the blocks. In [2, Erratum], we present another way of correcting the arguments of [2] thanks to a geometric viewpoint. In the present work, by adopting this viewpoint, we are able to completely relax the essential self-adjointness assumption of [19]. Additionally, our variational gap assumption is more general, as it covers a class of multi-center Dirac-Coulomb Hamiltonians in which the lower min-max levels fall below the threshold of the continuous spectrum (see e.g. [6] for a study of such operators): we shall use the image that some eigenvalues *dive* into the negative continuum.

Before going into the detail of our assumptions and results, let us start by briefly recalling the standard Friedrichs extension theorem and its proof. If a linear symmetric operator $A$ in a Hilbert space $\mathscr{H}$ is bounded from below, *i.e.*, if

$$m := \inf_{x \in \mathrm{Dom}(A) \setminus \{0\}} \frac{(x, A\,x)}{\|x\|^2} > -\infty ,$$

then $A$ has a natural self-adjoint extension $A_F$, which is called the *Friedrichs extension* and defined as follows (see *e.g.* [18] for more details). The quadratic form $q_A(x) = (x, A\,x)$ is closable in $\mathscr{H}$. Assume that $\overline{q}_A$ denotes its closure and $\overline{p}_A(\cdot,\cdot)$ its polar form. Take $E > -m$. By the Riesz isomorphism theorem, for each $f \in \mathscr{H}$, there is a unique $u_f \in \mathrm{Dom}(\overline{q}_A)$ such that $\overline{p}_A(v, u_f) + E\,(v, u_f) = (v, f)$ for all $v \in \mathrm{Dom}(\overline{q}_A)$. Note that $u_f$ is also the unique minimizer, in $\mathrm{Dom}(\overline{q}_A)$, of the functional $I_f(u) := \frac{1}{2}\left(\overline{q}_A(u) + E\,\|u\|^2\right) - (u, f)$. The map $f \mapsto u_f$ is linear, bounded and self-adjoint for $(\cdot,\cdot)$. Its inverse is $A_F + E\,\mathrm{id}_{\mathscr{H}}$ and one easily checks that $A_F$ does not depend on $E$: in fact, $A_F$ is just the restriction of $A^*$ to

$\mathrm{Dom}(\overline{q}_A)\cap\mathrm{Dom}(A^*)$. An important property of the Friedrichs extension is that its eigenvalues below its essential spectrum, if they exist, can be characterized by the Rayleigh-Ritz principle. In the special case of the Laplacian in a bounded domain $\Omega$ of $\mathbb{R}^d$ with smooth boundary, $A=-\Delta : C_c^\infty(\Omega)\to L^2(\Omega)$, one has $\mathrm{Dom}(\overline{q}_A)=H_0^1(\Omega)$ and the construction of $A_F$ corresponds to the weak formulation in $H_0^1(\Omega)$ of the Dirichlet problem: $-\Delta u=f$ in $\Omega$, $u=0$ on $\partial\Omega$. In other words, $u_f$ is the unique function in $H_0^1(\Omega)$ such that for all $v\in H_0^1(\Omega)$, $\int_\Omega \nabla u_f\cdot\nabla v\,dx=\int_\Omega f\,v\,dx$. So $A_F$ is the self-adjoint realization of the Dirichlet Laplacian. By regularity theory, we learn that $\mathrm{Dom}(A_F)=H^2(\Omega)\cap H_0^1(\Omega)$.

The statement of our main result requires some definitions and notations. We consider a Hilbert space $\mathscr{H}$ with scalar product $(\cdot,\cdot)$ and associated norm $\|\cdot\|$. When the sum of two subspaces $V$, $W$ of $\mathscr{H}$ is direct in the algebraic sense, we use the notation $V\dot{+}W$. We reserve the notation $V\oplus W$ to topological sums. Let $F$ be a dense subspace of $\mathscr{H}$ and let $A:\mathrm{Dom}(A)=F\to\mathscr{H}$ be a symmetric operator, *i.e.* an operator such that $(Ax,y)=(x,Ay)$ for any $x,y\in F$. Let $\mathscr{H}=\mathscr{H}_+\oplus\mathscr{H}_-$ be the orthogonal splitting of $\mathscr{H}$ as in (1) and note

$$\Lambda_\pm:\mathscr{H}\to\mathscr{H}_\pm$$

the associated projectors. We make the following assumptions:

$$F_+=\Lambda_+F \text{ and } F_-=\Lambda_-F \text{ are subspaces of } F \tag{H1}$$

and

$$a:=\sup_{x_-\in F_-\setminus\{0\}}\frac{(x_-,Ax_-)}{\|x_-\|^2}<+\infty. \tag{H2}$$

We also make the *variational gap assumption* that

$$\text{for some } k_0\geq 1, \text{ we have } \lambda_{k_0}>a \tag{H3}$$

where the min-max levels $\lambda_k$ are defined by

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

We shall use the more precise notation $(\mathrm{H3})_{k_0}$ for our variational gap assumption whenever we need to specify the value of $k_0:=\min\{k\geq 1:\lambda_k>a\}$.

The construction of a distinguished self-adjoint extension of $A$ is based on two closable quadratic forms. The first quadratic form is defined by

$$\mathscr{B}(x_-)=-(Ax_-,x_-)\quad\forall\,x_-\in F_-. \tag{3}$$

As a consequence of Assumption (H2) and of the symmetry of $-\Lambda_-A_{|F_-}$, $\mathscr{B}$ is bounded from below and closable in $\mathscr{H}_-$. Therefore, we can consider the Friedrichs extension $B:\mathrm{Dom}(B)\subset\mathscr{H}_-\to\mathscr{H}_-$ of $-\Lambda_-A_{|F_-}$ and, for any parameter $E>a$, the operator $L_E: F_+\to\mathrm{Dom}(B)\subset\mathscr{F}(B)\subset\mathscr{H}_-$ such that

$$L_Ex_+:=(B+E)^{-1}\Lambda_-Ax_+. \tag{4}$$

On the subspace of $\mathscr{H}$ defined by

$$\Gamma_E:=\{x_++L_Ex_+: x_+\in F_+\}\subset F_+\oplus\mathrm{Dom}(B), \tag{5}$$

we also consider the second quadratic form

$$Q_E(x_+ + L_E\,x_+) := \big(x_+, (A-E)\,x_+\big) + \big(L_E\,x_+, (B+E)\,L_E\,x_+\big)\,. \tag{6}$$

Denoting by $\overline{\Gamma}_E$ the closure of $\Gamma_E$ in $\mathscr{H}$, $Q_E$ is densely defined in the Hilbert space $\overline{\Gamma}_E$. Further details on this quadratic form are given in Section 2. Our main result is as follows.

**Theorem 1.** *Let $A$ be a symmetric operator on the Hilbert space $\mathscr{H}$. Assume* (H1)-(H2)-(H3) *and take $E > a$. With the above notations, the quadratic forms $\mathscr{B}$ and $Q_E$ are bounded from below, $\mathscr{B}$ is closable in $\mathscr{H}_-$, $Q_E$ is closable in $\overline{\Gamma}_E$ and they satisfy*

$$\mathrm{Dom}\big(\overline{Q}_E\big) \cap \mathrm{Dom}\big(\overline{\mathscr{B}}\big) = \{0\}\,.$$

*The operator $A$ admits a unique self-adjoint extension $\widetilde{A}$ such that*

$$\mathrm{Dom}\big(\widetilde{A}\big) \subset \mathrm{Dom}\big(\overline{Q}_E\big) \dot{+} \mathrm{Dom}\big(\overline{\mathscr{B}}\big)\,.$$

*The domain of this extension is*

$$\mathrm{Dom}\big(\widetilde{A}\big) = \mathrm{Dom}(A^*) \cap \Big(\mathrm{Dom}\big(\overline{Q}_E\big) \dot{+} \mathrm{Dom}\big(\overline{\mathscr{B}}\big)\Big)$$

*and it does not depend on $E$.*

*Writing*

$$b := \inf\big(\sigma_{\mathrm{ess}}(\widetilde{A}) \cap (a, +\infty)\big)\,,$$

*one has $\lambda_k \le b$ for all $k \ge 1$, hence $a < b$. In addition, the levels $\lambda_k$ satisfying $a < \lambda_k < b$ are all the eigenvalues – counted with multiplicity – of $\widetilde{A}$ in the spectral gap $(a, b)$.*

Theorem 1 deserves some comments.

• The abstract min-max version of Talman's principle stated in [2] and corrected in [2, Erratum] is similar to the second part of Theorem 1. An earlier work on the subject, [10], and also [13, 25], imply Talman's principle for the Dirac operator only with a bounded potential. Even in [2], the application to Dirac-Coulomb operators is valid only when the subspace of smooth compactly supported wave functions is a core, and this imposes the constraint $\nu \le \sqrt{3}/2$ for point-like atomic nuclei. The rigorous justification of Talman's min-max principle in the domain $\sqrt{3}/2 < \nu \le 1$ was done in the series of later works [14, 15, 6, 19]. In all those works, one assumes that $k_0 = 1$, which amounts to assumption $(\mathrm{H3})_1$. The abstract min-max principle for eigenvalues in the case $k_0 \ge 2$ was first considered in [5], but in that paper (H2) was replaced by a much more restrictive assumption. Allowing $k_0 \ge 2$ can be important in some applications: see Section 6.

• Compared with [9, 19], another novelty is that we do not assume that the operator $-\Lambda_- A_{|F_-}$ is self-adjoint or essentially self-adjoint in $\mathscr{H}_-$. As pointed out in [19], essential self-adjointness of $-\Lambda_- A_{|F_-}$ holds in many important situations. However there are also interesting examples for which it does not hold. An application to Dirac-Coulomb operators in which the essential adjointness of $-\Lambda_- A_{|F_-}$ does not hold true is described in Section 6. Let us give a simpler example.

**Example 1.** *On the domain $F := \big(C^\infty_c(\Omega, \mathbb{R})\big)^2$, consider the operator*

$$A \begin{pmatrix} u \\ v \end{pmatrix} := \begin{pmatrix} -\Delta u \\ \Delta v \end{pmatrix}$$

*taking values in $\mathscr{H} = \left(L^2(\Omega,\mathbb{R})\right)^2$, where $\Omega$ is a bounded open subset of $\mathbb{R}^d$ with smooth boundary. In this case one takes*

$$\Lambda_+ \begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} u \\ 0 \end{pmatrix}, \quad \Lambda_- \begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} 0 \\ v \end{pmatrix}$$

*and (H1) holds. If $\lambda(\Omega) > 0$ is the smallest eigenvalue of the Dirichlet Laplacian on $\Omega$, we can take $a = -\lambda(\Omega)$ in (H2) and we have $\lambda_1 = \lambda(\Omega) > a$, so Theorem 1 can be applied (with $k_0 = 1$). But $-\Lambda_- A_{|\Lambda_- F}$ is the Laplacian defined on the minimal domain $C_c^\infty(\Omega,\mathbb{R})$, and it is well-known that this operator is not essentially self-adjoint in $L^2(\Omega,\mathbb{R})$.*

This paper is organized as follows. In Section 2, we introduce a number of mathematical objects and state some preliminary results which explain the role of $Q_E$ in Theorem (1). For simplicity, we first consider the case $k_0 = 1$. The self-adjoint extension $\widetilde{A}$ of $A$ is constructed in Section 3 and the abstract version of Talman's principle for its eigenvalues is proved in Section 4. The case $k_0 \geq 2$ of Theorem 1 will be dealt with in Section 5. Section 6 is devoted to Dirac-Coulomb operators with charge configurations that are not covered by earlier results.

## 2. Functional set-up and preliminary results

In order to prove Theorem 1 we need to introduce a number of mathematical objects.

In the whole paper, $\mathscr{H}$ is a Hilbert space with scalar product $(\cdot,\cdot)$ and associated norm $\|\cdot\|$. If $T : \mathrm{Dom}(T) \subset \mathscr{H} \to \mathscr{H}$ is a linear operator, we define the corresponding norm by

$$\|x\|_{\mathrm{Dom}(T)} := \sqrt{\|x\|^2 + \|Tx\|^2}, \quad \forall\, x \in \mathrm{Dom}(T).$$

Recall that the fact that the quadratic form $\mathscr{B}$ defined by (3) is bounded from below and closable in $\mathscr{H}_-$ is just a consequence of Assumption (H2) and of the symmetry of $-\Lambda_- A_{|F_-}$. Of course $\mathrm{Dom}(\overline{\mathscr{B}})$ is dense in $\mathscr{H}_-$ since it contains $F_-$. Let $B : \mathrm{Dom}(B) \subset \mathscr{H}_- \to \mathscr{H}_-$ be the corresponding Friedrichs extension of the operator $-\Lambda_- A_{|F_-}$. The form-domain $\mathscr{F}(B)$ of $B$ is precisely $\mathrm{Dom}(\overline{\mathscr{B}})$. The subspace $F_-$ is dense in $\mathscr{F}(B)$ for the norm $\|\cdot\|_{\mathscr{F}(B)}$, *i.e.*, $(B+E)^{1/2} F_-$ is dense in $\mathscr{H}_-$ for any $E > a$, but we cannot say that $(B+E)F_-$ is dense in $\mathscr{H}_-$, since we do not assume that $-\Lambda_- A_{|F_-}$ is essentially self-adjoint.

Given $x_+ \in F_+$ and $E > a$, let $\varphi_{E,x_+} : F_- \to \mathbb{R}$ be defined by

$$\varphi_{E,x_+}(y_-) := \left(x_+ + y_-, (A-E)(x_+ + y_-)\right), \quad \forall\, y_- \in F_-,$$

and recall that $L_E$ is, according to (4), a well-defined operator on $F_+$ taking values in $\mathrm{Dom}(B) \subset \mathscr{F}(B) \subset \mathscr{H}_-$. In the sequel we will systematically take the condition

$$E > a$$

for granted. The heuristics is that $\varphi_{E,x_+}(y_-) = (x, Ax) - E\|x\|^2$ if $x = x_+ + y_-$ with $x_+ \in F_+$ and $y_- \in F_-$, so that, if $y_-$ is a critical point of $(x, Ax)/\|x\|^2$, then $y_- = L_E x_+$. Let us make this idea precise.

**Lemma 2.** *For each $x_+ \in F_+$ and $y_- \in F_-$,*

$$\varphi_{E,x_+}(y_-) = \left(x_+, (A-E)\,x_+\right) + \left(L_E\, x_+, (B+E)\, L_E x_+\right) - \left(y_- - L_E\, x_+, (B+E)\,(y_- - L_E\, x_+)\right).$$

*Proof.* With $z_- := y_- - L_E\, x_+ \in \mathrm{Dom}(B)$, we obtain

$$\begin{aligned}
\varphi_{E,x_+}(y_-) &= \big(x_+, (A-E)\, x_+\big) + 2\,\mathrm{Re}(A\, x_+, y_-) - \big(y_-, (B+E)\, y_-\big) \\
&= \big(x_+, (A-E)\, x_+\big) + 2\,\mathrm{Re}\big(L_E\, x_+, (B+E)\, y_-\big) - \big(y_-, (B+E)\, y_-\big) \\
&= \big(x_+, (A-E)\, x_+\big) + \big(L_E\, x_+, (B+E)\, L_E\, x_+\big) \\
&\qquad\qquad + \mathrm{Re}\big(L_E\, x_+, (B+E)\, z_-\big) - \mathrm{Re}\big(z_-, (B+E)\, y_-\big) \\
&= \big(x_+, (A-E)\, x_+\big) + \big(L_E\, x_+, (B+E)\, L_E\, x_+\big) - \big(z_-, (B+E)\, z_-\big)\,,
\end{aligned}$$

which completes the proof. □

Recall that in (5) we defined the *graph* $\Gamma_E$ of $L_E$ as

$$\Gamma_E := \big\{x_+ + L_E\, x_+ \,:\, x_+ \in F_+\big\} \subset F_+ \oplus \mathrm{Dom}(B)\,,$$

and that $\overline{\Gamma}_E$ denotes its closure in $\mathscr{H}$. As noticed in the proof of [19, Lemma 5],

$$\overline{\Gamma}_E \cap \mathscr{H}_- \subset \big((A-E)(F_-)\big)^\perp\,. \tag{7}$$

The subspace $\Lambda_-(A-E)(F_-)$ of $\mathscr{H}_-$ is not necessarily dense in $\mathscr{H}_-$ since we do not assume that $\Lambda_- A_{|_{F_-}}$ is essentially self-adjoint. For this reason, we cannot infer from (7) that $\overline{\Gamma}_E \cap \mathscr{H}_- = \{0\}$. *In other words, we do not know whether the operator $L_E$ is closable or not. This is why we have to resort to a geometric viewpoint in which the linear subspace $\overline{\Gamma}_E$ replaces the possibly nonexistent closure of $L_E$. Here is the main difference between the present work and* [19].

On $\Gamma_E$ we recall that the quadratic form is defined, according to (6), by

$$Q_E(x_+ + L_E\, x_+) = \big(x_+, (A-E)\, x_+\big) + \big(L_E\, x_+, (B+E)\, L_E\, x_+\big) = \varphi_{E,x_+}(L_E\, x_+)\,.$$

In the earlier works [2] and [19], $Q_E$ is seen as a quadratic form on $F_+$. For our argument, it is essential to define it on $\Gamma_E$: as we shall see, this will allow us to close it in $\overline{\Gamma}_E$.

Now, since $F_-$ is dense in $\mathscr{F}(B)$ for $\|\cdot\|_{\mathscr{F}(B)}$, there is a sequence $\{y_n\}_n$ in $F_-$ such that

$$\lim_{n\to+\infty} \big(y_n - L_E\, x_+, (B+E)\,(y_n - L_E\, x_+)\big) = 0\,.$$

Hence Lemma 2 tells us that

$$Q_E(x_+ + L_E\, x_+) = \sup_{y_-\in F_-} \varphi_{E,x_+}(y_-)\,.$$

Estimates on the variations of $\|x_+ + L_E\, x_+\|$ and $Q_E(x_+ + L_E\, x_+)$ as functions of $E$ are useful. The same statement can be found in [2, Lemma 2.1] and [19, Lemma 7], so we refer to these works for a proof.

**Lemma 3.** *Assume that* (H1)-(H2) *of Theorem 1 are satisfied. Then, for all $a < E < E'$ and for all $x_+ \in F_+$, we have*

$$\|x_+ + L_{E'}\, x_+\| \le \|x_+ + L_E\, x_+\| \le \frac{E'-a}{E-a}\,\|x_+ + L_{E'}\, x_+\| \tag{8}$$

*and*

$$(E'-E)\,\|x_+ + L_{E'}\, x_+\|^2 \le Q_E\big(x_+ + L_E\, x_+\big) - Q_{E'}\big(x_+ + L_{E'}\, x_+\big) \le (E'-E)\,\|x_+ + L_E\, x_+\|^2\,. \tag{9}$$

*Moreover, for any* $E > a$ :

$$\lambda_1 > E \quad \text{if and only if} \quad Q_E(x_+ + L_E\, x_+) > 0\,, \quad \forall\, x_+ \in F_+ \setminus \{0\}\,,$$
$$\lambda_1 \geq E \quad \text{if and only if} \quad Q_E(x_+ + L_E\, x_+) \geq 0\,, \quad \forall\, x_+ \in F_+\,.$$

*As a consequence, we have* $\lambda_1 > a$ *if and only if*

(iii') *For any* $E > a\,, \quad Q_E(x_+ + L_E\, x_+) \geq 0\,, \quad \forall\, x_+ \in F_+\,.$

For the sake of simplicity, up to the end of the current section, as well as in Sections 3 and 4, we impose the condition

$$\lambda_1 > a\,, \tag{10}$$

*i.e.*, we assume that $(\mathrm{H3})_1$, that is, (H3) with $k_0 = 1$, holds. See Section 5 for necessary changes to be done in the case $k_0 \geq 2$. For any $E > a$, let

$$\kappa_E := 1 + \max\{0, (E - \lambda_1)\} \left(\frac{E-a}{\lambda_1 - a}\right)^2 . \tag{11}$$

Then, from the above Lemma, one easily sees that $Q_E + \kappa_E \|\cdot\|^2 \geq \|\cdot\|^2$ on $\Gamma_E$ and we may define a new norm

$$\mathcal{N}_E := \sqrt{Q_E + \kappa_E \|\cdot\|^2}$$

on that space. Obviously, $\mathcal{N}_E \geq \|\cdot\|$ on $\Gamma_E$. Note that formulas (8) and (9) imply that, for $a < E < E'$, $\Gamma_E$ and $\Gamma_{E'}$ are isomorphic for the norm $\|\cdot\|$, as well as for the norms $\mathcal{N}_E$ and $\mathcal{N}'_E$. A detailed statement is as follows.

**Corollary 4.** *Under conditions* (H1), (H2) *and* $(\mathrm{H3})_1$, *for* $E,\, E' \in (a,\infty)$, *the map* $i_{E,E'}$ : $x_+ + L_E\, x_+ \longmapsto x_+ + L_{E'} x_+$ *is an isomorphism between* $\Gamma_E$ *and* $\Gamma_{E'}$ *for the norm* $\|\cdot\|$, *which can be uniquely extended to an isomorphism between* $\overline{\Gamma}_E$ *and* $\overline{\Gamma}_{E'}$. *Moreover there are two positive constants* $c(E,E')$ *and* $C(E,E')$ *such that*

$$c(E,E')\, \mathcal{N}_E(x_+ + L_E\, x_+) \leq \mathcal{N}_{E'}(x_+ + L_{E'} x_+) \leq C(E,E')\, \mathcal{N}_E(x_+ + L_E\, x_+)\,, \quad \forall\, x_+ \in F_+\,, \tag{12}$$

*so* $i_{E,E'}$ *is also an isomorphism for the norms* $\mathcal{N}_E$ *and* $\mathcal{N}'_E$.

Now, for $x \in \Gamma_E$ we may write $Q_E(x) = (x, S_E x)$, where

$$S_E := \Pi_E\big(\Lambda_+(A-E)\,\Lambda_+ + \Lambda_-(B+E)\,\Lambda_-\big)_{|\Gamma_E}$$

and $\Pi_E : \mathcal{H} \to \overline{\Gamma}_E$ is the orthogonal projector on $\overline{\Gamma}_E$. The operator $S_E$ is the analogue in our abstract context of the Schur complement of a block matrix. It is clearly symmetric, and we have seen that $Q_E$ is bounded from below, so $Q_E$ is closable in $\overline{\Gamma}_E$. If $G_E$ denotes the domain of its closure $\overline{Q}_E$, $\overline{P}_E$ the polar form of $\overline{Q}_E$ and $T_E$ the Friedrichs extension of $S_E$ in $\overline{\Gamma}_E$. The space $G_E$, endowed with the norm

$$\overline{\mathcal{N}_E} := \sqrt{\overline{Q}_E + \kappa_E \|\cdot\|^2}\,,$$

is complete. This space depends on $E$, since it is a subspace of $\overline{\Gamma_E}$, but (12) implies that, for every $E,\, E' > a$, the map $i_{E,E'}$ is the restriction to $\Gamma_E$ of a unique isomorphism between the two normed spaces $\big(G_E, \overline{\mathcal{N}}_E\big)$ and $\big(G_{E'}, \overline{\mathcal{N}}_{E'}\big)$. We have

$$\Gamma_E \subset \mathrm{Dom}(T_E) \subset G_E \subset \overline{\Gamma}_E \subset \mathcal{H}\,,$$

$\Gamma_E$ is dense in $\overline{\Gamma}_E$ for $\|\cdot\|$ and $\Gamma_E$ is dense in $G_E$ for the norm $\overline{\mathcal{N}}_E$. But we cannot say that $\Gamma_E$ is dense in $\mathrm{Dom}(T_E)$ for $\|\cdot\|_{\mathrm{Dom}(T_E)}$ since $S_E$ is not always essentially self-adjoint.

While we may have $\overline{\Gamma}_E \cap \mathscr{H}_- \neq \{0\}$, the following property holds.

**Lemma 5.** *Under conditions* (H1), (H2), $(\mathrm{H3})_1$ *and with the above notations,*

$$\overline{\Gamma}_E \cap \mathscr{F}(B) = \{0\}\,.$$

*Proof.* Notice that from (7),

$$\begin{aligned}\overline{\Gamma}_E \cap \mathscr{F}(B) &= \left(\overline{\Gamma}_E \cap \mathscr{H}_-\right) \cap \mathrm{Dom}\,\left((B+E)^{1/2}\right)\\ &\subset \left((B+E)(F_-)\right)^{\perp} \cap \mathrm{Dom}\left((B+E)^{1/2}\right) = (B+E)^{-1/2}\left(\left((B+E)^{1/2}F_-\right)^{\perp}\right) = \{0\}\,,\end{aligned}$$

since $(B+E)^{1/2}F_-$ is dense in $\mathscr{H}_-$ and $(B+E)^{1/2}$ is into. □

Summarizing the observations of Section 2, we learn that

**Proposition 6.** *Let $A$ be a symmetric operator on the Hilbert space $\mathscr{H}$. Assume* (H1)-(H2)-(H3) *and take $E > a$. With the above notations, if* (10) *holds, then the quadratic forms $\mathscr{B}$ and $\mathrm{Q}_E$ are bounded from below, $\mathscr{B}$ is closable in $\mathscr{H}_-$, $\mathrm{Q}_E$ is closable in $\overline{\Gamma}_E$ and their closures satisfy* $\mathrm{Dom}\big(\overline{\mathrm{Q}}_E\big) \cap \mathrm{Dom}\big(\overline{\mathscr{B}}\big) = \{0\}$.

## 3. The existence of a distinguished self-adjoint extension

In this section, we continue with the proof of Theorem 1 in the case $k_0 = 1$ by proving the following proposition.

**Proposition 7.** *Under the assumptions of Theorem 1, if* (10) *holds, then the operator $A$ admits a unique self-adjoint extension $\widetilde{A}$ such that* $\mathrm{Dom}\big(\widetilde{A}\big) \subset \mathrm{Dom}\big(\overline{\mathrm{Q}}_E\big) \dot{+} \mathrm{Dom}\big(\overline{\mathscr{B}}\big)$. *Its domain is* $\mathrm{Dom}\big(\widetilde{A}\big) = \mathrm{Dom}(A^*) \cap \big(\mathrm{Dom}\big(\overline{\mathrm{Q}}_E\big) \dot{+} \mathrm{Dom}\big(\overline{\mathscr{B}}\big)\big)$ *and this subspace does not depend on $E$.*

### 3.1. Self-adjoint extension.

We define an extension of $A$ as follows. For any $E > a$, on the subspace

$$\mathrm{Dom}\big(\widetilde{A}\big) := \big(G_E \dot{+} \mathscr{F}(B)\big) \cap \mathrm{Dom}\big(A^*\big)\,, \tag{13}$$

let us define

$$\widetilde{A}\,x := A^*\,x\,, \quad \forall\, x \in \mathrm{Dom}\,\big(\widetilde{A}\big)\,. \tag{14}$$

This defines a self-adjoint extension of $A$ because

$$F \subset \big(\Gamma_E \dot{+} \mathrm{Dom}\,(B)\big) \cap \mathrm{Dom}\big(A^*\big) \subset D\big(\widetilde{A}\big) \quad \text{and } A^*_{|F} = A\,.$$

We have to prove that $\widetilde{A}$ does not depend on $E$, that is, the subspace $\mathrm{Dom}\big(\widetilde{A}\big)$ is independent of $E$. Note that $G_E \dot{+} \mathscr{F}(B)$ is an algebraic direct sum, but the corresponding projectors are not necessarily continuous. We now prove

**Lemma 8.** *Assume that the conditions* (H1), (H2) *and* $(\mathrm{H3})_1$ *hold. Let $x,\, u \in G_E$ and $z_-$, $v_- \in \mathscr{F}(B)$ be such that $X = x + z_- \in Dom\,(A^*)$. Then, with $U = u + v_-$, we have*

$$\big((A^*-E)X, U\big) = \overline{P}_E(x,u) - \big((B+E)^{1/2} z_-, (B+E)^{1/2} v_-\big) \tag{15}$$

*for any $E > a$. As a consequence, $\widetilde{A}$ is symmetric.*

*Proof.* If $x$, $u$ are in $F$, formula (15) is already proved (see Lemma 2). If $X = x + z_-$ and $U = u + v_-$ satisfy the assumptions of the lemma, by density of $\Gamma_E$ in $G_E$, and by density of $F_-$ in $\mathscr{F}(B)$, there are sequences $\{X_n\}_n, \{U_n\}_n$ in $F$ such that, with

$$x_n := \Lambda_+ X_n + L_E \Lambda_+ X_n\,, \qquad z_n := \Lambda_- X_n - L_E \Lambda_+ X_n\,,$$
$$u_n := \Lambda_+ U_n + L_E \Lambda_+ U_n\,, \qquad v_n := \Lambda_- U_n - L_E \Lambda_+ U_n\,,$$

we have

$$\lim_{n\to+\infty} \overline{Q}_E(x - x_n) = \lim_{n\to+\infty} \overline{Q}_E(u - u_n) = 0\,,$$
$$\lim_{n\to+\infty} \big((B+E)^{1/2}(z_- - z_n), (B+E)^{1/2}(z_- - z_n)\big) = 0\,,$$
$$\lim_{n\to+\infty} \big((B+E)^{1/2}(v_- - v_n), (B+E)^{1/2}(v_- - v_n)\big) = 0\,.$$

As a consequence,

$$\lim_{n\to+\infty} \|X - X_n\| = \lim_{n\to+\infty} \|U - U_n\| = 0\,.$$

For $m$, $n \in \mathbb{N}$, $(X_n, U_n)$ satisfy the identity (15). Since $\big((A^* - E)X_m, U_n\big) = \big(X_m, (A - E)\,U_n\big)$ and $\big(X, (A - E)\,U_n\big) = \big((A^* - E)X, U_n\big)$, passing to the limit as $m \to +\infty$ for each $n$, we see that $(X, U_n)$ satisfies (15). Then, passing to the limit as $n \to +\infty$, we find that $(X, U)$ satisfies (15). □

Let us now prove that the domain of $\widetilde{A}$ does not depend on $E$. This immediately follows from formula (13) and from the next lemma:

**Lemma 9.** *Assume that the conditions (H1), (H2) and $(\text{H3})_1$ hold. Let $E$, $E' > a$, $E' \neq E$. Then*

$$G_E \dotplus \mathscr{F}(B) \subset G_{E'} \dotplus \mathscr{F}(B)\,. \tag{16}$$

*Proof.* If $x + z_- \in G_E \dotplus \mathscr{F}(B)$, there exists a sequence $y_n \in F_+$ such that

$$y_n \to \Lambda_+ x\,, \quad L_E y_n \to \Lambda_- x\,, \quad y_n + L_E y_n \to x\,.$$

Then, $y := \lim_{n\to+\infty}(y_n + L_{E'} y_n) \in \overline{\Gamma}_{E'}$ and

$$(L_E - L_{E'})\,y_n + z_- = (E' - E)\,(B+E)^{-1} L_{E'}\,y_n + z_- \in \mathrm{Dom}(B+E) + \mathscr{F}(B) \subset \mathscr{F}(B)\,.$$

We need only to prove that $y \in G_{E'}$. This is a consequence of Lemma 3. □

What remains to be done is to show that for any $E > a$, $\widetilde{A} - E$ is a bijection. In fact we are able to prove this for any $E$ in the variational gap $(a, \lambda_1)$.

Let $f \in \mathscr{H}$. We look for $X = x + z_-$ in $\mathrm{Dom}(A^*)$ with $x \in G_E = \mathscr{F}(T_E)$ and $z_- \in \mathscr{F}(B)$, such that $(A^* - E)X = f$. Thanks to Lemma 8, we can reformulate this problem as follows:

*Find $(x, z_-) \in G_E \dotplus \mathscr{F}(B)$ such that*

$$\begin{cases} \overline{P}_E(x, u) = (f, u)\,, & \forall\, u \in G_E\,, \\ \big((B+E)^{1/2} z_-, (B+E)^{1/2} v_-\big) = -(f, v_-)\,, & \forall\, v_- \in \mathscr{F}(B)\,. \end{cases} \tag{$\mathscr{P}_f$}$$

Indeed, Lemma 8 guarantees that any solution of $(A^*-E)X=f$ lying in $D\big(\widetilde{A}\big)$ must satisfy ($\mathscr{P}_f$). Conversely, if $(x,z_-)\in G_E\times\mathscr{F}(B)$ satisfies ($\mathscr{P}_f$), then, by Lemma 8, for any $U\in F$,

$$(X,(A-E)\,U)=\big(X,(A^*-E)U\big)=\overline{P}_E\,(x,\Lambda_+U+L_E\Lambda_+U)\\ -\big((B+E)^{1/2}z_-,(B+E)^{1/2}(\Lambda_-U-L_E\Lambda_+U)\big)=(f,U)\,,$$

so that $X\in\mathrm{Dom}(A^*)$ and $(A^*-E)X=f$.

Finally, since we assumed that $E\in(a,\lambda_1)$, $\overline{P}_E$ is a scalar product endowing $G_E$ with a Hilbert space structure, so the Riesz isomorphism theorem tells us that the first equation in ($\mathscr{P}_f$) has a unique solution $u\in G_E$. Similarly, since $E>a$, the second equation has a unique solution $z_-\in\mathscr{F}(B)$. This proves that $\widetilde{A}$ is a self-adjoint operator.

**Remark 10.** *Recalling that $\Pi_E$ (resp. $\Lambda_-$) is the orthogonal projector on $\overline{\Gamma}_E$ (resp. $\mathscr{H}_-$), the solution of the system of weak equations ($\mathscr{P}_f$) can be expressed in terms of these projectors and of the Friedrichs extensions $T_E$ and $B$:*

$$\begin{cases} x=T_E^{-1}\circ\Pi_E(f)\,,\\ z_-=-(B+E)^{-1}\circ\Lambda_-(f)\,. \end{cases}$$

*This shows that $x$ is in $Dom(T_E)$ and that $z_-$ belongs to $Dom(B)$. As a consequence, the domain of $\widetilde{A}$ may also be written as*

$$Dom\big(\widetilde{A}\big)=\big(Dom(T_E)\dotplus Dom(B)\big)\cap Dom\big(A^*\big)\,. \tag{17}$$

The extension $\widetilde{A}$ is thus built. Its uniqueness among those whose domain is contained in $G_E\dotplus\mathscr{F}(B)$ is almost trivial. Indeed, for any other self-adjoint extension $\hat{A}$, we must have $\mathrm{Dom}(\hat{A})\subset\mathrm{Dom}(A^*)$, hence, if $\mathrm{Dom}(\hat{A})\subset G_E\dotplus\mathscr{F}(B)$, then $\mathrm{Dom}(\hat{A})\subset\mathrm{Dom}\big(\widetilde{A}\big)$, which automatically implies $\hat{A}=\widetilde{A}$ since both operators are self-adjoint. This completes the proof of Proposition 7.

**Remark 11.** *In* [19], *it is proved that the extension $\widetilde{A}$ is unique among the self-adjoint extensions whose domain is included in $\Lambda_+G_E\oplus\mathscr{H}_-$, assuming that the operator $-\Lambda_-A_{|_{F_-}}$ is essentially self-adjoint. Coming back to Example 1, let us show that without this assumption, such a uniqueness result does not hold in general.*

*With the notations and assumptions of this example, one easily checks that $\mathscr{F}(B)=\{0\}\times H^1_0(\Omega)$, $G_E=H^1_0(\Omega,\mathbb{R})\times\{0\}$, and, if $\Delta^{(D)}$ denotes the Dirichlet Laplacian with domain $H^2\cap H^1_0(\Omega,\mathbb{R})$, one has*

$$\widetilde{A}=\begin{pmatrix}-\Delta^{(D)} & 0\\ 0 & \Delta^{(D)}\end{pmatrix}.$$

*But since $\Delta:C^\infty_c(\Omega,\mathbb{R})\to L^2(\Omega,\mathbb{R})$ is not essentially self-adjoint, there are infinitely many other self-adjoint extensions of $A$ with domain included in $\Lambda_+G_E\oplus\mathscr{H}_-$. An example is*

$$\widetilde{A}=\begin{pmatrix}-\Delta^{(D)} & 0\\ 0 & \Delta^{(N)}\end{pmatrix}$$

*with $\Delta^{(N)}$ the self-adjoint extension of $\Delta$ associated with the Neumann boundary condition $\nabla v\cdot n=0$.*

3.2. **Variational interpretation.** As a side remark, we give an interpretation of the self-adjoint extension $\widetilde{A}$ that generalizes the Rayleigh- Ritz principle for semibounded operators mentioned in the introduction. Assuming that $E \in (a, \lambda_1)$ and given $f \in \mathcal{H}$, let us consider the inf-sup level

$$\inf_{x_+ \in F_+} \sup_{y_- \in F_-} \left\{ \frac{1}{2} \Big( x_+ + y_-, (A - E)(x_+ + y_-) \Big) - (f, x_+ + y_-) \right\}.$$

Of course, in general, this inf-sup is not attained in $F_+ \oplus F_-$, but enlarging this space one can transform it into a min-max:

$$\begin{aligned} &\inf_{x_+ \in F_+} \sup_{z_- \in D(B)} \left\{ \frac{1}{2} \Big( (x_+, (A-E)\, x_+) + (L_E\, x_+, (B+E)\, L_E\, x_+) \Big) \right. \\ &\qquad\qquad\qquad \left. - (f, x_+ + L_E\, x_+) - \frac{1}{2} (z_-, (B+E)\, z_-) - (f, z_-) \right\} \\ &= \inf_{x_+ \in F_+} \left\{ \frac{1}{2} \Big( (x_+, (A-E)\, x_+) + (L_E\, x_+, (B+E)\, L_E\, x_+) \Big) - (f, x_+ + L_E\, x_+) \right\} \\ &\qquad\qquad\qquad - \inf_{z_- \in \mathrm{Dom}(B)} \left\{ \frac{1}{2} (z_-, (B+E)\, z_-) + (f, z_-) \right\} \\ &= \min_{x \in G_E} \left\{ \frac{1}{2} \overline{Q}_E(x) - (f, x) \right\} - \min_{z_- \in \mathcal{F}(B)} \left\{ \frac{1}{2} \Big( (B+E)^{1/2} z_-, (B+E)^{1/2} z_- \Big) + (f, z_-) \right\}. \end{aligned}$$

Each of these last two convex minimization problems has a unique solution, and the system of Euler-Lagrange equations solved by the two minimizers is just ($\mathscr{P}_f$), so their sum is $X = \big(\widetilde{A} - E\big)^{-1} f$.

## 4. The min-max principle

In this section, we establish the min-max principle for the eigenvalues of $\widetilde{A}$ in the case $k_0 = 1$. Even if our assumptions are weaker and our formalism slightly different, the arguments of this section are essentially the same as in [2, § 2], up to some missing details, and the more complete proof of [19, § 2.6].

**Proposition 12.** *Under assumptions of Theorem 1, if (10) holds, then for $k \geq k_0$ the numbers $\lambda_k$ lie in the interval $(a, b]$ and those $\lambda_k$ satisfying $\lambda_k < b$ are all the eigenvalues of $\widetilde{A}$ in the spectral gap $(a, b)$, counted with multiplicity.*

If assumptions (H1) and (H2) hold, to each $E > a$ we may associate the sequence of the min-max levels

$$\ell_k(E) := \inf_{\substack{V \text{ subspace of } \Gamma_E \\ \dim V = k}} \sup_{x \in V \setminus \{0\}} \frac{Q_E(x)}{\|x\|^2}. \tag{18}$$

We may also define the (possibly infinite) multiplicity numbers

$$m_k(E) := \mathrm{card}\Big\{ k' \geq 1 : \ell_{k'}(E) = \ell_k(E) \Big\} \geq 1. \tag{19}$$

The next lemma gives a direct relation between the min-max levels $\ell_k(E)$ of $Q_E$ and the min-max levels $\lambda_k$ of $A$ defined by (2). This result and its proof can be found in [2, Lemma 2.2] and in [19, Lemma 11]. The assumptions in these papers are stronger, but the proof in our case is very similar and rather straightforward, and actually an easy direct consequence of Lemma 3, so we omit it.

**Lemma 13.** *Under assumptions* (H1) *and* (H2)*, for any* $k \geq 1$ *and any* $\lambda > a$ *such that* $\lambda \neq \lambda_k$*, the signs of* $\lambda_k - \lambda$ *and* $\ell_k(\lambda)$ *are the same. If, in addition,* $\lambda_k > a$*, then* $\lambda_k$ *is the unique solution in* $(a, +\infty)$ *of the nonlinear equation*

$$\ell_k(\lambda) = 0\,. \tag{20}$$

*In other words,* 0 *is the* $k^{th}$ *min-max level for the Rayleigh-Ritz quotients of* $Q_{\lambda_k}$*, and this determines* $\lambda_k$ *in a unique way. As a consequence,* $m_k(\cdot)$ *defined by* (19) *is such that*

$$m_k(\lambda_k) = \operatorname{card}\Big\{k' \geq 1 \,:\, \lambda_{k'} = \lambda_k\Big\}\,.$$

Now, under assumptions (H1), (H2) and $(\mathrm{H3})_1$ one should recall that $\Gamma_E$ is dense in $G_E$ for the norm $\overline{\mathcal{N}_E}$, so that (18) is equivalent to

$$\ell_k(E) = \inf_{\substack{V \text{ subspace of } G_E \\ \dim V = k}} \ \sup_{x \in V \setminus \{0\}} \frac{\overline{Q}_E(x)}{\|x\|^2}\,, \quad \forall\, k \geq 1 \tag{21}$$

Then, by the classical Rayleigh-Ritz principle, we have $\ell_k(E) \leq \inf \sigma_{\rm ess}(T_E)$ and, in the case $\ell_k(E) < \inf \sigma_{\rm ess}(T_E)$, $\ell_k(E)$ is an eigenvalue of $T_E$ with multiplicity $m_k(E)$.

Since we have a relation between the spectrum of $T_E$ and the min-max levels $\ell_k(E)$, what remains to be done in order to end the proof of Theorem 1 is to find a relation between the spectra of $T_E$ and $\widetilde{A}$. In order to do so, we need some informations on the continuity of the decomposition of $X \in \operatorname{Dom}\big(\widetilde{A}\big)$ as a sum $X = x + z_-$, $x \in \operatorname{Dom}(T_E)$, $z_- \in \operatorname{Dom}(B)$. We already mentioned that this decomposition is not necessarily continuous for the $\|\cdot\|$ norm, but we have the following result.

**Lemma 14.** *Under assumptions* (H1), (H2) *and* $(\mathrm{H3})_1$*, for any* $E > a$*, the two projections*

$$\pi_E : X \in \operatorname{Dom}\big(\widetilde{A}\big) \mapsto x \in \operatorname{Dom}(T_E) \quad \textit{and} \quad \pi'_E : X \in \operatorname{Dom}\big(\widetilde{A}\big) \mapsto z_- \in \operatorname{Dom}(B)\,,$$

*uniquely defined by the condition* $X = x + z_-$*, are continuous for the norms* $\|X\|_{\operatorname{Dom}(\widetilde{A})}$*,* $\|x\|_{\operatorname{Dom}(T_E)}$ *and* $\|z_-\|_{\operatorname{Dom}(B)}$*. More precisely, there is a positive constant* $C_E$ *such that*

$$\|\pi'_E(X)\|_{\operatorname{Dom}(B)} \leq C_E\, \|\Lambda_-(\widetilde{A} - E)X\| \quad \textit{and} \quad \|\pi_E(X)\|_{\operatorname{Dom}(T_E)} \leq C_E\, \|X\|_{\operatorname{Dom}(\widetilde{A})}\,.$$

*Moreover the constant* $C_E$ *remains uniformly bounded when* $E$ *stays away from* $a$ *and* $\infty$.

*Proof.* In the arguments below the constant $C_E$ changes value from line to line but we keep the same notation for sake of simplicity. We use the weak formulation $(\mathscr{P}_f)$ of the equation $(\widetilde{A} - E)X = f$ introduced in Section 3. In that section, $f$ was given, $X$ was unknown and it was assumed that $E \in (a, \lambda_1)$ in order to make sure that $(\mathscr{P}_f)$ has a unique solution $X$. But we use $(\mathscr{P}_f)$ differently here. We take $E > a$, $X \in \operatorname{Dom}\big(\widetilde{A}\big)$ and we define $x := \pi_E(X)$, $z_- := \pi'_E(X)$, $f := (\widetilde{A} - E)X$. Then $(\mathscr{P}_f)$ must hold. Looking at the second equation of this system, we infer an estimate of the form $\|z_-\|_{\operatorname{Dom}(B)} \leq C_E\, \|\Lambda_- f\|$, hence the continuity of $\pi'_E$. Since $\|\cdot\|_{\operatorname{Dom}(B)} \geq \|\cdot\|$ and $x = X - z_-$, the estimate on $z_-$ implies in turn the estimate $\|x\| \leq C_E\, \|X\|_{\operatorname{Dom}(\widetilde{A})}$. Combining this information with the first equation in $(\mathscr{P}_f)$ we finally get the estimate $\|x\|_{\operatorname{Dom}(T_E)} \leq C_E\, \|X\|_{\operatorname{Dom}(\widetilde{A})}$, so $\pi_E$ is also continuous. □

**Remark 15.** *In the sequel, we do not use all the informations contained in Lemma 14: we only need the weaker estimates* $\|\pi'_E(X)\| \le C_E\,\|\Lambda_-(\widetilde{A}-E)X\|$ *and* $\|\pi_E(X)\| \le C_E\,\|X\|_{\mathrm{Dom}(\widetilde{A})}$.

We are now ready to prove the following result:

**Proposition 16.** *Under assumptions* (H1), (H2) *and* $(\mathrm{H3})_1$, *let* $E > a$ *and* $m \in \mathbb{N}^*$ *be such that for any* $\delta > 0$, $\mathrm{Rank}\big(\mathbb{1}_{(-\delta,\delta)}(T_E)\big) \ge m$. *Then for any* $\varepsilon > 0$, $\mathrm{Rank}\big(\mathbb{1}_{(E-\varepsilon,E+\varepsilon)}\big(\widetilde{A}\big)\big) \ge m$.

*Proof.* For $\delta > 0$ let $\mathscr{X}_\delta$ be a subspace of $\mathrm{R}\big(\mathbb{1}_{(-\delta,\delta)}(T_E)\big)$ of dimension $m$. Then we have $\mathscr{X}_\delta \subset \mathrm{Dom}(T_E) \subset G_E$. Using Lemmas 8 and 14 we find that for all $x \in \mathscr{X}_\delta$ and $y \in \mathrm{Dom}\big(\widetilde{A}\big)$,

$$|(x,(\widetilde{A}-E)y)| = |\overline{P_E}(x,\pi_E(y))| = |(T_E x,\pi_E(y))| \le \delta\,\|x\|\,\|\pi_E(y)\| \le C_E\,\delta\,\|x\|\,\|y\|_{\mathrm{Dom}(\widetilde{A})}.$$

Assume by contradiction that for some $\varepsilon_0 > 0$, $\mathrm{Rank}\big(\mathbb{1}_{(E-\varepsilon_0,E+\varepsilon_0)}\big(\widetilde{A}\big)\big) \le m-1$. Then for each $\delta > 0$ there is $x_\delta$ in $\mathscr{X}_\delta$ such that $\|x_\delta\| = 1$ and $\mathbb{1}_{(E-\varepsilon_0,E+\varepsilon_0)}\big(\widetilde{A}\big)x_\delta = 0$. So there is $y_\delta \in \mathrm{Dom}\big(\widetilde{A}\big)$ such that $(\widetilde{A}-E)y_\delta = x_\delta$ and $\|y_\delta\| \le \varepsilon_0^{-1}$. We thus get $\big(x_\delta,\big(\widetilde{A}-E\big)y_\delta\big) = \|x_\delta\|^2 = 1$ and $C_E\|x_\delta\|\|y_\delta\|_{\mathrm{Dom}(\widetilde{A})}$ is bounded independently of $\delta$. So, taking $\delta$ small enough we obtain $\big|\big(x_\delta,\big(\widetilde{A}-E\big)y_\delta\big)\big| > C_E\,\delta\,\|x_\delta\|\,\|y_\delta\|_{\mathrm{Dom}(\widetilde{A})}$ and this is absurd. We have thus proved the Proposition by contradiction. □

The converse of Proposition 16 is also true:

**Proposition 17.** *Under assumptions* (H1), (H2) *and* $(\mathrm{H3})_1$, *let* $E > a$ *and* $m \in \mathbb{N}^*$ *be such that for any* $\varepsilon > 0$, $\mathrm{Rank}\big(\mathbb{1}_{(E-\varepsilon,E+\varepsilon)}\big(\widetilde{A}\big)\big) \ge m$. *Then for all* $\delta > 0$, $\mathrm{Rank}\big(\mathbb{1}_{(-\delta,\delta)}(T_E)\big) \ge m$.

*Proof.* For $\varepsilon > 0$, let $\mathscr{Y}_\varepsilon$ be a subspace of $\mathrm{R}(\mathbb{1}_{(E-\varepsilon,E+\varepsilon)}\big(\widetilde{A}\big))$ of dimension $m$. Then we have $\mathscr{Y}_\varepsilon \subset \mathrm{Dom}\big(\widetilde{A}\big) \subset \mathrm{Dom}(T_E)\dot{+}\mathrm{Dom}(B)$. Using Lemma 8 we find that for all $x \in \mathrm{Dom}(T_E)$ and $Y \in \mathscr{Y}_\varepsilon$,

$$\big|\big(T_E x,\pi_E(Y)\big)\big| = \big|\overline{P_E}\big(x,\pi_E(Y)\big)\big| = \big|\big(x,\big(\widetilde{A}-E\big)Y\big)\big| \le \varepsilon\,\|x\|\,\|Y\|.$$

Moreover for any $Y \in \mathscr{Y}_\varepsilon$, from Lemma 14 one has

$$\big\|\pi'_E(Y)\big\| \le C_E\,\big\|\Lambda_-\big(\widetilde{A}-E\big)Y\big\| \le C_E\,\varepsilon\,\|y\|.$$

So, imposing $\varepsilon \le \frac{1}{2C_E}$ and using the triangular inequality, we get the estimate $\|Y\| \le 2\,\|\pi_E(Y)\|$ for any $Y \in \mathscr{Y}_\varepsilon$. As a consequence, the subspace $V_\varepsilon := \pi_E(\mathscr{Y}_\varepsilon) \subset \mathrm{Dom}(T_E)$ is $m$-dimensional and for all $x \in \mathrm{Dom}(T_E)$ and $y \in V_\varepsilon$, one has

$$|(T_E x, y)| \le 2\,\varepsilon\,\|x\|\,\|y\|.$$

To end the proof of the Proposition, let us assume by contradiction that there exists $\delta_0 > 0$ such that $\mathrm{Rank}\big(\mathbb{1}_{(-\delta_0,\delta_0)}(T_E)\big) \le m-1$. Then for each small $\varepsilon$ there is $y_\varepsilon$ in $V_\varepsilon$ such that $\|y_\varepsilon\| = 1$ and $\mathbb{1}_{(-\delta_0,\delta_0)}(T_E)y_\varepsilon = 0$. So there is $x_\varepsilon \in \mathrm{Dom}(T_E)$ such that $T_E x_\varepsilon = y_\varepsilon$ and $\|x_\varepsilon\| \le \delta_0^{-1}$. We thus get $(T_E x_\varepsilon, y_\varepsilon) = \|y_\varepsilon\|^2 = 1$ and $\|x_\varepsilon\|\,\|y_\varepsilon\| \le \delta_0^{-1}$. So, taking $\varepsilon$ small enough we get $|(x_\varepsilon,(\widetilde{A}-E)y_\varepsilon)| > 2\,\varepsilon\,\|x_\varepsilon\|\,\|y_\varepsilon\|$ and this is absurd. We have thus proved the Proposition by contradiction. □

Combining Lemma 13 with Propositions 16 and 17 completes the proof of Proposition 12.
□

## 5. End of the proof of the main result

With Propositions 6, 7 and 12, the proof of Theorem 1 is complete if $k_0 = 1$ in assumption (H3). In the more general case $k_0 \geq 1$, one can define the Friedrichs extension $B$ exactly as before, as well as the operator $L_E$, its graph $\Gamma_E$ and the quadratic form $Q_E(x) = (x, S_E x)$ with $S_E = \Pi_E\left(\Lambda_+(A-E)\Lambda_+ + \Lambda_-(B+E)\,\Lambda_-\right)_{|\Gamma_E}$, $\Pi_E : \mathscr{H} \to \overline{\Gamma}_E$ being the orthogonal projector on $\overline{\Gamma}_E$.

Lemma 2 still holds, as well as the inequalities (8) and (9) of Lemma 3. But of course, when $k_0 \geq 2$ there is no value of $E > a$ such that $Q_E \geq 0$. However we have the following result:

**Lemma 18.** *Under assumptions* (H1), (H2) *and* (H3), *for any $E > a$, there is $\kappa_E > 0$ such that $Q_E + \kappa_E \|\cdot\|^2 \geq \|\cdot\|^2$ on $\Gamma_E$.*

*Proof.* Note that formula (11) for $\kappa_E$ given for $k_0 = 1$, does not work for $\lambda_1 = a$. We thus need a new argument when $k_0 \geq 2$. Fortunately, as in the case $k_0 = 1$, we just have to find a constant $\kappa_E$ for *any* $E > a$: then the inequalities (8) and (9) will immediately imply its existence for *any* $E > a$. We take $E \in (a, \lambda_{k_0})$. Since $\lambda_{k_0-1} = a < E$, by Lemma 13 we have $\ell_{k_0-1}(E) \in [-\infty, 0)$. So there is a $(k_0-1)$-dimensional subspace $W$ of $\Gamma_E$ such that

$$\ell' := \sup_{w \in W\setminus\{0\}} \frac{Q_E(w)}{\|w\|^2} \in (-\infty, 0)\,.$$

Let $C := \sup\left\{\|S_E w\| \,:\, w \in W,\, \|w\| \leq 1\right\}$. This constant is finite, since $W$ is finite-dimensional. We now consider an arbitrary vector $x$ in $\Gamma_E$ and we look for a lower bound on $Q_E(x)$. We distinguish two cases.

• *First case:* $x \in W$. Then $Q_E(x) = (x, S_E x) \geq -C\|x\|^2$.

• *Second case:* $x \notin W$. Then the vector space $\mathrm{span}\{x\} \oplus W$ has dimension $k_0$. Since we have $\lambda_{k_0} > E > a$, by Lemma 13 we obtain $\ell_{k_0}(E) > 0$, so there is a vector $w_0 \in W$ such that $Q_E(x + w_0) \geq 0$. Then we have

$$Q_E(x) = Q_E(x+w_0) - 2\,\mathrm{Re}(x, S_E w_0) - Q_E(w_0) \geq -2\,C\,\|x\|\,\|w_0\| + |\ell'|\,\|w_0\|^2 \geq -\frac{C^2}{|\ell'|}\,\|x\|^2\,.$$

So in all cases, if we choose $\kappa_E = 1 + \max\left\{C, C^2/|\ell'|\right\}$, we get $Q_E(x) + \kappa_E\,\|x\|^2 \geq \|x\|^2$. This ends the proof of the lemma. □

Now, using Lemma 18, we can construct $\mathscr{N}_E$, $G_E$, $\overline{Q}_E$, $\overline{\mathscr{N}}_E$ and $\widetilde{A}$ exactly as in the case $k_0 = 1$. Then Corollary 4 and Lemmas 5, 8, 9 remain true under the more general hypothesis $(\mathrm{H3})_{k_0}$ instead of $(\mathrm{H3})_1$, and their proofs are unchanged.

When $E \in (a, \lambda_{k_0})$, the problem $(\mathscr{P}_f)$ defined in Section 3.1 has a unique solution $(u, z_-) \in G_E \times \mathscr{F}(B)$, as in the case $k_0 = 1$. For the existence and uniqueness of $z_-$ satisfying the second equation in $(\mathscr{P}_f)$, the argument is exactly the same: one appeals to the Riesz isomorphism theorem. But when $k_0 \geq 2$, $\overline{Q}_E$ is no longer positive definite, so we cannot use the Riesz isomorphism theorem for the existence and uniqueness of $u$. Instead, we recall that from Lemma 13, $\ell_{k_0-1}(E) < 0$ and $\ell_{k_0}(E) > 0$. By the Rayleigh-Ritz principle, $\sigma(T_E) \cap \left(\ell_{k_0-1}(E), \ell_{k_0}(E)\right)$ is empty, so $T_E$ is an isomorphism between $\mathrm{Dom}(T_E)$

and $\overline{\Gamma}_E$ that extends to an isomorphism between $G_E$ and its topological dual. This implies the existence and uniqueness of $u$ satisfying the first equation in ($\mathscr{P}_f$). The other arguments in Section 3.1 are unchanged. Note, however, that the variational interpretation of ($\mathscr{P}_f$) given in Section 3.2 is no longer valid when $k_0 \geq 2$, but it was just a side remark that plays no role in the proof of Theorem 1. So the first part of this theorem is proved for any value of $k_0$.

In Section 4, all statements remain true if one replaces assumption $(H3)_1$ by the more general assumption $(H3)_{k_0}$ with $k_0 \geq 1$, and their proof is unchanged. The only difference is that the condition $\lambda_k > a$ appearing in Lemma 13 is only true for $k \geq k_0$ instead of $k \geq 1$. This completes the proof of Theorem 1 when $k_0 \geq 2$.

## 6. Applications to Dirac-Coulomb operators

Let us consider the *Dirac-Coulomb operator* in dimension 3 given by

$$A = -i\,\alpha\nabla + \beta + V$$

and start by the case of a point-like nucleus corresponding to the potential $V(x) = -\nu/|x|$. Using Talman's splitting $\Lambda_+(\psi) = (\phi, 0)$, $\Lambda_-(\psi) = (0, \chi)$ of four-spinors $\psi = (\phi, \chi)$ into upper and lower two-spinors, thanks to Theorem 1 with $k_0 = 1$ we can define a distinguished self-adjoint extension of $A$ with minimal domain $C_c^\infty(\mathbb{R}^3 \setminus \{0\}, \mathbb{C}^4)$ for any $0 \leq \nu \leq 1$ and we can also characterize all the eigenvalues of this extension in the spectral gap $(-1, 1)$ by the min-max principle (2). This is not a new result: see [2, 8, 6, 19], where it was also noted that $V$ can be replaced by more general attractive potentials which are bounded from below by $-1/|x|$ near the origin.

A more delicate situation arises when

$$V(x) = -\frac{\nu_1}{|x|} + \frac{\nu_2}{|x - x_0|} \quad \text{with} \quad x_0 \neq 0, \quad 0 < \nu_1 \leq 1 \quad \text{with} \quad \frac{3}{4} < \nu_2 \leq \frac{2}{\frac{\pi}{2} + \frac{2}{\pi}}.$$

In such a case, Talman's decomposition in upper and lower spinors cannot be used: assumption (H2) does not hold. Instead, as projectors we choose

$$\Lambda_\pm = \mathbb{1}_{\mathbb{R}_\pm}(-i\,\alpha\nabla + \beta),$$

and as domain $F$ we take the Schwartz class $\mathscr{S}(\mathbb{R}^3, \mathbb{C}^4)$, so that (H1) is satisfied. By the upper bound on $\nu_2$, it follows from an inequality of Tix [24] that the Brown-Ravenhall operator $-\Lambda_-\big(A + 1 - \nu_2\big)_{|\Lambda_- F}$ is non-negative so that (H2) holds with $a = -1 + \nu_2$. On the other hand, since $\nu_1 \leq 1$, [2, inequality (36)] implies that $\lambda_1 \geq 0$, so $(H3)_1$ holds as well and thus, Theorem 1 can be applied with $k_0 = 1$. But as shown in [23, Corollary 3], $-\Lambda_- A_{|\Lambda_- F}$ is not essentially self-adjoint, since $\nu_2 > 3/4$, so one cannot use the abstract result of [19].

Interesting cases of application of Theorem 1 with $k_0 \geq 2$ are Dirac operators perturbed by an attractive electrostatic potential $V(x) = -\sum_i \frac{\nu_i}{|x - x_i|}$ generated by several nuclei, each having at most $Z_i$ protons with $Z_i \leq Z_* \approx 137.04$ so that $\nu_i = Z_i/Z_* < 1$. If the total number of protons $\sum_i Z_i$ is larger than 137, a finite number $N$ of eigenvalues of the distinguished extension in the spectral gap $(-1, 1)$ can *dive* in the negative continuum when the nuclei get sufficiently close. If this happens, the $N$ first min-max levels $\lambda_k$ (with Talman's splitting for instance) become equal to $a = -1$ and one has to take $k_0 = N+1$ (see the recent work [7] for more details).

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