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

JEAN DOLBEAULT, MARIA J. ESTEBAN, AND ERIC SÉRÉ

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 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 goal by making only minimal assumptions. Our result applied to the Dirac-Coulomb-like Hamiltonians 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 $\mathcal{D}_V = \mathcal{D} + V$ where $\mathcal{D} = -i\alpha \cdot \nabla + \beta$ is the linear Dirac operator with standard notations (see [26] for details), 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 $\mathcal{D}_{-\nu/|x|}$ 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 ν lies in the interval $(0, \sqrt{3}/2]$. In other words, its closure is self-adjoint and there is no other self-adjoint extension. For larger constants ν one must define a distinguished, physically relevant, self-adjoint extension and this can be done when $\nu \leq 1$. 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., [24, 30, 31, 32, 20, 21, 15, 14]. In these papers, general classes of potentials V are considered, but in the case $V = -\nu/|x|$ one always assumes that ν 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 [25] 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 deals with a self-adjoint operator A defined in a Hilbert space \mathcal{H} and satisfying a *variational gap* condition, to be specified later, related to a block decomposition under an orthogonal splitting

$$\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_-. \quad (1)$$

Such an abstract principle was proved for the first time in [13], but its hypotheses were rather restrictive and the application to the distinguished self-adjoint realization of \mathcal{D}_V only gave Talman's principle for bounded electric potentials (see also [16, 29] for related abstract principles). In [12] Talman's principle was proved for the unbounded potential $-v/|x|$ with $v \in (0, 0.305]$. In [3], thanks to a different abstract approach, the range of essential self-adjointness $v \in (0, \sqrt{3}/2]$ was dealt with. The articles [18, 19, 8, 23, 9] followed and the full range $v \in (0, 1]$ is now covered.

Using some of the tools of [3], Esteban and Loss [10, 11] 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 $v \in (0, 1]$. In [8, 9], connections were established between this new approach and the earlier constructions for Dirac-Coulomb operators with general electric potentials V .

Important closability issues had been overlooked in some arguments of [3] and some domain invariance issues are present in [10, 11] (see some comments about this at the beginning of Subsection 3.2). In [23] these issues are clarified and the self-adjoint extension problem considered in [10, 11] is connected to the min-max principle for eigenvalues of self-adjoint operators studied in [3]. The abstract results in [23] 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 [3, Corrigendum], we present another way of correcting the arguments of [3] thanks to a new geometric viewpoint. In the present work, by adopting this viewpoint, we are able to completely relax the essential self-adjointness assumption of [23]. 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, we fix some general notations that will be used in the whole paper. We consider a Hilbert space \mathcal{H} with scalar product $\langle \cdot, \cdot \rangle$ and associated norm $\| \cdot \|$. When the sum $V + W$ of two subspaces V, W of \mathcal{H} is direct in the algebraic sense, we use the notation $V \dot{+} W$. We reserve the notation $V \oplus W$ to topological sums. We adopt the convention of using the same letter to denote a quadratic form $q(\cdot)$ and its polar form $q(\cdot, \cdot)$. We use the notations $\mathcal{D}(q)$ for the domain of a quadratic form q and $\mathcal{D}(L)$ for the domain of a linear operator L . The space $\mathcal{D}(L)$ is endowed with the norm

$$\|x\|_{\mathcal{D}(L)} := \sqrt{\|x\|^2 + \|Lx\|^2}, \quad \forall x \in \mathcal{D}(L).$$

Let us briefly recall the standard Friedrichs extension method. Let $S : \mathcal{D}(S) \rightarrow \mathcal{H}$ be a densely defined operator. Assume that S is symmetric, which means that $\langle Sx, y \rangle = \langle x, Sy \rangle$ for all $x, y \in \mathcal{D}(S)$. If the quadratic form $s(x) = \langle x, Sx \rangle$ associated to S is bounded from below, *i.e.*, if

$$\ell_1 := \inf_{x \in \mathcal{D}(S) \setminus \{0\}} \frac{s(x)}{\|x\|^2} > -\infty,$$

then S has a natural self-adjoint extension T , which is called the *Friedrichs extension* of S and that can be constructed as follows (see *e.g.* [22] for more details). First of all, since the quadratic form s is bounded from below and associated to a densely defined symmetric operator, it is closable in \mathcal{H} . Denote its closure by \bar{s} . Take $\ell < \ell_1$, so that $\bar{s}(\cdot, \cdot) - \ell \langle \cdot, \cdot \rangle$ is a scalar product on $\mathcal{D}(\bar{s})$ giving it a Hilbert space structure. By the Riesz isomorphism theorem, for each $f \in \mathcal{H}$, there is a unique $u_f \in \mathcal{D}(\bar{s})$ such that $\bar{s}(v, u_f) - \ell \langle v, u_f \rangle = \langle v, f \rangle$ for all $v \in \mathcal{D}(\bar{s})$. Note that u_f is also the unique minimizer of the functional $I_f(u) := \frac{1}{2} (\bar{s}(u) - \ell \|u\|^2) - \langle u, f \rangle$ in $\mathcal{D}(\bar{s})$. The map $f \mapsto u_f$ is linear, bounded and self-adjoint for $\langle \cdot, \cdot \rangle$. Its inverse is $T - \ell \text{id}_{\mathcal{H}}$ and one easily checks that T does not depend on ℓ : this operator is just the restriction of S^* to $\mathcal{D}(\bar{s}) \cap \mathcal{D}(S^*)$. An important property of the Friedrichs extension is that the eigenvalues of T below its essential spectrum, if they exist, can be characterized by the classical Courant-Fisher min-max principle: for every positive integer k , the level

$$\ell_k := \inf_{\substack{V \text{ subspace of } \mathcal{D}(S) \\ \dim V = k}} \sup_{x \in V \setminus \{0\}} \frac{s(x)}{\|x\|^2}$$

is either the bottom of $\sigma_{\text{ess}}(T)$ (in the case $\ell_j = \ell_k$ for all $j \geq k$) or the k -th eigenvalue of T (counted with multiplicity) below $\sigma_{\text{ess}}(T)$.

In the special case of the Laplacian in a bounded domain Ω of \mathbb{R}^d with smooth boundary, $S = -\Delta : C_c^\infty(\Omega) \rightarrow L^2(\Omega)$, one has $\mathcal{D}(\bar{s}) = H_0^1(\Omega)$ and the construction of the Friedrichs extension T corresponds to the weak formulation in $H_0^1(\Omega)$ of the Dirichlet problem: $-\Delta u = f$ in Ω , $u = 0$ 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 T is the self-adjoint realization of the Dirichlet Laplacian. By regularity theory, we learn that $\mathcal{D}(T) = H^2(\Omega) \cap H_0^1(\Omega)$.

From now on in this paper, we consider a dense subspace F of \mathcal{H} and a symmetric operator $A : F \rightarrow \mathcal{H}$. We do *not* assume that the quadratic form $a(x) = \langle x, Ax \rangle$ is bounded from below, so we cannot apply the standard Friedrichs extension theorem to A . We introduce an orthogonal splitting $\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_-$ of \mathcal{H} as in (1). We denote by

$$\Lambda_\pm : \mathcal{H} \rightarrow \mathcal{H}_\pm$$

the orthogonal projectors associated to this splitting. We make the following assumptions:

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

and

$$\lambda_0 := \sup_{x_- \in F_- \setminus \{0\}} \frac{a(x_-)}{\|x_-\|^2} < +\infty. \tag{H2}$$

We also make the *variational gap assumption* that

$$\text{for some } k_0 \geq 1, \text{ we have } \lambda_{k_0} > \lambda_0 = \lambda_{k_0-1} \quad (\text{H3})$$

where the min-max levels λ_k ($k \geq 1$) are defined by

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

In order to construct a distinguished self-adjoint extension of A , for $E > \lambda_0$, we are going to decompose the quadratic form $a - E\|\cdot\|^2$ as the difference of two quadratic forms q_E and \bar{b}_E with q_E bounded from below and closable, while \bar{b}_E is positive and closed. Before stating our main result, let us define these quadratic forms.

We first introduce a quadratic form b on F_- :

$$b(x_-) = -a(x_-) = \langle x, (-\Lambda_- A \upharpoonright_{F_-}) x \rangle \quad \forall x_- \in F_-. \quad (3)$$

For $E > \lambda_0$ it is convenient to define the associated form

$$b_E(x_-) = b(x_-) + E\|x_-\|^2 \quad \forall x_- \in F_-. \quad (4)$$

As a consequence of Assumption (H2) and of the symmetry of $-\Lambda_- A \upharpoonright_{F_-}$, we have that

$$b_E \text{ is positive definite for all } E > \lambda_0 \text{ and } b \text{ is closable in } \mathcal{H}_-. \quad (b)$$

We denote by \bar{b} the closure of b and by $\bar{b}_E = \bar{b} + E\|\cdot\|^2$ the closure of b_E , their domain being $\mathcal{D}(\bar{b})$. We can consider the Friedrichs extension B of $-\Lambda_- A \upharpoonright_{F_-}$. For every parameter $E > \lambda_0$, the operator $B + E : \mathcal{D}(B) \rightarrow \mathcal{H}_-$ is invertible with bounded inverse. This allows us to define the operator $L_E : F_+ \rightarrow \mathcal{D}(B)$ such that

$$L_E x_+ := (B + E)^{-1} \Lambda_- A x_+, \quad \forall x_+ \in F_+. \quad (5)$$

We then introduce the subspace

$$\Gamma_E := \{x_+ + L_E x_+ : x_+ \in F_+\} \subset F_+ \oplus \mathcal{D}(B). \quad (6)$$

Making an abuse of terminology justified by the isomorphism $F_+ \oplus \mathcal{D}(B) \approx F_+ \times \mathcal{D}(B)$, we call Γ_E the *graph* of L_E . On this space, we define a quadratic form q_E by

$$q_E(x_+ + L_E x_+) := \langle x_+, (A - E)x_+ \rangle + \langle L_E x_+, (B + E)L_E x_+ \rangle. \quad (7)$$

Denoting by $\bar{\Gamma}_E$ the closure of Γ_E in \mathcal{H} and by Π_E the orthogonal projection on $\bar{\Gamma}_E$, we may write

$$q_E(x) = \langle x, S_E x \rangle, \quad \forall x \in \Gamma_E,$$

where

$$S_E := \Pi_E (\Lambda_+ (A - E) \Lambda_+ + \Lambda_- (B + E) \Lambda_-) \upharpoonright_{\Gamma_E}. \quad (8)$$

The operator S_E is symmetric and densely defined in the Hilbert space $(\bar{\Gamma}_E, \langle \cdot, \cdot \rangle \upharpoonright_{\bar{\Gamma}_E \times \bar{\Gamma}_E})$. It is one of the two Schur complements associated with the block decomposition of the operator $A - E \text{id}_{\mathcal{H}}$ under the orthogonal splitting $\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_-$. Further details on q_E , S_E are given in Section 2. In particular, in Subsection 2.1 the decomposition of $a - E\|\cdot\|^2$ in terms of q_E , \bar{b}_E is given. Note that in [3] (before its Corrigendum) as well as in [10, 11, 23],

the form \bar{b} was already present and a form analogous to q_E was defined, but its domain was F_+ instead of Γ_E .

The main result of this paper is as follows.

Theorem 1. *Let A be a symmetric operator on the Hilbert space \mathcal{H} . Assume (H1)-(H2)-(H3) and take $E > \lambda_0$. With the above notations, the quadratic forms b and q_E are bounded from below, b is closable in \mathcal{H}_- , q_E is closable in $\bar{\Gamma}_E$ and they satisfy*

$$\mathcal{D}(\bar{q}_E) \cap \mathcal{D}(\bar{b}) = \{0\}.$$

The operator A admits a unique self-adjoint extension \tilde{A} such that

$$\mathcal{D}(\tilde{A}) \subset \mathcal{D}(\bar{q}_E) \dot{+} \mathcal{D}(\bar{b}).$$

The domain of this extension is

$$\mathcal{D}(\tilde{A}) = \mathcal{D}(A^*) \cap \left(\mathcal{D}(\bar{q}_E) \dot{+} \mathcal{D}(\bar{b}) \right)$$

and it does not depend on E .

Writing

$$\lambda_\infty := \lim \lambda_k \in (\lambda_0, \infty]$$

one has

$$\lambda_\infty = \inf(\sigma_{\text{ess}}(\tilde{A}) \cap (\lambda_0, +\infty)).$$

In addition, the numbers λ_k ($k \geq 1$) satisfying $\lambda_0 < \lambda_k < \lambda_\infty$ are all the eigenvalues – counted with multiplicity – of \tilde{A} in the spectral gap $(\lambda_0, \lambda_\infty)$.

Theorem 1 deserves some comments.

- In the earlier works [13, 12, 3, 4, 5, 18, 19, 8, 23] on Talman's min-max principle, one assumes that $k_0 = 1$, which amounts to consider assumption (H3) with $k_0 = 1$. Allowing $k_0 \geq 2$ can be important in some applications: see Section 6. The abstract min-max principle for eigenvalues in the case $k_0 \geq 2$ was first considered in [6], but in that paper (H2) was replaced by a much more restrictive assumption. Moreover, the proof in [6] was based on the arguments of [3], so it suffered from the same closability issue solved in [23] and [3, Corrigendum]: the closure of L_E was used but its existence was not proved.
- Compared with [11, 23], another important novelty is that for constructing \tilde{A} we do not need the operator $-\Lambda_- A \upharpoonright_{F_-}$ to be self-adjoint or essentially self-adjoint in \mathcal{H}_- . This assumption was used in [23] to prove that L_E is closable, while in the present work this closability is not needed thanks to a new geometric viewpoint: instead of trying to close L_E we consider the subspace $\bar{\Gamma}_E$, which of course always exists, but is not necessarily a graph. As pointed out in [23], essential self-adjointness of $-\Lambda_- A \upharpoonright_{F_-}$ holds true in many important situations. However there are also interesting examples for which it does not hold true. An application to Dirac-Coulomb operators in which the essential adjointness of $-\Lambda_- A \upharpoonright_{F_-}$ does not hold true is described in Section 6. Let us give a simpler example: on the domain $F := (C_c^\infty(\Omega, \mathbb{R}))^2$ consider the operator

$$A \begin{pmatrix} u \\ v \end{pmatrix} := \begin{pmatrix} -\Delta u \\ \Delta v \end{pmatrix} \tag{9}$$

taking values in $\mathcal{H} = (L^2(\Omega, \mathbb{R}))^2$, where Ω 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 true. If $\lambda(\Omega) > 0$ is the smallest eigenvalue of the Dirichlet Laplacian on Ω , we have $\lambda_0 = -\lambda(\Omega)$ in (H2) and $\lambda_1 = \lambda(\Omega) > \lambda_0$, so (H3) with $k_0 = 1$ holds true. But $-\Lambda_- A \upharpoonright_{F_-}$ is the Laplacian defined on the minimal domain $\{0\} \times C_c^\infty(\Omega, \mathbb{R})$, and it is well-known that this operator is not essentially self-adjoint in $\{0\} \times L^2(\Omega, \mathbb{R})$, so one cannot apply the abstract results of [11, 23].

In this example, the distinguished extension given by Theorem 1 is easily obtained. One checks that $\mathcal{D}(\bar{b}) = \{0\} \times H_0^1(\Omega, \mathbb{R})$, $\mathcal{D}(\bar{q}_E) = H_0^1(\Omega, \mathbb{R}) \times \{0\}$. Moreover, if $\Delta^{(D)}$ denotes the Dirichlet Laplacian with domain $H^2(\Omega, \mathbb{R}) \cap H_0^1(\Omega, \mathbb{R})$, one has

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

- In [23], it is proved that the extension \tilde{A} is unique among the self-adjoint extensions whose domain is included in $\Lambda_+ \mathcal{D}(\bar{q}_E) \oplus \mathcal{H}_-$, assuming that the operator $-\Lambda_- A \upharpoonright_{F_-}$ is essentially self-adjoint. But the above example shows that without this assumption, such a uniqueness result does not hold true in general. Indeed, since $\Delta : C_c^\infty(\Omega, \mathbb{R}) \rightarrow L^2(\Omega, \mathbb{R})$ is not essentially self-adjoint, the operator A given by (9) has infinitely many self-adjoint extensions with domains included in $\Lambda_+ \mathcal{D}(\bar{q}_E) \oplus \mathcal{H}_-$. For instance, one can take

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

with $\Delta^{(N)}$ the self-adjoint extension of Δ associated with the Neumann boundary condition $\nabla v \cdot n = 0$, where n denotes the outward normal unit vector on $\partial\Omega$. Obviously, $\hat{A} \neq \tilde{A}$.

- In [18], the closability of L_E is claimed without proof, exactly as in [3]. The present work does not contain the result of [18] as a particular case: the self-adjoint operator is constructed in a different way in that paper, and the subspaces F_\pm involved in the min-max principle are larger. But it seems likely that the geometric approach of the present paper could be adapted to [18] in order to avoid the closability issue.

Concerning the proof of Theorem 1, we emphasize three main facts:

(1) *The quadratic form $q_E(x) = \langle x, S_E x \rangle$ is bounded from below for all $E > \lambda_0$, so that it has a closure \bar{q}_E in $\bar{\Gamma}_E$ and S_E has a Friedrichs extension T_E . This fact will allow us to define the distinguished extension \tilde{A} as the restriction of A^* to $\mathcal{D}(A^*) \cap (\mathcal{D}(\bar{q}_E) + \mathcal{D}(\bar{b}))$. We will prove its symmetry thanks to a formula expressing the product $\langle (\tilde{A} - E)X, U \rangle$ in terms of \bar{q}_E and \bar{b}_E , which will be deduced by density arguments from a decomposition of $a - E\|\cdot\|^2$ as the difference of q_E and \bar{b}_E .*

(2) *The self-adjoint operator T_E is invertible for all $\lambda_0 < E < \lambda_{k_0}$.* Combined with the (obvious) invertibility of $B + E$, this fact will allow us to construct the inverse of the distinguished extension $\tilde{A} - E$, by using once again the formula relating $\langle (\tilde{A} - E)X, U \rangle$ to \bar{q}_E and \bar{b}_E . Then, by a classical argument, we will conclude that \tilde{A} is self-adjoint.

(3) Although we are not able to prove that $\bar{\Gamma}_E$ is a graph above \mathcal{H}_+ , we will see that the sum $\bar{\Gamma}_E + \mathcal{D}(\bar{b})$ is direct in the algebraic sense. More importantly, if we denote by $\pi_E : \bar{\Gamma}_E + \mathcal{D}(\bar{b}) \rightarrow \bar{\Gamma}_E$ and $\pi'_E : \bar{\Gamma}_E + \mathcal{D}(\bar{b}) \rightarrow \mathcal{D}(\bar{b})$ the associated projectors, *the linear map*

$$X \in \mathcal{D}(\tilde{A}) \mapsto (\pi_E X, \pi'_E X) \in \bar{\Gamma}_E \times \mathcal{D}(\bar{b})$$

is continuous for the norms $\|X\|_{\mathcal{D}(\tilde{A})}$ and $\|\pi_E X\| + \|\pi'_E X\|$. Thanks to this fact, we will be able to give a relation between the spectra of \tilde{A} and T_E which will allow us to prove the min-max principle for the eigenvalues of \tilde{A} above λ_0 .

For $k_0 = 1$ the facts (1) and (2) are a consequence of the positivity of q_E for $E \in (\lambda_0, \lambda_1)$ and of the Riesz isomorphism theorem. When $k_0 \geq 2$ the positivity is lost, but these two key facts still hold true for other reasons to be given in the proofs of Proposition 6 and Lemma 7 and in Remark 8.

The paper is organized as follows. In Section 2, we study the quadratic form q_E under Assumptions (H1)-(H2). In Section 3, under the additional condition (H3) we prove that q_E is bounded from below, then we study its closure \bar{q}_E and the Friedrichs extension T_E . The self-adjoint extension \tilde{A} is constructed in Section 4 and the abstract version of Talman's principle for its eigenvalues is proved in Section 5, which ends the proof of Theorem 1. Section 6 is devoted to Dirac-Coulomb operators with charge configurations that are not covered by earlier abstract results.

2. THE QUADRATIC FORM q_E

The results of this section are essentially contained in the earlier works [3, 11, 23], we recall them here for the reader's convenience. We first give a more intuitive interpretation of the objects L_E, q_E that have been defined in the Introduction. Then we define a sequence of min-max levels for q_E that will be related to the min-max levels λ_k of A in Section 5.

2.1. A family of maximization problems. In this subsection we motivate the definition of L_E and q_E given in the Introduction. Consider the eigenvalue equation $(A - E)x = 0$ with unknowns $x \in F$ and $E \in \mathbb{R}$. Writing $x_+ := \Lambda_+ x$, $y_- := \Lambda_- x$ and projecting both sides of the equation on \mathcal{H}_- , one gets

$$\Lambda_- A x_+ + \Lambda_- (A - E) y_- = 0$$

which is also the Euler-Lagrange equation for the problem

$$\sup_{y_- \in F_-} \langle x_+ + y_-, (A - E)(x_+ + y_-) \rangle.$$

Given x_+ in F_+ one can try to look for a solution y_- . In general the problem is not solvable in F_- but one can consider a larger space in which a solution exists. We denote by $L_E x_+$

the generalized solution. In order to make these explanations more precise, we need to express the quadratic form $a - E\|\cdot\|^2$ in terms of q_E, \bar{b}_E .

Given $x_+ \in F_+$ and $E > \lambda_0$, let $\varphi_{E,x_+} : F_- \rightarrow \mathbb{R}$ be defined by

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

One easily sees that φ_{E,x_+} has a unique continuous extension to $\mathcal{D}(\bar{b})$ which is the strictly concave function

$$\bar{\varphi}_{E,x_+} : y_- \in \mathcal{D}(\bar{b}) \mapsto \langle x_+, (A - E)(x_+) \rangle + 2\operatorname{Re}\langle Ax_+, y_- \rangle - \bar{b}_E(y_-).$$

The main result of this subsection is

Proposition 2. *Let A be a symmetric operator on the Hilbert space \mathcal{H} . Assume (H1)-(H2), take $E > \lambda_0$ and remember the definition (7) of q_E . Then:*

- One has the decomposition

$$\langle X, (A - E)X \rangle = q_E(\Lambda_+ X + L_E \Lambda_+ X) - \bar{b}_E(\Lambda_- X - L_E \Lambda_+ X), \quad \forall X \in F. \quad (10)$$

- For each $x_+ \in F_+$, $L_E x_+$ is the unique maximizer of $\bar{\varphi}_{E,x_+}$ and one has

$$q_E(x_+ + L_E x_+) = \bar{\varphi}_{E,x_+}(L_E x_+) = \max_{y_- \in F_-} \bar{\varphi}_{E,x_+}(y_-) = \sup_{y_- \in F_-} \varphi_{E,x_+}(y_-). \quad (11)$$

Proof. If $X \in F$, taking $x_+ := \Lambda_+ X \in F_+$, $y_- := \Lambda_- X \in F_-$ and $z_- := y_- - L_E x_+ \in \mathcal{D}(B)$ we obtain

$$\begin{aligned} \langle X, (A - E)X \rangle &= \langle x_+, (A - E)x_+ \rangle + 2\operatorname{Re}\langle Ax_+, y_- \rangle - \langle y_-, (B + E)y_- \rangle \\ &= \langle x_+, (A - E)x_+ \rangle + 2\operatorname{Re}\langle L_E x_+, (B + E)y_- \rangle - \langle y_-, (B + E)y_- \rangle \\ &= \langle x_+, (A - E)x_+ \rangle + \langle L_E x_+, (B + E)L_E x_+ \rangle \\ &\quad + \operatorname{Re}\langle L_E x_+, (B + E)z_- \rangle - \operatorname{Re}\langle z_-, (B + E)y_- \rangle \\ &= \langle x_+, (A - E)x_+ \rangle + \langle L_E x_+, (B + E)L_E x_+ \rangle - \langle z_-, (B + E)z_- \rangle, \end{aligned}$$

which proves (10). Now, given $x_+ \in F_+$ this identity can be rewritten in the form

$$\varphi_{E,x_+}(y_-) = q_E(x_+ + L_E x_+) - \bar{b}_E(y_- - L_E x_+), \quad \forall y_- \in F_-.$$

By density of F_- in the Hilbert space $(\mathcal{D}(\bar{b}), \bar{b}_E(\cdot, \cdot))$ one thus has

$$\bar{\varphi}_{E,x_+}(y_-) = q_E(x_+ + L_E x_+) - \bar{b}_E(y_- - L_E x_+), \quad \forall y_- \in \mathcal{D}(\bar{b})$$

and by the positivity of \bar{b}_E one concludes that (11) holds true, which completes the proof. \square

2.2. The min-max levels for q_E . If assumptions (H1) and (H2) hold true, to each $E > \lambda_0$ we may associate the nondecreasing sequence of min-max levels $(\ell_k(E))_{k \geq 1}$ defined by

$$\ell_k(E) := \inf_{\substack{V \text{ subspace of } \Gamma_E \\ \dim V = k}} \sup_{x \in V \setminus \{0\}} \frac{q_E(x)}{\|x\|^2} \in [-\infty, +\infty). \quad (12)$$

We may also define the (possibly infinite) multiplicity numbers

$$m_k(E) := \text{card}\{k' \geq 1 : \ell_{k'}(E) = \ell_k(E)\} \geq 1. \quad (13)$$

In this subsection we analyse the dependence on E of the quadratic form q_E and its associated min-max levels. The results are summarized in the following proposition:

Proposition 3. *Assume that (H1)-(H2) of Theorem 1 are satisfied. Then:*

- For all $\lambda_0 < E < E'$ and for all $x_+ \in F_+$, we have

$$\|x_+ + L_{E'}x_+\| \leq \|x_+ + L_E x_+\| \leq \frac{E' - \lambda_0}{E - \lambda_0} \|x_+ + L_{E'}x_+\| \quad (14)$$

and

$$(E' - E) \|x_+ + L_{E'}x_+\|^2 \leq q_E(x_+ + L_E x_+) - q_{E'}(x_+ + L_{E'}x_+) \leq (E' - E) \|x_+ + L_E x_+\|^2. \quad (15)$$

- For every positive integer k and all $\lambda > \lambda_0$, one has

$$\ell_k(\lambda) \leq \lambda_k - \lambda. \quad (16)$$

- For every positive integer k , if $\lambda_k > \lambda_0$ then for all $\lambda > \lambda_0$, one has

$$\ell_k(\lambda) \geq (\lambda_k - \lambda) \left(\frac{\lambda - \lambda_0}{\lambda_k - \lambda_0} \right)^2. \quad (17)$$

As a consequence, when $\lambda_k > \lambda_0$ the min-max level $\ell_k(\lambda)$ is finite for every $\lambda > \lambda_0$. It is positive when $\lambda_0 < \lambda < \lambda_k$, negative when $\lambda > \lambda_k$ and one has $\ell_k(\lambda) = 0$ if and only if $\lambda = \lambda_k$. Therefore, the formula $m_k(\lambda_k) = \text{card}\{k' \geq 1 : \lambda_{k'} = \lambda_k\}$ holds true.

Proof. Formulas (14), (15) and their detailed proof can be found in [3, Lemma 2.1] and [23, Lemma 2.4], so here we just give the main arguments. In order to prove (14) one can start from the fact that for all $t \geq -\lambda_0$, $(t + E')^{-1} \leq (t + E)^{-1} \leq \frac{E' - \lambda_0}{E - \lambda_0} (t + E')^{-1}$. Then one can use the inclusion $\sigma(B) \subset [-\lambda_0, \infty)$ and the definition of L_E . In order to prove (15), one notices that this formula is equivalent to the two inequalities $\bar{\varphi}_E(L_{E'}x_+) \leq q_E(x_+ + L_E x_+)$ and $\bar{\varphi}_{E'}(L_E x_+) \leq q_{E'}(x_+ + L_{E'}x_+)$, which both hold true thanks to (11).

We now prove (16) and (17).

By definition of λ_k , for each $\varepsilon > 0$ there is a k -dimensional subspace V_ε of F_+ such that for all $x_+ \in V_\varepsilon$ and $y_- \in F_-$, $a(X) \leq (\lambda_k + \varepsilon) \|X\|^2$ with $X = x_+ + y_-$. If $E \in (\lambda_0, \infty)$ this inequality can be rewritten as $\varphi_{E, x_+}(y_-) \leq (\lambda_k - E + \varepsilon) \|x_+ + y_-\|^2$. By a density argument one infers that the inequality

$$\bar{\varphi}_{E, x_+}(y_-) \leq (\lambda_k - E + \varepsilon) \|x_+ + y_-\|^2$$

holds true for all $y_- \in \mathcal{D}(\bar{b})$. Choosing $y_- = L_E x_+$ and using (11), one gets the estimate $q_E(x) \leq (\lambda_k - E + \varepsilon) \|x\|^2$ with $x = x_+ + L_E x_+$, hence

$$\sup_{x \in W_\varepsilon \setminus \{0\}} \frac{q_E(x)}{\|x\|^2} \leq \lambda_k - E + \varepsilon$$

with $W_\varepsilon := \{x \in \Gamma_E : \Lambda_+ x \in V_\varepsilon\}$. Since ε is arbitrary and $\dim(W_\varepsilon) = k$, we conclude that (16) holds true.

On the other hand, using once again the definition of λ_k , we find that for each $\varepsilon > 0$ and each k -dimensional subspace W of Γ_{λ_k} , there is a nonzero vector x_ε in the k -dimensional space $V := \Lambda_+ W \subset F_+$ and a vector $y_\varepsilon \in F_-$ such that $a(X_\varepsilon) \geq (\lambda_k - \varepsilon) \|X_\varepsilon\|^2$ with $X_\varepsilon = x_\varepsilon + y_\varepsilon$. If $\lambda_k > \lambda_0$, after imposing $\varepsilon < \lambda_k - \lambda_0$ we get $\varphi_{\lambda_k - \varepsilon, x_\varepsilon}(y_\varepsilon) \geq 0$, hence, invoking (11), $q_{\lambda_k - \varepsilon}(x_\varepsilon + L_{\lambda_k - \varepsilon} x_\varepsilon) \geq 0$. Then, using (14), (15) with the choices $E = \lambda_k - \varepsilon$, $E' = \lambda_k$, we get

$$q_{\lambda_k}(x_\varepsilon + L_{\lambda_k} x_\varepsilon) \geq q_{\lambda_k - \varepsilon}(x_\varepsilon + L_{\lambda_k - \varepsilon} x_\varepsilon) - \varepsilon \|x_\varepsilon + L_{\lambda_k - \varepsilon} x_\varepsilon\|^2 \geq -\varepsilon \left(\frac{\lambda_k - \lambda_0}{\lambda_k - \varepsilon - \lambda_0} \right)^2 \|x_\varepsilon + L_{\lambda_k} x_\varepsilon\|^2.$$

Since W and ε are arbitrary, we thus have $\ell_k(\lambda_k) \geq 0$. Combining this with (16), we see that $\ell_k(\lambda_k) = 0$.

It remains to study the case $\lambda_k > \lambda_0$ and $\lambda \in (\lambda_0, \infty) \setminus \{\lambda_k\}$. We take an arbitrary k -dimensional subspace \widehat{W} of Γ_λ . We define $V := \Lambda_+ \widehat{W} \subset F_+$ and $W := \{x = x_+ + L_{\lambda_k} x_+ : x_+ \in V\} \subset \Gamma_{\lambda_k}$. Then W is also k -dimensional, so one has $\sup_{x \in W \setminus \{0\}} \frac{q_{\lambda_k}(x)}{\|x\|^2} \geq 0$, from what we have just seen. So, by compactness of the unit sphere for $\|\cdot\|$ of the k -dimensional space W and the continuity of q_{λ_k} on this space, there is $x_0 \in V$ such that $\|x_0 + L_{\lambda_k} x_0\| = 1$ and $q_{\lambda_k}(x_0 + L_{\lambda_k} x_0) \geq 0$. In order to bound $q_\lambda(x_0 + L_\lambda x_0)$ from below, we use (14), (15) with $E = \min(\lambda, \lambda_k)$ and $E' = \max(\lambda, \lambda_k)$. We get

$$q_\lambda(x_0 + L_\lambda x_0) \geq (\lambda_k - \lambda) \|x_0 + L_{\lambda_k} x_0\|^2 \geq (\lambda_k - \lambda) \left(\frac{\lambda - \lambda_0}{\lambda_k - \lambda_0} \right)^2 \|x_0 + L_\lambda x_0\|^2.$$

Since \widehat{W} is arbitrary, we conclude that (17) holds true.

The last statements of Proposition 3 - finiteness and sign of $\ell_k(\lambda)$, the fact that λ_k is the unique zero of ℓ_k - are an immediate consequence of (16) and (17). Note that this characterization of λ_k as unique solution of a nonlinear equation was already stated and proved in [3, Lemma 2.2 (c)] and [23, Lemma 2.8 (iii)]. \square

Remark 4. *Assumptions (H1)-(H2) are rather easy to check in practice, but checking (H3) is more delicate. The second point in Proposition 3 provides a way to do this: one just has to prove that for some $k_0 \geq 1$ and $E_0 > \lambda_0$ the level $\ell_{k_0}(E_0)$ is nonnegative, which implies that $\lambda_{k_0} \geq E_0$. We will see two examples of application of this method in Section 6: for the one-center Dirac-Coulomb operator and the multicenter Dirac-Coulomb operator (with attractive centers).*

Remark 5. *The numerical calculation of eigenvalues in a spectral gap is a delicate issue, due to a well-known phenomenon called spectral pollution: as the discretization is refined, one sometimes observes more and more spurious eigenvalues that do not approximate any eigenvalue of the exact operator (see [17]). It is possible to eliminate these spurious eigenvalues thanks to Talman's min-max principle. A method inspired of Talman's work was proposed in [7, 5]. The idea was to calculate each eigenvalue λ_k as the unique solution of the problem $\ell_k(\lambda) = 0$. This method is free of spectral pollution, but solving nonlinear equations has a computational cost. The estimates (16) and (17) proved in the present work suggest a fast and stable iterative algorithm that could reduce this cost. Starting from a value $E^{(0)}$ comprised between λ_0 and λ_k , one can compute a sequence of approximations by the formula $E^{(j+1)} = E^{(j)} + \ell_k(E^{(j)})$. From (16), one proves by induction that*

for all $j \geq 0$, one has $E^{(j)} \in (\lambda_0, \lambda_k)$, $E^{(j+1)} - E^{(j)} = \ell_k(E^{(j)}) > 0$ and $E^{(j)}$ converges monotonically to λ_k . Moreover, combining the inequalities (16) and (17) one finds that for $|h|$ small, $h + \ell_k(\lambda_k + h) = \mathcal{O}(h^2)$. So $E^{(j)}$ converges quadratically to λ_k . It would be interesting to perform numerical tests of this algorithm in practical situations.

3. THE CLOSURE \bar{q}_E AND THE FRIEDRICHS EXTENSION T_E

In this section, under assumptions (H1)-(H2)-(H3) we prove that the form q_E is bounded from below and closable, so that the Schur complement S_E has a Friedrichs extension T_E . We then relate the spectrum of T_E to the min-max levels λ_k . Finally, we construct a natural isomorphism between the domains of \bar{q}_E and $\bar{q}_{E'}$ for all $E, E' > \lambda_0$.

3.1. Construction of \bar{q}_E and T_E . In this subsection we are going to prove the following result:

Proposition 6. *Let A be a symmetric operator on the Hilbert space \mathcal{H} . Assuming (H1)-(H2)-(H3) and with the above notations:*

- For each $E > \lambda_0$, the quadratic form $q_E(x) = \langle x, S_E x \rangle$ is bounded from below hence closable in $\bar{\Gamma}_E$ and S_E has a Friedrichs extension T_E .
- If $E \in (\lambda_0, \lambda_\infty) \setminus \{\lambda_k : k \geq 1\}$ then $T_E : \mathcal{D}(T_E) \rightarrow \bar{\Gamma}_E$ is invertible with bounded inverse. If $\lambda_0 < \lambda_k < \lambda_\infty$ then 0 is the k -th eigenvalue of T_{λ_k} counted with multiplicity. Moreover its multiplicity is finite and equal to $\text{card}\{k' \geq 1 : \lambda_{k'} = \lambda_k\}$. If $\lambda_k = \lambda_\infty$ for some positive integer k , then $0 = \min \sigma_{\text{ess}}(T_{\lambda_k})$.

The main tool in the proof of Proposition 6 is the following result:

Lemma 7. *Under assumptions (H1), (H2) and (H3), for every $E > \lambda_0$, there is $\kappa_E > 0$ such that $q_E + \kappa_E \|\cdot\|^2 \geq \|\cdot\|^2$ on Γ_E .*

Proof. We distinguish two cases depending on the value of $k_0 = \min\{k \geq 1 : \lambda_k > \lambda_0\}$.

When $k_0 = 1$, one has $\lambda_1 > \lambda_0$ and $q_{\lambda_1}(x) \geq 0$ for all $x \in \Gamma_{\lambda_1}$. So, using the inequalities (14) and (15), one finds that for all $E > \lambda_0$ and $x \in \Gamma_E$, $q_E(x) + \kappa_E \|x\|^2 \geq \|x\|^2$, with

$$\kappa_E := 1 + \max\{0, (E - \lambda_1)\} \left(\frac{E - \lambda_0}{\lambda_1 - \lambda_0} \right)^2.$$

When $k_0 \geq 2$ we need a different argument and the formula for κ_E is less explicit. As in the case $k_0 = 1$, we just have to find a constant κ_E for some $E > \lambda_0$; then the inequalities (14) and (15) will immediately imply its existence for all $E > \lambda_0$. We take $E \in (\lambda_0, \lambda_{k_0})$. Since $\lambda_{k_0-1} = \lambda_0 < E$, by the second point of Proposition 3 we have $\ell_{k_0-1}(E) \in [-\infty, 0)$. So there is a $(k_0 - 1)$ -dimensional subspace W of Γ_E such that

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

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

- *First case:* $x \in W$. Then $q_E(x) = \langle x, S_E x \rangle \geq -C \|x\|^2$.
- *Second case:* $x \notin W$. Then the vector space $\text{span}\{x\} \oplus W$ has dimension k_0 . Since we have $\lambda_{k_0} > E > \lambda_0$, by the third point of Proposition 3 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

$$q_E(x) = q_E(x + w_0) - 2 \operatorname{Re} \langle x, S_E w_0 \rangle - q_E(w_0) \geq -2C \|x\| \|w_0\| + |\ell'| \|w_0\|^2 \geq -\frac{C^2}{|\ell'|} \|x\|^2.$$

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

Proof of Proposition 6. As mentioned in the Introduction, we have $q_E(x) = \langle x, S_E x \rangle$ where $S_E : \Gamma_E \rightarrow \bar{\Gamma}_E$ is the Schur complement of the block decomposition of $A - E$ under the splitting $\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_-$ given by formula (8). The operator S_E is densely defined in the Hilbert space $\bar{\Gamma}_E$ and it is clearly symmetric, moreover we have just seen that q_E is bounded from below, so q_E is closable in $\bar{\Gamma}_E$. We denote its closure by \bar{q}_E . We call T_E the Friedrichs extension of S_E in $\bar{\Gamma}_E$. With

$$\ell_\infty(E) := \lim_{k \rightarrow \infty} \ell_k(E),$$

the classical min-max principle implies that the levels $\ell_k(E)$ such that $\ell_k(E) < \ell_\infty(E)$ are all the eigenvalues of T_E below $\ell_\infty(E)$ counted with multiplicity, and one has $\ell_\infty(E) = \inf \sigma_{\text{ess}}(T_E)$. So:

If $E \in (\lambda_0, \lambda_\infty) \setminus \{\lambda_k : k \geq 1\}$ then by Proposition 3, one has $0 < \ell_\infty(E)$ and 0 is not in the set $\{\ell_k(E) : k \geq 1\}$. As a consequence, it is not in the spectrum of T_E , so T_E is invertible with bounded inverse.

If $E = \lambda_k$ with $\lambda_0 < \lambda_k < \lambda_\infty$ then, using once again Proposition 3, we find that $\ell_k(E) = 0$ and $\ell_\infty(E) > 0$. So 0 is an eigenvalue of T_E of finite multiplicity equal to $m_k(\lambda_k)$ where m_k has been defined in (13). From Proposition 3, $m_k(\lambda_k)$ equals $\text{card}\{k' \geq 1 : \lambda_{k'} = \lambda_k\}$.

If $\lambda_k = \lambda_\infty$, then for all $k' \geq k$ one has $\lambda_{k'} = \lambda_k$, so $0 = \ell_{k'}(\lambda_k)$ by Proposition 3. In other words, $0 = \ell_\infty(\lambda_k)$. Then the classical min-max theorem implies that $0 = \min \sigma_{\text{ess}}(T_{\lambda_k})$.

Proposition 6 is thus proved. \square

Remark 8. When $k_0 = 1$ and $\lambda_0 < E < \lambda_1$, the closed quadratic form \bar{q}_E is positive definite and the invertibility of T_E is just a consequence of the Riesz isomorphism theorem.

3.2. A family of isomorphisms. In the earlier works [3] (before its Corrigendum), [10, 11] and [23], q_E was seen as a quadratic form on F_+ and the domain of its closure was independent of E . Note, however, that the existence of the closure was claimed without proof in [3] (and this was a serious gap), while the proof of the domain invariance was based on an incorrect estimate in [10, Proposition 2] and was incomplete in [11] (but this domain invariance problem can be easily fixed using [3, inequalities (10), (11)]).

In the present situation, since we do not know whether L_E is closable or not, it is essential to define q_E on Γ_E then to close it in $\bar{\Gamma}_E$. So the domain of q_E cannot be independent of E : indeed it is a subspace of $\bar{\Gamma}_E$ which itself depends on E . However, if we endow

each space $\mathcal{D}(\bar{q}_E)$ with the norm $\|x\|_{\mathcal{D}(\bar{q}_E)} := \sqrt{\bar{q}_E(x) + \kappa_E \|x\|^2}$, there is a natural isomorphism $\hat{i}_{E,E'}$ between any two Banach spaces $\mathcal{D}(\bar{q}_E)$ and $\mathcal{D}(\bar{q}_{E'})$, as explained in the next proposition:

Proposition 9. *Under conditions (H1), (H2) and (H3), for $E, E' \in (\lambda_0, \infty)$, the linear map $i_{E,E'} : x_+ + L_E x_+ \mapsto x_+ + L_{E'} x_+$ can be uniquely extended to an isomorphism $\hat{i}_{E,E'}$ between the Banach spaces $\mathcal{D}(\bar{q}_E)$ and $\mathcal{D}(\bar{q}_{E'})$ which can itself be uniquely extended to an isomorphism $\bar{i}_{E,E'}$ between $\bar{\Gamma}_E$ and $\bar{\Gamma}_{E'}$ for the norm $\|\cdot\|$. Moreover one has the formula*

$$\bar{i}_{E,E'}(x) = x + (E' - E)(B + E')^{-1} \Lambda_- x, \quad \forall x \in \bar{\Gamma}_E. \quad (18)$$

Proof. The linear map $i_{E,E'}$ is obviously a bijection between Γ_E and $\Gamma_{E'}$, of inverse $i_{E',E}$. The estimates (14), (15) of Lemma 3 imply that $i_{E,E'}$ is an isomorphism for the norm $\|\cdot\|$ as well as for the norms $\|\cdot\|_{\mathcal{D}(\bar{q}_E)}$ and $\|\cdot\|_{\mathcal{D}(\bar{q}_{E'})}$, hence the existence and uniqueness of the successive continuous extensions $\hat{i}_{E,E'}$ and $\bar{i}_{E,E'}$, that are isomorphisms of inverses $\hat{i}_{E',E}$ and $\bar{i}_{E',E}$.

From the formula $L_E x_+ = (B + E)^{-1} \Lambda_- A x_+$ one easily gets the resolvent identity

$$L_{E'} x_+ = L_E x_+ + (E - E')(B + E')^{-1} L_E x_+, \quad \forall x_+ \in F_+$$

which is the same as

$$\bar{i}_{E,E'}(x) = x + (E - E')(B + E')^{-1} \Lambda_- x, \quad \forall x \in \Gamma_E.$$

By continuity of $\bar{i}_{E,E'}$, $(B + E')^{-1}$ and Λ_- for the norm $\|\cdot\|$, one can extend the above formula to $\bar{\Gamma}_E$ and this ends the proof of the proposition. \square

Proposition 9 has the following consequence which will be useful in the next section:

Corollary 10. *Assume that the conditions (H1), (H2) and (H3) hold true. Let $E, E' > \lambda_0$. Then*

$$\mathcal{D}(\bar{q}_{E'}) + \mathcal{D}(\bar{b}) = \mathcal{D}(\bar{q}_E) + \mathcal{D}(\bar{b}). \quad (19)$$

Proof. From formula (18), for each $x \in \mathcal{D}(\bar{q}_E)$ one has $\hat{i}_{E,E'}(x) - x \in \mathcal{D}(B)$, hence

$$\mathcal{D}(\bar{q}_{E'}) \subset \mathcal{D}(\bar{q}_E) + \mathcal{D}(B) \subset \mathcal{D}(\bar{q}_E) + \mathcal{D}(\bar{b}),$$

which of course implies the inclusion

$$\mathcal{D}(\bar{q}_{E'}) + \mathcal{D}(\bar{b}) \subset \mathcal{D}(\bar{q}_E) + \mathcal{D}(\bar{b}).$$

Exchanging E and E' one gets the reverse inclusion, so (19) is proved. \square

4. THE DISTINGUISHED SELF-ADJOINT EXTENSION

In this section, we continue with the proof of Theorem 1 by constructing the distinguished self-adjoint extension \tilde{A} and studying some properties of its domain that will be useful in the sequel. But before doing this, we need to establish a decomposition of the product $\langle (A^* - E)X, U \rangle$ under weak assumptions on the vectors X, U .

4.1. A useful identity. In this subsection we state and prove an identity that plays a crucial role in the construction and study of \tilde{A} :

Proposition 11. *Assume that the conditions (H1), (H2) and (H3) hold true. Let $x, u \in \mathcal{D}(\bar{q}_E)$ and $z_-, v_- \in \mathcal{D}(\bar{b})$ be such that $X = x + z_- \in \mathcal{D}(A^*)$. Then, with $U = u + v_-$, we have*

$$\langle (A^* - E)X, U \rangle = \bar{q}_E(x, u) - \bar{b}_E(z_-, v_-) \quad (20)$$

for every $E > \lambda_0$.

Proof. Formula (10) of Lemma 2 exactly says that for all $X = x + z_- \in F$ with $x = \Lambda_+ X + L_E \Lambda_+ X$ and $z_- = \Lambda_- X - L_E \Lambda_+ X$, one has

$$\langle X, (A - E)X \rangle = \langle x, S_E x \rangle - \langle z_-, (B + E)z_- \rangle.$$

This relation between quadratic forms directly implies a formula involving their polar forms: for all $X = x + z_- \in F$ and $U = u + v_- \in F$ with $x = \Lambda_+ X + L_E \Lambda_+ X$, $u = \Lambda_+ U + L_E \Lambda_+ U$, $z_- = \Lambda_- X - L_E \Lambda_+ X$ and $v_- = \Lambda_- U - L_E \Lambda_+ U$, one has

$$\langle x + z_-, (A - E)U \rangle = \langle x, S_E u \rangle - \langle z_-, (B + E)v_- \rangle. \quad (21)$$

In order to prove Lemma 11, we have to generalize (21) to larger classes of vectors X, U . We proceed in two steps.

First step: we fix $U = u + v_-$ in F , with $u = \Lambda_+ U + L_E \Lambda_+ U$ and $v_- = \Lambda_- U - L_E \Lambda_+ U$.

If $x = 0$ and $X = z_- \in F_-$, the identity (21) holds true and reduces to

$$\langle z_-, (A - E)U \rangle = -\langle z_-, (B + E)v_- \rangle. \quad (22)$$

Both sides of (22) are continuous in z_- for the norm $\|\cdot\|$, and we recall that F_- is dense in \mathcal{H}_- . So (22) remains true for all $z_- \in \mathcal{H}_-$.

As a consequence, for $X \in F$ we may apply (22) to $z_- = \Lambda_- X - L_E \Lambda_+ X \in \mathcal{H}_-$ and we may subtract this identity from (21). This gives

$$\langle x, (A - E)U \rangle = \langle x, S_E u \rangle, \quad \forall x \in \Gamma_E. \quad (23)$$

Both sides of (23) are continuous in x for the norm $\|\cdot\|$, so (23) remains true for all $x \in \bar{\Gamma}_E$.

Then, for $x \in \bar{\Gamma}_E$ and $z_- \in \mathcal{H}_-$, we may add (22) and (23). We conclude that (21) remains valid for all $x \in \bar{\Gamma}_E$ and $z_- \in \mathcal{H}_-$. In particular, when $X = x + z_- \in \mathcal{D}(A^*)$ with $x \in \mathcal{D}(\bar{q}_E)$ and $z_- \in \mathcal{D}(\bar{b})$, (21) still holds true and may be rewritten as follows:

$$\langle (A^* - E)X, u + v_- \rangle = \bar{q}_E(x, u) - \bar{b}_E(z_-, v_-). \quad (24)$$

This formula is the same as (20) under the additional assumptions $U \in F$, $u \in \Gamma_E$ and $v_- = U - u \in \mathcal{D}(B)$.

Second step: we fix $X = x + z_- \in \mathcal{D}(A^*)$ with $x \in \mathcal{D}(\bar{q}_E)$, $z_- \in \mathcal{D}(\bar{b})$.

If $u = 0$ and $v_- = U \in F_-$, the identity (24) holds true and reduces to

$$\langle (A^* - E)X, v_- \rangle = -\bar{b}_E(z_-, v_-). \quad (25)$$

Both sides of (25) are continuous in v_- for the norm $\|\cdot\|_{\mathcal{D}(\bar{b})}$ and we recall that F_- is dense in $\mathcal{D}(\bar{b})$ for this norm. So (25) remains true for all $v_- \in \mathcal{D}(\bar{b})$.

As a consequence, for $U \in F$ we may apply (25) to $v_- = \Lambda_- U - L_E \Lambda_+ U \in \mathcal{D}(B) \subset \mathcal{D}(\bar{b})$ and we may subtract this identity from (24). This gives

$$\langle (A^* - E)X, u \rangle = \bar{q}_E(x, u), \quad \forall u \in \Gamma_E. \quad (26)$$

Both sides of (26) are continuous in u for the norm $\|\cdot\|_{\mathcal{D}(\bar{q}_E)}$, and we recall that Γ_E is dense in $\mathcal{D}(\bar{q}_E)$ for this norm. So (26) remains true for all $u \in \mathcal{D}(\bar{q}_E)$.

Then, for $u \in \mathcal{D}(\bar{q}_E)$ and $v_- \in \mathcal{D}(\bar{b})$, we may add (25) and (26) and we finally get (20) in the general case. \square

4.2. Construction of the self-adjoint extension. In this subsection we prove

Proposition 12. *Under conditions (H1), (H2) and (H3), the operator A admits a unique self-adjoint extension \tilde{A} such that $\mathcal{D}(\tilde{A}) \subset \mathcal{D}(\bar{q}_E) + \mathcal{D}(\bar{b})$. Its domain is $\mathcal{D}(\tilde{A}) = \mathcal{D}(A^*) \cap (\mathcal{D}(\bar{q}_E) + \mathcal{D}(\bar{b}))$ and this subspace does not depend on E .*

Proof. For $E > \lambda_0$, on the subspace

$$\mathcal{D}(\tilde{A}) := (\mathcal{D}(\bar{q}_E) + \mathcal{D}(\bar{b})) \cap \mathcal{D}(A^*), \quad (27)$$

let us define

$$\tilde{A}x := A^*x, \quad \forall x \in \mathcal{D}(\tilde{A}). \quad (28)$$

The operator \tilde{A} is indeed an extension of A , since

$$F \subset (\Gamma_E + \mathcal{D}(B)) \cap \mathcal{D}(A^*) \subset \mathcal{D}(\tilde{A}) \quad \text{and} \quad A^* \upharpoonright_F = A.$$

By Corollary 10, the domain of \tilde{A} does not depend on E . Moreover this extension is symmetric: this immediately follows from Proposition 11. So, in order to prove that it is self-adjoint, we just have to show that for some $E > \lambda_0$, $\tilde{A} - E$ is a bijection.

Let $f \in \mathcal{H}$. We look for $X = x + z_-$ in $\mathcal{D}(A^*)$ with $x \in \mathcal{D}(\bar{q}_E)$ and $z_- \in \mathcal{D}(\bar{b})$, such that $(A^* - E)X = f$. Using once again Proposition 11, we can reformulate this equation as a system of two equations written in weak form:

$$\begin{aligned} & \text{Find } (x, z_-) \in \mathcal{D}(\bar{q}_E) \times \mathcal{D}(\bar{b}) \text{ such that} \\ & \begin{cases} \bar{q}_E(x, u) = \langle f, u \rangle, & \forall u \in \mathcal{D}(\bar{q}_E), \\ \bar{b}_E(z_-, v_-) = -\langle f, v_- \rangle, & \forall v_- \in \mathcal{D}(\bar{b}). \end{cases} \end{aligned} \quad (\mathcal{D}_f)$$

Indeed, Proposition 11 guarantees that any solution of $(A^* - E)X = f$ lying in $D(\tilde{A})$ must be a sum $X = x + z_-$ where (x, z_-) satisfies (\mathcal{D}_f) . Conversely, if $(x, z_-) \in \mathcal{D}(\bar{q}_E) \times \mathcal{D}(\bar{b})$ satisfies (\mathcal{D}_f) and $X = x + z_-$, then, by Proposition 11, for all $U \in F$,

$$\begin{aligned} \langle X, (A - E)U \rangle &= \langle X, (A^* - E)U \rangle \\ &= \bar{q}_E(x, \Lambda_+ U + L_E \Lambda_+ U) - \bar{b}_E(z_-, \Lambda_- U - L_E \Lambda_+ U) = \langle f, U \rangle, \end{aligned}$$

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

Now, the problem (\mathcal{P}_f) can be rewritten as follows in terms of the Friedrichs extensions T_E and B :

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

This system has a unique solution for every E in $(\lambda_0, \lambda_\infty) \setminus \{\lambda_k, k \geq k_0\}$. Indeed, for $E > \lambda_0$ we have seen that $B + E$ is invertible with bounded inverse, and by Lemma 6 the same is true with T_E if in addition $E \notin \{\lambda_k, k \geq k_0\}$. So (\mathcal{P}_f) has a unique solution given by

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

As a consequence, $\tilde{A} - E$ is a bijection. Then the resolvent operator $R_E(\tilde{A}) = (E - \tilde{A})^{-1}$, being everywhere defined and symmetric, is self-adjoint, and this proves the self-adjointness of $\tilde{A} = E - R_E(\tilde{A})^{-1}$. \square

Remark 13. From the formulas for x and z_- , we see that x is in $\mathcal{D}(T_E)$ and that z_- belongs to $\mathcal{D}(B)$. As a consequence, the domain of \tilde{A} may also be written as

$$\mathcal{D}(\tilde{A}) = (\mathcal{D}(T_E) + \mathcal{D}(B)) \cap \mathcal{D}(A^*). \quad (29)$$

The self-adjoint extension \tilde{A} is thus built. Its uniqueness among those whose domain is contained in $\mathcal{D}(\bar{q}_E) + \mathcal{D}(\bar{b})$ is almost trivial. Indeed, if \hat{A} is a self-adjoint extension of A , we must have $\mathcal{D}(\hat{A}) \subset \mathcal{D}(A^*)$, hence, if in addition $\mathcal{D}(\hat{A}) \subset \mathcal{D}(\bar{q}_E) + \mathcal{D}(\bar{b})$ then $\mathcal{D}(\hat{A}) \subset \mathcal{D}(\tilde{A})$, which automatically implies $\hat{A} = \tilde{A}$ since both operators are self-adjoint. This completes the proof of Proposition 12.

4.3. Direct sums. Recall that in (6) we defined the graph Γ_E of L_E as

$$\Gamma_E := \{x_+ + L_E x_+ : x_+ \in F_+\} \subset F_+ \oplus \mathcal{D}(B).$$

A natural question is whether its closure $\bar{\Gamma}_E$ in \mathcal{H} has the graph property $\bar{\Gamma}_E \cap \mathcal{H}_- = \{0\}$. A partial answer to this question is given in the next lemma:

Lemma 14. Under conditions (H1), (H2) and with the above notations,

$$\bar{\Gamma}_E \cap \mathcal{H}_- \subset ((B + E)(F_-))^\perp. \quad (30)$$

Proof. The arguments below are essentially contained in the proof of [23, Lemma 2.2], but we repeat them here for the reader's convenience. If $y \in \bar{\Gamma}_E \cap \mathcal{H}_-$ then there is a sequence (x_n) in F_+ such that $\|x_n\| \rightarrow 0$ and $\|L_E x_n - y\| \rightarrow 0$. Then, for $z \in (B + E)(F_-)$ we may write $\langle y, z \rangle = \lim \langle L_E x_n, z \rangle$. On the other hand, $|\langle L_E x_n, z \rangle| = |\langle x_n, A(B + E)^{-1} z \rangle| \leq \|x_n\| \|A(B + E)^{-1} z\| \rightarrow 0$, so $\langle y, z \rangle = 0$. \square

If one assumes as in [23] that $\Lambda_- A \upharpoonright_{F_-}$ is essentially self-adjoint, then the subspace $(B + E)(F_-)$ of \mathcal{H}_- is dense in \mathcal{H}_- and one concludes that $\bar{\Gamma}_E$ has the graph property. But we do not make this assumption, and for this reason we cannot infer from (30) that $\bar{\Gamma}_E \cap \mathcal{H}_- = \{0\}$. 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 strategy in which the linear subspace $\bar{\Gamma}_E$ replaces the possibly nonexistent closure of L_E . Here is the main difference between the present work and [23].

While we may have $\bar{\Gamma}_E \cap \mathcal{H}_- \neq \{0\}$, the following property holds true, as a consequence of Lemma 14:

Proposition 15. *Under conditions (H1), (H2) and with the above notations,*

$$\bar{\Gamma}_E \cap \mathcal{D}(\bar{b}) = \{0\}.$$

Proof. From (30), we have

$$\begin{aligned} \bar{\Gamma}_E \cap \mathcal{D}(\bar{b}) &= (\bar{\Gamma}_E \cap \mathcal{H}_-) \cap \mathcal{D}((B+E)^{1/2}) \\ &\subset ((B+E)(F_-))^\perp \cap \mathcal{D}((B+E)^{1/2}) = (B+E)^{-1/2} \left((B+E)^{1/2} F_- \right)^\perp = \{0\}, \end{aligned}$$

since $(B+E)^{1/2} F_-$ is dense in \mathcal{H}_- . \square

Proposition 15 tells us that the sum of $\bar{\Gamma}_E$ and $\mathcal{D}(\bar{b})$ is algebraically direct. Let us denote by $\pi_E : \bar{\Gamma}_E \dot{+} \mathcal{D}(\bar{b}) \rightarrow \bar{\Gamma}_E$ and $\pi'_E : \bar{\Gamma}_E \dot{+} \mathcal{D}(\bar{b}) \rightarrow \mathcal{D}(\bar{b})$ the associated projectors. In Section 5 we will need some informations on the continuity of the restrictions $\pi_E \upharpoonright_{\mathcal{D}(\tilde{A})}$ and $\pi'_E \upharpoonright_{\mathcal{D}(\tilde{A})}$. These operators are not necessarily continuous for the $\|\cdot\|$ norm, but we have the following result.

Proposition 16. *Under assumptions (H1), (H2) and (H3), for all $E > \lambda_0$, one has*

$$\pi_E(\mathcal{D}(\tilde{A})) \subset \mathcal{D}(T_E) \text{ and } \pi'_E(\mathcal{D}(\tilde{A})) \subset \mathcal{D}(B).$$

Moreover the operator $\pi_E \upharpoonright_{\mathcal{D}(\tilde{A})}$ is continuous for the norms $\|\cdot\|_{\mathcal{D}(\tilde{A})}$, $\|\cdot\|_{\mathcal{D}(T_E)}$ and the operator $\pi'_E \upharpoonright_{\mathcal{D}(\tilde{A})}$ is continuous for the norms $\|\cdot\|_{\mathcal{D}(\tilde{A})}$, $\|\cdot\|_{\mathcal{D}(B)}$. More precisely, there is a positive constant C_E such that for all $X \in \mathcal{D}(\tilde{A})$,

$$\|\pi'_E(X)\|_{\mathcal{D}(B)} \leq C_E \|\Lambda_-(\tilde{A}-E)X\| \quad \text{and} \quad \|\pi_E(X)\|_{\mathcal{D}(T_E)} \leq C_E \|X\|_{\mathcal{D}(\tilde{A})}.$$

Moreover the constant C_E remains uniformly bounded when E stays away from λ_0 and ∞ .

Proof. In the arguments below the constant C_E changes value from line to line but we keep the same notation for the sake of simplicity. We use the weak formulation (\mathcal{P}_f) of the equation $(\tilde{A}-E)X = f$ introduced in Section 4. In that section, f was given, X was unknown and it was assumed that $E \in (\lambda_0, \lambda_1)$ in order to make sure that (\mathcal{P}_f) had a unique solution X . But here we use (\mathcal{P}_f) differently. We take $E > \lambda_0$, $X \in \mathcal{D}(\tilde{A})$ and we define $x := \pi_E(X)$, $z_- := \pi'_E(X)$, $f := (\tilde{A}-E)X$. Then (\mathcal{P}_f) must hold true. The second equation of this system means that $z_- = -(B+E)^{-1} \Lambda_- f$, which implies that z_- is in $\mathcal{D}(B)$ with an estimate of the form $\|z_-\|_{\mathcal{D}(B)} \leq C_E \|\Lambda_- f\|$. Since $\|\cdot\|_{\mathcal{D}(B)} \geq \|\cdot\|$ and $x = X - z_-$, the estimate on z_- implies in turn the estimate $\|x\| \leq C_E \|X\|_{\mathcal{D}(\tilde{A})}$. Moreover, the first equation in (\mathcal{P}_f) means that x is in $\mathcal{D}(T_E)$ and $T_E x = \Pi_E(\tilde{A}-E)X$, so we finally get the estimate $\|x\|_{\mathcal{D}(T_E)} \leq C_E \|X\|_{\mathcal{D}(\tilde{A})}$ and this ends the proof of Proposition 16. \square

Remark 17. *In Section 5, we do not use all the informations contained in Proposition 16: we only need the weaker estimates*

$$\|\pi'_E(X)\| \leq C_E \|\Lambda_-(\tilde{A}-E)X\| \quad \text{and} \quad \|\pi_E(X)\| \leq C_E \|X\|_{\mathcal{D}(\tilde{A})}. \quad (31)$$

4.4. Variational interpretation when $k_0 = 1$. In the special case $k_0 = 1$, for $\lambda_0 < E < \lambda_1$ the quadratic form \bar{q}_E is positive definite as well as \bar{b}_E and the existence and uniqueness of a solution to the weak problem (\mathcal{P}_f) directly follows from the Riesz isomorphism theorem. One can even give an interpretation of (\mathcal{P}_f) that generalizes the minimization principle for the Friedrichs extension of semibounded operators mentioned in the introduction. We describe it in this short subsection, as a side remark.

Assuming that $E \in (\lambda_0, \lambda_1)$ and given $f \in \mathcal{H}$, let us consider the inf-sup problem

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

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:

$$\begin{aligned} & \inf_{x_+ \in F_+} \sup_{z_- \in \mathcal{D}(B)} \left\{ \frac{1}{2} q_E(x_+ + L_E x_+) - \langle f, x_+ + L_E x_+ \rangle - \frac{1}{2} \bar{b}_E(z_-) - \langle f, z_- \rangle \right\} \\ &= \inf_{x_+ \in F_+} \left\{ \frac{1}{2} q_E(x_+ + L_E x_+) - \langle f, x_+ + L_E x_+ \rangle \right\} - \inf_{z_- \in \mathcal{D}(B)} \left\{ \frac{1}{2} \bar{b}_E(z_-) + \langle f, z_- \rangle \right\} \\ &= \min_{x \in \mathcal{D}(\bar{q}_E)} \left\{ \frac{1}{2} \bar{q}_E(x) - \langle f, x \rangle \right\} - \min_{z_- \in \mathcal{D}(\bar{b})} \left\{ \frac{1}{2} \bar{b}_E(z_-) + \langle f, z_- \rangle \right\}. \end{aligned}$$

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 (\mathcal{P}_f) , so their sum is $X = (\tilde{A} - E)^{-1} f$.

5. THE MIN-MAX PRINCIPLE

In this section, we establish the min-max principle for the eigenvalues of \tilde{A} that constitutes the last part of Theorem 1:

Proposition 18. *Under assumptions (H1), (H2) and (H3), for $k \geq k_0$ the numbers λ_k satisfying $\lambda_k < \lambda_\infty$ are all the eigenvalues of \tilde{A} in the spectral gap $(\lambda_0, \lambda_\infty)$ counted with multiplicity. Moreover one has*

$$\lambda_\infty = \inf(\sigma_{\text{ess}}(\tilde{A}) \cap (\lambda_0, \infty)).$$

Even if our assumptions are weaker and our formalism slightly different, the arguments in the proof of Proposition 18 are essentially the same as in [3, § 2] (but some details are missing in that reference) and [23, § 2.6]. This proof is based on two facts:

- A relation between the min-max levels λ_k and the spectrum of T_E which is provided by the second part of Proposition 6.
- A relation between the spectra of T_E and \tilde{A} which is provided by the next lemma, and whose proof relies on Proposition 11 and on the estimates (31) of Remark 17.

Lemma 19. *Under assumptions (H1), (H2) and (H3), let $E > \lambda_0$ and let r be a positive integer. The two following properties are equivalent:*

- (i) For all $\delta > 0$, $\text{Rank}(\mathbb{1}_{(-\delta, \delta)}(T_E)) \geq r$.
- (ii) For all $\varepsilon > 0$, $\text{Rank}(\mathbb{1}_{(E-\varepsilon, E+\varepsilon)}(\tilde{A})) \geq r$.

In other words: $0 \in \sigma_{\text{ess}}(T_E)$ if and only if $E \in \sigma_{\text{ess}}(\tilde{A})$; $0 \in \sigma_{\text{disc}}(T_E)$ if and only if $E \in \sigma_{\text{disc}}(\tilde{A})$ and when this happens they have the same multiplicity; $0 \in \rho(T_E)$ if and only if $E \in \rho(\tilde{A})$.

Proof. If (i) holds true, for each $\delta > 0$ there is a subspace \mathcal{X}_δ of $\mathbb{R}(\mathbb{1}_{(-\delta, \delta)}(T_E))$ of dimension r . Then we have $\mathcal{X}_\delta \subset \mathcal{D}(T_E) \subset \mathcal{D}(\overline{q}_E)$. Using Proposition 11 and the second estimate of (31) we find that for all $x \in \mathcal{X}_\delta$ and $Y \in \mathcal{D}(\tilde{A})$,

$$|\langle x, (\tilde{A} - E)Y \rangle| = |\overline{q}_E(x, \pi_E(Y))| = |\langle T_E x, \pi_E(Y) \rangle| \leq \delta \|x\| \|\pi_E(Y)\| \leq C_E \delta \|x\| \|Y\|_{\mathcal{D}(\tilde{A})}.$$

Assume, in addition, that the property (ii) does not hold true. This means that for some $\varepsilon_0 > 0$, $\text{Rank}(\mathbb{1}_{(E-\varepsilon_0, E+\varepsilon_0)}(\tilde{A})) \leq r - 1$. Then for each $\delta > 0$ there is x_δ in \mathcal{X}_δ such that $\|x_\delta\| = 1$ and $\mathbb{1}_{(E-\varepsilon_0, E+\varepsilon_0)}(\tilde{A})x_\delta = 0$. So there is $Y_\delta \in \mathcal{D}(\tilde{A})$ such that $(\tilde{A} - E)Y_\delta = x_\delta$ and $\|Y_\delta\| \leq \varepsilon_0^{-1}$. We thus get $\langle x_\delta, (\tilde{A} - E)Y_\delta \rangle = \|x_\delta\|^2 = 1$ and $C_E \|x_\delta\| \|Y_\delta\|_{\mathcal{D}(\tilde{A})}$ is bounded independently of δ . So, taking δ small enough we obtain $|\langle x_\delta, (\tilde{A} - E)Y_\delta \rangle| > C_E \delta \|x_\delta\| \|Y_\delta\|_{\mathcal{D}(\tilde{A})}$ and this is absurd. We have thus proved by contradiction that (i) implies (ii).

It remains to show that (ii) implies (i). If (ii) holds true, then for each $\varepsilon > 0$ there is a subspace \mathcal{Y}_ε of $\mathbb{R}(\mathbb{1}_{(E-\varepsilon, E+\varepsilon)}(\tilde{A}))$ of dimension r , and we have $\mathcal{Y}_\varepsilon \subset \mathcal{D}(\tilde{A}) \subset \mathcal{D}(T_E) \dot{+} \mathcal{D}(B)$. Using Proposition 11 we find that for all $x \in \mathcal{D}(T_E)$ and $Y \in \mathcal{Y}_\varepsilon$,

$$|\langle T_E x, \pi_E(Y) \rangle| = |\overline{q}_E(x, \pi_E(Y))| = |\langle x, (\tilde{A} - E)Y \rangle| \leq \varepsilon \|x\| \|Y\|.$$

Moreover for all $Y \in \mathcal{Y}_\varepsilon$, from the first estimate of (31) one has

$$\|\pi'_E(Y)\| \leq C_E \|\Lambda_-(\tilde{A} - E)Y\| \leq C_E \varepsilon \|Y\|.$$

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

$$|\langle T_E x, y \rangle| \leq 2\varepsilon \|x\| \|y\|.$$

Assume, in addition, that (i) does not hold true. This means that there exists $\delta_0 > 0$ such that $\text{Rank}(\mathbb{1}_{(-\delta_0, \delta_0)}(T_E)) \leq r - 1$. Then for each small ε there is y_ε in V_ε such that $\|y_\varepsilon\| = 1$ and $\mathbb{1}_{(-\delta_0, \delta_0)}(T_E)y_\varepsilon = 0$. So there is $x_\varepsilon \in \mathcal{D}(T_E)$ such that $T_E x_\varepsilon = y_\varepsilon$ and $\|x_\varepsilon\| \leq \delta_0^{-1}$. We thus get $\langle T_E x_\varepsilon, y_\varepsilon \rangle = \|y_\varepsilon\|^2 = 1$ and $\|x_\varepsilon\| \|y_\varepsilon\| \leq \delta_0^{-1}$. So, taking ε small enough we get $|\langle T_E x_\varepsilon, y_\varepsilon \rangle| > 2\varepsilon \|x_\varepsilon\| \|y_\varepsilon\|$ and this is absurd. We have thus proved by contradiction that (ii) implies (i), so the two properties are equivalent.

Now, given $E > \lambda_0$, 0 is in $\sigma_{\text{ess}}(T_E)$ if and only if (i) holds true for every r , and this is equivalent to saying that (ii) holds true for every r , which exactly means that $E \in \sigma_{\text{ess}}(\tilde{A})$. Similarly, we can say that 0 is in $\sigma_{\text{disc}}(T_E)$ and has multiplicity μ_E as an eigenvalue if and only if (i) holds true for μ_E but not for $\mu_E - 1$, and this is equivalent to saying that (ii) holds true for μ_E but not for $\mu_E - 1$, which exactly means that $E \in \sigma_{\text{disc}}(\tilde{A})$ with multiplicity μ_E . The last statement on $\rho(\tilde{A})$ follows immediately, since for any operator L , $\sigma_{\text{ess}}(L)$, $\sigma_{\text{disc}}(L)$ and $\rho(L)$ form a partition of \mathbb{C} . This ends the proof of the lemma. \square

Proof of Proposition 18. Let us define

$$\underline{\lambda} := \inf(\sigma_{\text{ess}}(\tilde{A}) \cap (\lambda_0, \infty)) \in [\lambda_0, \infty].$$

By Proposition 6, if $E \in (\lambda_0, \lambda_\infty)$ then 0 is either an element of $\rho(T_E)$ or an eigenvalue of T_E of finite multiplicity μ_E . The second case occurs when $E = \lambda_k$ for some positive integer k . Then $\mu_E = \text{card}\{k' : \lambda_{k'} = \lambda_k\}$. So, by Lemma 19, $(\lambda_0, \lambda_\infty) \cap \sigma_{\text{ess}}(\tilde{A})$ is empty hence $\lambda_\infty \leq \underline{\lambda}$, and the levels λ_k in $(\lambda_0, \lambda_\infty)$ are all the eigenvalues of \tilde{A} in this open interval, counted with multiplicity.

It remains to prove that $\underline{\lambda} \leq \lambda_\infty$. The nontrivial case is when the sequence (λ_k) is bounded, so that $\lambda_\infty \in (\lambda_0, \infty)$. If the sequence is nonstationary and bounded, then $\{\lambda_k : k \geq k_0\}$ is an infinite subset of $\sigma_{\text{disc}}(\tilde{A})$, so its limit point λ_∞ is in $\sigma_{\text{ess}}(\tilde{A})$. If the sequence is stationary, let k be such that $\lambda_k = \lambda_\infty$. Then, by Proposition 6, $0 \in \sigma_{\text{ess}}(T_{\lambda_\infty})$ so, by Lemma 19, we find once again that $\lambda_\infty \in \sigma_{\text{ess}}(\tilde{A})$. In conclusion, one always has $\underline{\lambda} \leq \lambda_\infty$ and this ends the proof of Proposition 18. \square

Proof of Theorem 1. Propositions 12, 15 and 18 together imply Theorem 1. \square

6. APPLICATIONS TO DIRAC-COULOMB OPERATORS

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

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

and start by the case of a point-like nucleus corresponding to the potential $V(x) = -v/|x|$. As domain of A , take $F = C_c^\infty(\mathbb{R}^3 \setminus \{0\}, \mathbb{C}^4)$. Consider Talman's splitting $\Lambda_+(\psi) = (\phi, 0)$, $\Lambda_-(\psi) = (0, \chi)$ of four-spinors $\psi = (\phi, \chi)$ into upper and lower two-spinors. Assumptions (H1)-(H2) are easily checked with $\lambda_0 = -1$. One can check Assumption (H3) with $k_0 = 1$ by the method mentioned in Remark 4: from a Hardy-type inequality proved in [3, 2] one finds that $\ell_1(0) \geq 0$, and one concludes using the second point in Proposition 3. So, using Theorem 1 with $k_0 = 1$ we can define a distinguished self-adjoint extension of A for $0 < v \leq 1$ 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 [3, 10, 8, 23], and it is known 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

$$V(x) = -\frac{v_1}{|x|} + \frac{v_2}{|x - x_0|} \quad \text{with } x_0 \neq 0, \quad 0 < v_1 \leq 1 \quad \text{with } \frac{3}{4} < v_2 \leq \frac{\pi}{2} + \frac{2}{\pi}.$$

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

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

and as domain F we take the Schwartz class $\mathcal{S}(\mathbb{R}^3, \mathbb{C}^4)$. In the Fourier domain, Λ_\pm becomes the multiplication operator by the matrix

$$M_\pm(p) = \frac{1}{2} \left(I_4 \pm \frac{\alpha \cdot p + \beta}{\sqrt{|p|^2 + 1}} \right).$$

This matrix depends smoothly on p and is bounded on \mathbb{R}^3 as well as all its derivatives. As a consequence, the multiplication by M_\pm preserves the Schwartz class, so (H1) is

satisfied. By the upper bound on ν_2 , it follows from an inequality of Tix [28] that the Brown-Ravenhall operator $-\Lambda_-(A+1-\nu_2) \upharpoonright_{F_-}$ is non-negative, so (H2) holds true with $\lambda_0 = -1 + \nu_2$. On the other hand, since $\nu_1 \leq 1$, [3, inequality (38)] implies that $\lambda_1 \geq 0$, so (H3) with $k_0 = 1$ holds true as well and thus, Theorem 1 can be applied with $k_0 = 1$. But as shown in [27, Corollary 3], $-\Lambda_- A \upharpoonright_{F_-}$ is not essentially self-adjoint, since $\nu_2 > 3/4$. So one cannot use the abstract result of [23].

Interesting cases of application of Theorem 1 with $k_0 \geq 2$ are Dirac operators perturbed by an attractive electrostatic potential $V(x) = -\sum_{i=1}^K \frac{\nu_i}{|x-x_i|}$ generated by K nuclei, each having at most Z_i protons with $Z_i < Z_* \approx 137.04$ so that $\nu_i = Z_i/Z_* < 1$ (we suppose that $K \geq 2$ and $x_i \neq x_j, \forall i \neq j$). One can define such operators on the minimal domain $F = C_c^\infty(\mathbb{R}^3 \setminus \{x_1, \dots, x_K\}, \mathbb{C}^4)$. Their distinguished self-adjoint extension was constructed in [21, 14] by a method completely different from the one considered in the present work. Talman's min-max principle for the eigenvalues of the extension was studied in [9]. But that paper appealed to the abstract result of [6] and as mentioned in the Introduction, the arguments in [6] suffered from the same closability issue as [3]. Theorem 1 solves this issue, moreover it provides a unified treatment: construction of the extension and justification of the min-max principle, provided Assumptions (H1)-(H2)-(H3) have been checked for Talman's splitting. Assumptions (H1)-(H2) obviously hold true with $\lambda_0 = -1$, as in the one-center case. But checking (H3) is more delicate. The difficulty is that k_0 may be larger than 1. Indeed, when the total number of protons $\sum_i Z_i$ is larger than 137.04, if the nuclei are close to each other one expects some eigenvalues of the distinguished extension to *dive* into the negative continuum. If this happens, the corresponding min-max levels λ_k should become equal to λ_0 . To check Assumption (H3) in such a situation, by Proposition 3 it is sufficient to prove that there exists a positive integer k_0 (depending on the nuclear configuration) such that $\ell_{k_0}(0) \geq 0$. One can argue by contradiction: otherwise, there would be a sequence $(V_k)_{k \geq 1}$ of k -dimensional subspaces of F_+ such that $q_0(\psi) < 0$ for all $\psi \in (V_k \oplus F_-) \setminus \{0\}$. Then one could build a sequence (ϕ_k) in $C_c^\infty(\mathbb{R}^3 \setminus \{x_1, \dots, x_K\}, \mathbb{C}^2)$ such that $(\phi_k, 0) \in V_k$ and $\langle \phi_k, \phi_l \rangle_{L^2(\mathbb{R}^3, \mathbb{C}^2)} = \delta_{kl}$. But the sequence of unit vectors ϕ_k would converge weakly to 0 in L^2 and this would imply the absurd conclusion that $q_0(\phi_k, 0) \geq 0$ for k large enough, as shown in [9, Section 6, Step 4, p. 1448-1449]. So the assumptions of Theorem 1 are satisfied, with k_0 possibly larger than 1.

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REFERENCES

- [1] S. N. DATTA AND G. DEVAIAH, *The minimax technique in relativistic Hartree-Fock calculations*, *Pramana*, 30 (1988), pp. 387–405.
- [2] J. DOLBEAULT, M. J. ESTEBAN, M. LOSS, AND L. VEGA, *An analytical proof of Hardy-like inequalities related to the Dirac operator*, *J. Funct. Anal.*, 216 (2004), pp. 1–21.
- [3] J. DOLBEAULT, M. J. ESTEBAN, AND E. SÉRÉ, *On the eigenvalues of operators with gaps. Application to Dirac operators*, *J. Funct. Anal.*, 174 (2000), pp. 208–226. *Corrigendum*: *J. Funct. Anal.*, 284 (2023), 109651.
- [4] ———, *Variational characterization for eigenvalues of Dirac operators*, *Calc. Var. Partial Differential Equations*, 10 (2000), pp. 321–347.
- [5] ———, *A variational method for relativistic computations in atomic and molecular physics*, *Int. J. Quantum Chem.*, 93 (2003), pp. 149–155.
- [6] ———, *General results on the eigenvalues of operators with gaps, arising from both ends of the gaps. Application to Dirac operators*, *J. Eur. Math. Soc. (JEMS)*, 8 (2006), pp. 243–251.
- [7] J. DOLBEAULT, M. J. ESTEBAN, E. SÉRÉ, AND M. VANBREUGEL, *Minimization methods for the one-particle dirac equation*, *Phys. Rev. Lett.*, 85 (2000), pp. 4020–4023.
- [8] M. J. ESTEBAN, M. LEWIN, AND E. SÉRÉ, *Domains for Dirac-Coulomb min-max levels*, *Rev. Mat. Iberoam.*, 35 (2019), pp. 877–924.
- [9] M. J. ESTEBAN, M. LEWIN, AND E. SÉRÉ, *Dirac-Coulomb operators with general charge distribution I. Distinguished extension and min-max formulas*, *Annales Henri Lebesgue*, 4 (2021), pp. 1421–1456.
- [10] M. J. ESTEBAN AND M. LOSS, *Self-adjointness for Dirac operators via Hardy-Dirac inequalities*, *J. Math. Phys.*, 48 (2007), pp. 112107, 8.
- [11] ———, *Self-adjointness via partial Hardy-like inequalities*, in *Mathematical results in quantum mechanics*, World Sci. Publ., Hackensack, NJ, 2008, pp. 41–47.
- [12] M. GRIESEMER, R. T. LEWIS, AND H. SIEDENTOP, *A minimax principle for eigenvalues in spectral gaps: Dirac operators with coulomb potentials.*, *Doc. Math.*, 4 (1999), pp. 275–283.
- [13] M. GRIESEMER AND H. SIEDENTOP, *A minimax principle for the eigenvalues in spectral gaps*, *J. London Math. Soc. (2)*, 60 (1999), pp. 490–500.
- [14] M. KLAUS, *Dirac operators with several Coulomb singularities*, *Helv. Phys. Acta*, 53 (1980), pp. 463–482 (1981).
- [15] M. KLAUS AND R. WÜST, *Characterization and uniqueness of distinguished selfadjoint extensions of Dirac operators*, *Commun. Math. Phys.*, 64 (1978/79), pp. 171–176.
- [16] M. KRAUS, M. LANGER, AND C. TRETTER, *Variational principles and eigenvalue estimates for unbounded block operator matrices and applications*, *J. Comput. Appl. Math.*, 171 (2004), pp. 311–334.
- [17] M. LEWIN AND E. SÉRÉ, *Spectral pollution and how to avoid it (with applications to Dirac and periodic Schrödinger operators)*, *Proc. London Math. Soc.*, 100 (2010), pp. 864–900.
- [18] S. MOROZOV AND D. MÜLLER, *On the minimax principle for Coulomb-Dirac operators*, *Mathematische Zeitschrift*, 280 (2015), pp. 733–747.
- [19] D. MÜLLER, *Minimax principles, Hardy-Dirac inequalities, and operator cores for two and three dimensional Coulomb-Dirac operators*, *Doc. Math.*, 21 (2016), pp. 1151–1169.
- [20] G. NENCIU, *Self-adjointness and invariance of the essential spectrum for Dirac operators defined as quadratic forms*, *Commun. Math. Phys.*, 48 (1976), pp. 235–247.
- [21] ———, *Distinguished self-adjoint extension for Dirac operator with potential dominated by multicenter Coulomb potentials*, *Helv. Phys. Acta*, 50 (1977), pp. 1–3.
- [22] M. REED AND B. SIMON, *Methods of modern mathematical physics. II. Fourier analysis, self-adjointness*, Academic Press [Harcourt Brace Jovanovich, Publishers], New York-London, 1975.
- [23] L. SCHIMMER, J. P. SOLOVEJ, AND S. TOKUS, *Friedrichs extension and min-max principle for operators with a gap*, *Ann. Henri Poincaré*, 21 (2020), pp. 327–357.
- [24] U.-W. SCHMINCKE, *Distinguished selfadjoint extensions of Dirac operators*, *Math. Z.*, 129 (1972), pp. 335–349.

- [25] J. D. TALMAN, *Minimax principle for the Dirac equation*, Phys. Rev. Lett., 57 (1986), pp. 1091–1094.
- [26] B. THALLER, *The Dirac equation*, Springer-Verlag, Berlin, 1992.
- [27] C. TIX, *Self-adjointness and spectral properties of a pseudo-relativistic Hamiltonian due to Brown and Ravenhall*, Preprint, mp-arc 97–441, url: https://web.ma.utexas.edu/mp_arc-bin/mpa?yn=97-441, (1997).
- [28] C. TIX, *Strict positivity of a relativistic Hamiltonian due to Brown and Ravenhall*, Bull. London Math. Soc., 30 (1998), pp. 283–290.
- [29] C. TRETTER, *Spectral theory of block operator matrices and applications*, World Scientific, 2008.
- [30] R. WÜST, *A convergence theorem for selfadjoint operators applicable to Dirac operators with cutoff potentials*, Math. Z., 131 (1973), pp. 339–349.
- [31] ———, *Distinguished self-adjoint extensions of Dirac operators constructed by means of cut-off potentials*, Math. Z., 141 (1975), pp. 93–98.
- [32] ———, *Dirac operations with strongly singular potentials. Distinguished self-adjoint extensions constructed with a spectral gap theorem and cut-off potentials*, Math. Z., 152 (1977), pp. 259–271.

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