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► **To cite this version:**

Jean Dolbeault, Maria J Esteban, Eric Séré. Distinguished self-adjoint extension and eigenvalues of operators with gaps. Application to Dirac-Coulomb operators. 2023. hal-03702964v2

HAL Id: hal-03702964

<https://hal.science/hal-03702964v2>

Preprint submitted on 2 Feb 2023 (v2), last revised 3 Aug 2023 (v4)

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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

2020 *Mathematics Subject Classification*. Primary: 47B25. Secondary: 47A75, 49R50, 81Q10.

Key words and phrases. variational methods; self-adjoint operators; symmetric operators; quadratic forms; spectral gaps; eigenvalues; min-max principle; Rayleigh-Ritz quotients; Dirac operators.

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 $\overline{\varphi}_E(L_{E'}x_+) \leq q_E(x_+ + L_E x_+)$ and $\overline{\varphi}_{E'}(L_E x_+) \leq q_{E'}(x_+ + L_{E'}x_+)$, 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

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

holds true for all $y_- \in \overline{\mathcal{D}(\overline{b})}$. 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 $V(x) = -\nu/|x|$. 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 $0 < \nu \leq 1$ 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 [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

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

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.

Acknowledgment: The authors wish to thank the referees for their very careful reading of the manuscript, and for many comments and suggestions that greatly improved the quality of this paper.

J.D. has been partially supported by the Project EFI (ANR-17-CE40-0030) and M.J.E. and E.S. by the project molQED (ANR-17-CE29-0004) of the French National Research Agency (ANR).

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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