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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 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

In three space dimensions, the *free Dirac operator* is of the form  $D = -i \alpha \cdot \nabla + \beta$  with

$$\beta = \begin{pmatrix} I_2 & 0 \\ 0 & -I_2 \end{pmatrix}, \quad \alpha_k = \begin{pmatrix} 0 & \sigma_k \\ \sigma_k & 0 \end{pmatrix} \quad (k = 1, 2, 3),$$

$\sigma_1, \sigma_2, \sigma_3$  being the Pauli matrices (see [30]). The *Dirac-Coulomb operator* is  $D_V = D + V$  where  $V$  is the Coulomb potential  $-\frac{\nu}{|x|}$  ( $\nu > 0$ ) or, more generally, the convolution of  $-\frac{1}{|x|}$  with an extended charge density. Usually, one first defines  $D_{-\nu/|x|}$  on the so-called minimal domain  $C_c^\infty(\mathbb{R}^3 \setminus \{0\}, \mathbb{C}^4)$ . The resulting minimal operator is symmetric but not closed in the Hilbert space  $L^2(\mathbb{R}^3, \mathbb{C}^4)$ . It is essentially self-adjoint when  $\nu$  lies in the interval  $(0, \sqrt{3}/2]$ . In other words, its closure is self-adjoint and there is no other self-adjoint extension. For larger constants  $\nu$  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 Dirac-Coulomb operators were made in the 1970's, see, e.g., [27, 34, 35, 36, 23, 24, 18, 17]. In these papers, general classes of potentials  $V$  are considered, but in the case  $V = -\nu/|x|$  one always assumes that  $\nu$  is smaller than 1.

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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 [29] and Datta-Devaiah [2] proposed a min-max principle involving Rayleigh quotients and the decomposition of four-spinors into their so-called large and small two-components. A related min-max principle based on another decomposition using the free-energy projectors  $\mathbb{1}_{\mathbb{R}_{\pm}}(D)$  was proposed in [14] and justified rigorously in [5] for  $\nu \in (0, \frac{2}{\pi/2+2/\pi})$ . An abstract version of these min-max principles 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

$$\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_-. \quad (1.1)$$

Such an abstract principle was proved for the first time in [16], but its hypotheses were rather restrictive and the application to the distinguished self-adjoint realization of  $D_V$  only gave Talman's principle for bounded electric potentials (see also [19, 33] for related abstract principles). In [15], an improved abstract min-max principle was applied to  $D_V$  with the splitting given by the free-energy projectors, for the unbounded potential  $-\nu/|x|$  with  $\nu \in (0, 0.305]$ . In [4], thanks to a different abstract approach, the range of essential self-adjointness  $\nu \in (0, \sqrt{3}/2]$  was dealt with, both for Talman's splitting and the free projectors. The articles [21, 22, 10, 26, 11] followed and the full range  $\nu \in (0, 1]$  is now covered.

Using some of the tools of [4], Esteban and Loss [12, 13] proposed a new strategy to build a distinguished, Friedrichs-like, self-adjoint extension of an abstract *symmetric* operator with variational gap and applied it to the minimal Dirac-Coulomb operator, with  $\nu \in (0, 1]$ . In [10, 11], connections were established between this new approach and the earlier constructions for Dirac-Coulomb operators.

Important closability issues had been overlooked in some arguments of [4] and some domain invariance questions had not been addressed properly in [12, 13] (see the beginning of Subsection 3.2). In [26] these issues are clarified and the self-adjoint extension problem considered in [12, 13] is connected to the min-max principle for the eigenvalues of self-adjoint operators studied in [4]. The abstract results in [26] 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 the corrigendum [8], we present another way of correcting the arguments of [4] 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 [26]. 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  $q$ ,  $\mathcal{D}(L)$  for the domain of a linear operator  $L$  and  $\mathcal{R}(L)$  for its range. The space  $\mathcal{D}(L)$  is endowed with the norm

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

We denote the resolvent set, spectrum, essential spectrum and discrete spectrum of a self-adjoint operator  $T$  by  $\rho(T)$ ,  $\sigma(T)$ ,  $\sigma_{\text{ess}}(T)$  and  $\sigma_{\text{disc}}(T)$  respectively.

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 can be constructed as follows (see *e.g.* [25] 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  $\mathcal{J}_f(u) := \frac{1}{2} (\bar{s}(u) - \ell \|u\|^2) - \langle u, f \rangle$  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  $\ell$ : 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  $\Omega$  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  $\Omega$ ,  $u = 0$  on  $\partial\Omega$ . In other words,  $u_f$  is the unique function in  $H_0^1(\Omega)$  such that for all  $v \in H_0^1(\Omega)$ ,  $\int_\Omega \nabla u_f \cdot \nabla v \, dx = \int_\Omega f v \, dx$ . So  $T$  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 (1.1). We denote by

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

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

$$F_+ := \Lambda_+ F \text{ and } F_- := \Lambda_- F \text{ are subspaces of } F \quad (\text{H1})$$

and

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

We also make the *variational gap assumption* that

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

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

$$\lambda_k := \inf_{\substack{V \text{ subspace of } F_+ \\ \dim V = k}} \sup_{x \in (V \oplus F_-) \setminus \{0\}} \frac{a(x)}{\|x\|^2}. \quad (1.2)$$

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  $F_-$ :

$$b(x_-) = -a(x_-) = \langle x_-, (-\Lambda_- A \upharpoonright_{F_-}) x_- \rangle \quad \forall x_- \in F_-. \quad (1.3)$$

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

$$b_E(x_-) = b(x_-) + E\|x_-\|^2 \quad \forall x_- \in F_-. \quad (1.4)$$

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

$$L_E x_+ := (B + E)^{-1} \Lambda_- A x_+, \quad \forall x_+ \in F_+. \quad (1.5)$$

We then introduce the subspace

$$\Gamma_E := \{x_+ + L_E x_+ : x_+ \in F_+\} \subset F_+ \oplus \mathcal{D}(B). \quad (1.6)$$

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

$$q_E(x_+ + L_E x_+) := \langle x_+, (A - E)x_+ \rangle + \langle L_E x_+, (B + E)L_E x_+ \rangle. \quad (1.7)$$

Denoting by  $\bar{\Gamma}_E$  the closure of  $\Gamma_E$  in  $\mathcal{H}$  and by  $\Pi_E$  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

$$S_E := \Pi_E(\Lambda_+(A - E)\Lambda_+ + \Lambda_-(B + E)\Lambda_-) \upharpoonright_{\Gamma_E}. \quad (1.8)$$

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 [4] (before its corrigendum [8]) as well as in [12, 13, 26], the form  $\bar{b}$  was already present and a form analogous to  $q_E$  was defined, but its domain was  $F_+$  instead of  $\Gamma_E$ .

The main result of this paper is as follows.

**Theorem 1.** *Let  $A$  be a densely defined symmetric operator on the Hilbert space  $\mathcal{H}$  with domain  $F$ . 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  $\lambda_k$  ( $k \geq 1$ ) 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 some situations, one encounters a symmetric operator  $A$  that does not satisfy (H1) but has the weaker property  $\Lambda_\pm \mathcal{D}(A) \subset \mathcal{D}(\bar{A})$ , where  $\bar{A}$  denotes the closure of  $A$ . This happens for instance if one defines a Dirac-Coulomb operator on a “minimal” domain consisting of compactly supported smooth functions, and one considers the splitting associated with the free energy projectors  $\Lambda_\pm = \mathbb{1}_{\mathbb{R}_\pm}(D)$ : see the example of Subsection 6.2. In such a case one can replace  $A$  by its symmetric extension  $\bar{A} \upharpoonright_{\Lambda_+ \mathcal{D}(A) \oplus \Lambda_- \mathcal{D}(A)}$ . Then (H1) is automatically satisfied by the new domain and it remains to check that the new operator satisfies (H2)-(H3) before applying Theorem 1.

- In the earlier works [16, 15, 4, 5, 6, 21, 22, 10, 26] on the min-max principle in gaps, one assumes that  $\lambda_1 > \lambda_0$ , 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 [7], but in that paper (H2) was replaced by a much more restrictive assumption. Moreover, the proof in [7] was based on the arguments of [4], so it suffered from the same closability issue solved in [26] and the corrigendum [8] of [4]: the closure of  $L_E$  was used but its existence was not proved.

- Compared with [13, 26], 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 [26] 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 [26], 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 self-adjointness of  $-\Lambda_- A \upharpoonright_{F_-}$  does not hold true is described in Subsection 6.2. Let us give a simpler example: on the domain  $F := (C_c^\infty(\Omega, \mathbb{R}))^2$  consider the operator

$$A \begin{pmatrix} u \\ v \end{pmatrix} := \begin{pmatrix} -\Delta u \\ \Delta v \end{pmatrix} \quad (1.9)$$

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

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

and (H1) holds true. If  $\lambda(\Omega) > 0$  is the smallest eigenvalue of the Dirichlet Laplacian on  $\Omega$ , 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 [13, 26]. In this example, the distinguished extension given by Theorem 1 is easily obtained as follows. One checks that  $\mathcal{D}(\bar{b}) = \{0\} \times H_0^1(\Omega, \mathbb{R})$ ,  $\mathcal{D}(\bar{q}_E) = H_0^1(\Omega, \mathbb{R}) \times \{0\}$  and  $\mathcal{D}(A^*) = (H^2(\Omega, \mathbb{R}))^2$ . So, denoting by  $\Delta^{(D)}$  the Dirichlet Laplacian with domain  $H^2(\Omega, \mathbb{R}) \cap H_0^1(\Omega, \mathbb{R})$ , one finds that

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

- In [26], 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 (1.9) 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  $\Delta$  associated with the Neumann boundary condition  $\nabla \nu \cdot n = 0$ , where  $n$  denotes the outward normal unit vector on  $\partial\Omega$ . Obviously,  $\hat{A} \neq \tilde{A}$ .

• As we will see in Subsection 6.1, when dealing with the Dirac-Coulomb operator  $D_{-\nu/|x|}$  with Talman's splitting it is natural to choose  $F = C_c^\infty(\mathbb{R}^3 \setminus \{0\}, \mathbb{C}^4)$ . Then the large and small two-components appearing in Talman's min-max principle are taken in  $C_c^\infty(\mathbb{R}^3 \setminus \{0\}, \mathbb{C}^2)$ . But other functional spaces can be used for these components. In [21, 22] an abstract min-max principle is stated in the setting of quadratic forms and applied to Talman's min-max principle with  $H^{1/2}(\mathbb{R}^3, \mathbb{C}^2)$  as space of large and small two-components, under the condition  $\nu \in (0, 1)$ . However it seems that some closability issues are present in the proof of the abstract principle, as in [4]. We do not know whether the geometric approach of the present paper could be adapted to the framework of [21] in order to avoid these closability issues without additional assumptions. Note that by a completely different approach, Talman's min-max principle is proved in [10] for all  $\nu \in (0, 1]$ , with arbitrary spaces of large and small two-components lying between  $C_c^\infty(\mathbb{R}^3 \setminus \{0\}, \mathbb{C}^2)$  and  $H^{1/2}(\mathbb{R}^3, \mathbb{C}^2)$ .

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  $\mathcal{D}(A^*) \cap \left( \mathcal{D}(\bar{q}_E) + \mathcal{D}(\bar{b}) \right)$ . 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  $\bar{b}_E$ , for  $X \in \mathcal{D}(\tilde{A})$  and  $U \in \mathcal{D}(\bar{q}_E) + \mathcal{D}(\bar{b})$ . This formula 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  $\lambda_0$ .

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 [4, 13, 26], 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  $\lambda_k$  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  $\varphi_{E, x_+}$  has a unique continuous extension to  $\mathcal{D}(\bar{b})$  which is the strictly concave function

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

The main result of this subsection is

**Proposition 2.** *Let  $A$  be a symmetric operator on the Hilbert space  $\mathcal{H}$ . Assume hypotheses (H1)-(H2), take  $E > \lambda_0$  and remember the definition (1.7) of  $q_E$ . Then:*

- One has the decomposition

$$\langle X, (A - E)X \rangle = q_E(\Lambda_+ X + L_E \Lambda_+ X) - \bar{b}_E(\Lambda_- X - L_E \Lambda_+ X), \quad \forall X \in F. \quad (2.1)$$

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

$$q_E(x_+ + L_E x_+) = \bar{\varphi}_{E, x_+}(L_E x_+) = \max_{y_- \in F_-} \bar{\varphi}_{E, x_+}(y_-) = \sup_{y_- \in F_-} \varphi_{E, x_+}(y_-). \quad (2.2)$$

*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

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

which proves (2.1). 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 (2.2) 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

$$\ell_k(E) := \inf_{\substack{V \text{ subspace of } \Gamma_E \\ \dim V = k}} \sup_{x \in V \setminus \{0\}} \frac{q_E(x)}{\|x\|^2} \in [-\infty, +\infty). \quad (2.3)$$

We may also define the (possibly infinite) multiplicity numbers

$$m_k(E) := \operatorname{card}\{k' \geq 1 : \ell_{k'}(E) = \ell_k(E)\} \geq 1. \quad (2.4)$$

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

$$\|x_+ + L_{E'} x_+\| \leq \|x_+ + L_E x_+\| \leq \frac{E' - \lambda_0}{E - \lambda_0} \|x_+ + L_{E'} x_+\| \quad (2.5)$$

and

$$(E' - E) \|x_+ + L_{E'} x_+\|^2 \leq q_E(x_+ + L_E x_+) - q_{E'}(x_+ + L_{E'} x_+) \leq (E' - E) \|x_+ + L_E x_+\|^2. \quad (2.6)$$

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

$$\ell_k(\lambda) \leq \lambda_k - \lambda. \quad (2.7)$$

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

$$\ell_k(\lambda) \geq (\lambda_k - \lambda) \left( \frac{\lambda - \lambda_0}{\lambda_k - \lambda_0} \right)^2. \quad (2.8)$$

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.* Both formula (2.5) and (2.6) as well as their detailed proof can be found in [4, Lemma 2.1] and [26, Lemma 2.4], so here we just give the main arguments. In order to prove (2.5) 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 (2.6), 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 (2.2).

We now prove (2.7) and (2.8).

By definition of  $\lambda_k$ , for each  $\varepsilon > 0$  there is a  $k$ -dimensional subspace  $V_\varepsilon$  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  $y_- \in \mathcal{D}(\overline{b})$ . Choosing  $y_- = L_E x_+$  and using (2.2), 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  $\varepsilon$  is arbitrary and  $\dim(W_\varepsilon) = k$ , we conclude that (2.7) holds true.

On the other hand, using once again the definition of  $\lambda_k$ , we find that for each  $\varepsilon > 0$  and each  $k$ -dimensional subspace  $W$  of  $\Gamma_{\lambda_k}$ , there is a nonzero vector  $x_\varepsilon$  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 (2.2),  $q_{\lambda_k - \varepsilon}(x_\varepsilon + L_{\lambda_k - \varepsilon} x_\varepsilon) \geq 0$ . Then, using (2.5), (2.6) 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  $\varepsilon$  are arbitrary, we thus have  $\ell_k(\lambda_k) \geq 0$ . Combining this with (2.7), 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  $\Gamma_\lambda$ . 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  $q_{\lambda_k}$  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 (2.5), (2.6)

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 (2.8) holds true.

The last statements of Proposition 3 - finiteness and sign of  $\ell_k(\lambda)$ , the fact that  $\lambda_k$  is the unique zero of  $\ell_k$  - are an immediate consequence of (2.7) and (2.8). Note that this characterization of  $\lambda_k$  as unique solution of a nonlinear equation was already stated and proved in [4, Lemma 2.2 (c)] and [26, 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  $\lambda_{k_0} \geq E_0$ . In Section 6 we will apply this method to one-center and multi-center Dirac-Coulomb operators.

**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 [20]). 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 [9, 6]. The idea was to calculate each eigenvalue  $\lambda_k$  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 (2.7) and (2.8) 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  $\lambda_0$  and  $\lambda_k$ , one can compute a sequence of approximations by the formula  $E^{(j+1)} = E^{(j)} + \ell_k(E^{(j)})$ . From (2.7), 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  $\lambda_k$ . Moreover, combining the inequalities (2.7) and (2.8) one finds that for  $|h|$  small,  $h + \ell_k(\lambda_k + h) = \mathcal{O}(h^2)$ . So  $E^{(j)}$  converges quadratically to  $\lambda_k$ . It would be interesting to perform numerical tests of this algorithm in practical situations.

### 3. THE CLOSURE $\overline{q}_E$ 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  $\lambda_k$ . Finally, we construct a natural isomorphism between the domains of  $\overline{q}_E$  and  $\overline{q}_{E'}$  for all  $E, E' > \lambda_0$ .

**3.1. Construction of  $\overline{q}_E$  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  $\overline{\Gamma}_E$  and  $S_E$  has a Friedrichs extension  $T_E$ .

• If  $E \in (\lambda_0, \lambda_\infty) \setminus \{\lambda_k : k \geq k_0\}$  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  $T_{\lambda_k}$  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)-(H3), for every  $E > \lambda_0$ , there is  $\kappa_E > 0$  such that  $q_E + \kappa_E \|\cdot\|^2 \geq \|\cdot\|^2$  on  $\Gamma_E$ .*

*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 (2.5) and (2.6), 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  $\kappa_E$  is less explicit. As in the case  $k_0 = 1$ , we just have to find a constant  $\kappa_E$  for *some*  $E > \lambda_0$ ; then the inequalities (2.5) and (2.6) 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  $\Gamma_E$  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  $\Gamma_E$  and we look for a lower bound on  $q_E(x)$ . We distinguish two cases.

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

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

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 (1.8). 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 we have the following cases:

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 (2.4). 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 [4] (before its corrigendum [8]), [12, 13] and [26],  $q_E$  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 [4] and this was a serious gap. Moreover the proof of the domain invariance was based on an incorrect estimate in [12, Proposition 2] and was incomplete in [13], but this domain invariance problem is easily fixed using the inequalities (10)-(11) of [4] which are called (2.5)-(2.6) in the present work.

In our situation, since we do not know whether  $L_E$  is closable or not, it is essential to define  $q_E$  on  $\Gamma_E$  and 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)-(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

$$\bar{i}_{E,E'}(x) = x + (E - E')(B + E')^{-1} \Lambda_- x, \quad \forall x \in \bar{\Gamma}_E. \quad (3.1)$$

*Proof.* The linear map  $i_{E,E'}$  is obviously a bijection between  $\Gamma_E$  and  $\Gamma_{E'}$ , of inverse  $i_{E',E}$ . The estimates (2.5), (2.6) of Proposition 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  $\Lambda_-$  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 conditions (H1)-(H2)-(H3) hold true. Let  $E, E' > \lambda_0$ . Then*

$$\mathcal{D}(\bar{q}_{E'}) + \mathcal{D}(\bar{b}) = \mathcal{D}(\bar{q}_E) + \mathcal{D}(\bar{b}). \quad (3.2)$$

*Proof.* From formula (3.1), 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 (3.2) 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 conditions (H1)-(H2)-(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*

$$\langle (A^* - E)X, U \rangle = \bar{q}_E(x, u) - \bar{b}_E(z_-, v_-) \quad (4.1)$$

for every  $E > \lambda_0$ .

*Proof.* Formula (2.1) of Proposition 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

$$\langle x + z_-, (A - E)U \rangle = \langle x, S_E u \rangle - \langle z_-, (B + E)v_- \rangle. \quad (4.2)$$

In order to prove Proposition 11, we have to generalize (4.2) 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 (4.2) holds true and reduces to

$$\langle z_-, (A - E)U \rangle = -\langle z_-, (B + E)v_- \rangle. \quad (4.3)$$

Both sides of (4.3) are continuous in  $z_-$  for the norm  $\|\cdot\|$ , and we recall that  $F_-$  is dense in  $\mathcal{H}_-$ . So (4.3) remains true for all  $z_- \in \mathcal{H}_-$ .

Now, in the special case  $X = x_+ \in F_+$ ,  $x = x_+ + L_E x_+$  and  $z_- = -L_E x_+$ , the identity (4.2) becomes

$$\langle x_+, (A - E)U \rangle = \langle x, S_E u \rangle + \langle L_E x_+, (B + E)v_- \rangle.$$

We may also apply (4.3) to  $z_- = -L_E x_+$  and we get

$$-\langle L_E x_+, (A - E)U \rangle = \langle L_E x_+, (B + E)v_- \rangle.$$

Subtracting these two identities, we find

$$\langle x, (A - E)U \rangle = \langle x, S_E u \rangle, \quad \forall x \in \Gamma_E. \quad (4.4)$$

Both sides of (4.4) are continuous in  $x$  for the norm  $\|\cdot\|$ , so (4.4) remains true for all  $x \in \bar{\Gamma}_E$ .

Then, for  $x \in \bar{\Gamma}_E$  and  $z_- \in \mathcal{H}_-$ , we may add (4.3) and (4.4). We conclude that (4.2) remains valid for all  $x \in \bar{\Gamma}_E$  and  $z_- \in \mathcal{H}_-$ . When  $x \in \mathcal{D}(\bar{q}_E)$  and  $z_- \in \mathcal{D}(\bar{b})$ , this identity may be rewritten in the form

$$\langle x + z_-, (A - E)U \rangle = \bar{q}_E(x, u) - \bar{b}_E(z_-, v_-). \quad (4.5)$$

In particular, when  $X = x + z_- \in \mathcal{D}(A^*)$  with  $x \in \mathcal{D}(\bar{q}_E)$  and  $z_- \in \mathcal{D}(\bar{b})$ , one obtains the equality

$$\langle (A^* - E)X, U \rangle = \bar{q}_E(x, u) - \bar{b}_E(z_-, v_-). \quad (4.6)$$

This formula is the same as (4.1) 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 (4.6) holds true and reduces to

$$\langle (A^* - E)X, v_- \rangle = -\bar{b}_E(z_-, v_-). \quad (4.7)$$

Both sides of (4.7) 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 (4.7) remains true for all  $v_- \in \mathcal{D}(\bar{b})$ .

Now, in the special case  $U = u_+ \in F_+$ ,  $u = u_+ + L_E u_+$  and  $v_- = -L_E u_+$ , the identity (4.6) becomes

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

We may also apply (4.7) to  $v_- = -L_E u_+ \in \mathcal{D}(B) \subset \mathcal{D}(\bar{b})$  and we get

$$-\langle (A^* - E)X, L_E u_+ \rangle = \bar{b}_E(z_-, L_E u_+).$$

Subtracting these two identities, we find

$$\langle (A^* - E)X, u \rangle = \bar{q}_E(x, u), \quad \forall u \in \Gamma_E. \quad (4.8)$$

Both sides of (4.8) are continuous in  $u$  for the norm  $\|\cdot\|_{\mathcal{D}(\bar{q}_E)}$ , and we recall that  $\Gamma_E$  is dense in  $\mathcal{D}(\bar{q}_E)$  for this norm. So (4.8) 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 (4.7) and (4.8) and we finally get (4.1) in the general case.  $\square$

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

**Proposition 12.** *Under conditions (H1) (H2)-(H3), given  $E > \lambda_0$  the operator  $A$  admits a unique self-adjoint extension  $\tilde{A}$  such that  $\mathcal{D}(\tilde{A}) \subset \mathcal{D}(\bar{q}_E) + \mathcal{D}(\bar{b})$ . This extension is independent of  $E$  and defined by*

$$\tilde{A}x := A^*x, \quad \forall x \in \mathcal{D}(\tilde{A}) \quad (4.9)$$

where

$$\mathcal{D}(\tilde{A}) := (\mathcal{D}(\bar{q}_E) + \mathcal{D}(\bar{b})) \cap \mathcal{D}(A^*). \quad (4.10)$$

Moreover, for each  $E$  in  $(\lambda_0, \lambda_\infty) \setminus \{\lambda_k : k_0 \leq k < \infty\}$ , the operator  $\tilde{A} - E$  is invertible with bounded inverse given by the formula

$$(\tilde{A} - E)^{-1} = T_E^{-1} \circ \Pi_E - (B + E)^{-1} \circ \Lambda_-. \quad (4.11)$$

*Proof.* For  $E > \lambda_0$ , the operator  $\tilde{A}$  defined by (4.9)-(4.10) is indeed an extension of  $A$ , since

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

By Corollary 10,  $\mathcal{D}(\tilde{A})$  is independent of  $E$ , as well as  $\tilde{A} = A^* \upharpoonright_{\mathcal{D}(\tilde{A})}$ . Moreover the extension  $\tilde{A}$  is symmetric: this immediately follows from Proposition 11.

Now, given  $f \in \mathcal{H}$  and  $E > \lambda_0$  we want to study the equation  $(\tilde{A} - E)X = f$ . For this purpose, we introduce the following problem written in weak form:

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

We recall the identity (4.5), which is a special case of formula (4.1) stated in Proposition 11: if  $(x, z_-) \in \mathcal{D}(\bar{q}_E) \times \mathcal{D}(\bar{b})$  then, for all  $U \in F$ , one has

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

with  $X = x + z_-$ ,  $u = \Lambda_+U + L_E\Lambda_+U$  and  $v_- = U - u$ . Thanks to this identity, we see that for any solution  $(x, z_-)$  of  $(\mathcal{P}_f)$ , the sum  $X = x + z_-$  satisfies

$$\langle X, (A - E)U \rangle = \langle f, U \rangle, \quad \forall U \in F.$$

As a consequence,  $X$  is in  $\mathcal{D}(A^*)$  and solves  $(A^* - E)X = f$ . But this vector is also in  $\mathcal{D}(\bar{q}_E) + \mathcal{D}(\bar{b})$ , so it solves  $(\tilde{A} - E)X = f$ .

On the other hand, we can rewrite  $(\mathcal{P}_f)$  in terms of the Friedrichs extensions  $T_E$  and  $B$ :

$$\begin{aligned} & \text{Find } (x, z_-) \in \mathcal{D}(T_E) \times \mathcal{D}(B) \text{ such that} \\ & \begin{cases} T_E x = \Pi_E(f), \\ (B + E)z_- = -\Lambda_-(f). \end{cases} \end{aligned} \quad (4.12)$$

Since  $E > \lambda_0$ , the operator  $B + E$  is invertible with bounded inverse, and by Proposition 6 the same is true with  $T_E$  if  $E$  is in  $(\lambda_0, \lambda_\infty) \setminus \{\lambda_k, k \geq k_0\}$ . Then (4.12) has a unique solution

given by

$$\begin{cases} x = T_E^{-1} \circ \Pi_E(f), \\ z_- = -(B + E)^{-1} \circ \Lambda_-(f) \end{cases} \quad (4.13)$$

and the vector  $X = (T_E^{-1} \circ \Pi_E - (B + E)^{-1} \circ \Lambda_-)(f)$  solves  $(\tilde{A} - E)X = f$ .

The above discussion shows that for  $E$  in  $(\lambda_0, \lambda_\infty) \setminus \{\lambda_k, k \geq k_0\}$  the symmetric operator  $\tilde{A} - E$  is surjective and admits the bounded operator  $T_E^{-1} \circ \Pi_E - (B + E)^{-1} \circ \Lambda_-$  as a right inverse. But it is well-known that the surjectivity of a symmetric operator implies its injectivity, since its kernel is orthogonal to its range. So  $\tilde{A} - E$  is invertible and (4.11) holds true. Another classical result is that a densely defined surjective symmetric operator is always self-adjoint: see, e.g., [28, Corollary 3.12]. Applying this to  $\tilde{A} - E$ , we conclude that  $\tilde{A}$  is self-adjoint.

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.  $\square$

**4.3. Direct sums.** Recall that in (1.6) we defined the *graph*  $\Gamma_E$  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 13.** *Under conditions (H1)-(H2) and with the above notations,*

$$\bar{\Gamma}_E \cap \mathcal{H}_- \subset ((B + E)(F_-))^\perp. \quad (4.14)$$

*Proof.* The arguments below are essentially contained in the proof of [26, 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 [26] 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 (4.14) 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 [26].*

While we may have  $\bar{\Gamma}_E \cap \mathcal{H}_- \neq \{0\}$ , the following property holds true, as a consequence of Lemma 13:

**Proposition 14.** *Under conditions (H1)-(H2) and with the above notations,*

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

*Proof.* From (4.14), 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 14 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 15.** *Under assumptions (H1)-(H2)-(H3), for all  $E > \lambda_0$ , one has*

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

*As a consequence, the domain of  $\tilde{A}$  may also be written as*

$$\mathcal{D}(\tilde{A}) = (\mathcal{D}(T_E) \dot{+} \mathcal{D}(B)) \cap \mathcal{D}(A^*). \quad (4.15)$$

*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  $X \in \mathcal{D}(\tilde{A})$ ,*

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

*The constant  $C_E$  remains uniformly bounded when  $E$  stays away from  $\lambda_0$  and  $\infty$ .*

*Proof.* Note that Formula (4.11) for the inverse of  $\tilde{A}-E$  already proves the two inclusions  $\pi_E(\mathcal{D}(\tilde{A})) \subset \mathcal{D}(T_E)$  and  $\pi'_E(\mathcal{D}(\tilde{A})) \subset \mathcal{D}(B)$  when  $E$  is in  $(\lambda_0, \lambda_\infty) \setminus \{\lambda_k : k_0 \leq k < \infty\}$ . But we want to prove a statement for *all* values of  $E$  in  $(\lambda_0, \infty)$  and this requires some additional work.

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 shall use the weak form  $(\mathcal{D}_f)$  of the equation  $(\tilde{A}-E)X = f$  and the equivalent system of strong equations (4.12), introduced in the proof of Proposition 12. In that proof,  $f$  was given,  $X = x + z_-$  was unknown and it was shown that for each  $E > \lambda_0$  the solvability of  $(\mathcal{D}_f)$  is a sufficient condition for the solvability of  $(\tilde{A}-E)X = f$ . But it turns out that this condition is also necessary. Indeed, taking  $E > \lambda_0$ ,  $X \in \mathcal{D}(\tilde{A})$  and defining

$$x := \pi_E(X), \quad z_- := \pi'_E(X), \quad f := (\tilde{A}-E)X,$$

we can apply Formula (4.1) of Proposition 11 with the successive choices  $U = u \in \mathcal{D}(\bar{q}_E)$ ,  $U = v_- \in \mathcal{D}(\bar{b})$  and this tells us that  $(x, z_-)$  satisfies  $(\mathcal{D}_f)$ . Then, the second equation of the equivalent system (4.12) implies that  $z_- = -(B+E)^{-1} \Lambda_-(\tilde{A}-E)X$ , so  $z_-$  is in  $\mathcal{D}(B)$

with an estimate of the form

$$\|z_-\|_{\mathcal{D}(B)} \leq C_E \|\Lambda_-(\tilde{A} - E)X\|.$$

This estimate on  $z_-$  implies in turn the estimate  $\|x\| \leq C_E \|X\|_{\mathcal{D}(\tilde{A})}$ , since  $x = X - z_-$ ,  $\|X\| \leq \|X\|_{\mathcal{D}(\tilde{A})}$  and  $\|z_-\| \leq \|z_-\|_{\mathcal{D}(B)}$ . Moreover, the first equation in (4.12) exactly 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

$$\|x\|_{\mathcal{D}(T_E)} \leq C_E \|X\|_{\mathcal{D}(\tilde{A})}.$$

We thus have the desired inclusions  $\pi_E(\mathcal{D}(\tilde{A})) \subset \mathcal{D}(T_E)$  and  $\pi'_E(\mathcal{D}(\tilde{A})) \subset \mathcal{D}(B)$ , hence  $\mathcal{D}(\tilde{A}) \subset \mathcal{D}(T_E) \dot{+} \mathcal{D}(B)$ . Then, remembering the definition  $\mathcal{D}(\tilde{A}) = (\mathcal{D}(\bar{q}_E) \dot{+} \mathcal{D}(\bar{b})) \cap \mathcal{D}(A^*)$  and the inclusions  $\mathcal{D}(T_E) \subset \mathcal{D}(\bar{q}_E)$ ,  $\mathcal{D}(B) \subset \mathcal{D}(\bar{b})$ , one easily gets (4.15). This ends the proof of Proposition 15.  $\square$

**Remark 16.** *In Section 5, we do not use all the information contained in Proposition 15: we only need the weaker estimates*

$$\|\pi'_E(X)\| \leq C_E \|\Lambda_-(\tilde{A} - E)X\| \quad \text{and} \quad \|\pi_E(X)\| \leq C_E \|X\|_{\mathcal{D}(\tilde{A})}. \quad (4.16)$$

**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

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

Of course, in general,  $I_{E,f}$  is not attained, but using the decomposition (2.1) and replacing  $F = F_+ \oplus F_-$  by the larger space  $\mathcal{D}(\bar{q}_E) \dot{+} \mathcal{D}(\bar{b})$ , one can transform it into a min-max:

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

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 17.** *Under assumptions (H1)-(H2)-(H3), for  $k \geq k_0$  the numbers  $\lambda_k$  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 17 are essentially the same as in [4, § 2] (but some details are missing in that reference) and [26, § 2.6]. This proof is based on two facts:

- A relation between the min-max levels  $\lambda_k$  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 (4.16) of Remark 16.

**Lemma 18.** *Under assumptions (H1) (H2)-(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  $\mathcal{X}_\delta$  of  $\mathcal{R}(\mathbb{1}_{(-\delta, \delta)}(T_E))$  of dimension  $r$  (we recall the notation  $\mathcal{R}(L)$  for the range of an operator  $L$ ). Then we have  $\mathcal{X}_\delta \subset \mathcal{D}(T_E) \subset \mathcal{D}(\bar{q}_E)$ . Using Proposition 11 and the second estimate of (4.16) 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  $x_\delta$  in  $\mathcal{X}_\delta$  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  $\delta$ . So, taking  $\delta$  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  $\mathcal{Y}_\varepsilon$  of  $\mathcal{R}(\mathbb{1}_{(E-\varepsilon, E+\varepsilon)}(\tilde{A}))$  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 (4.16) 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  $\varepsilon$  there is  $y_\varepsilon$  in  $V_\varepsilon$  such that  $\|y_\varepsilon\| = 1$  and  $\mathbb{1}_{(-\delta_0, \delta_0)}(T_E)y_\varepsilon = 0$ . So there is  $x_\varepsilon \in \mathcal{D}(T_E)$  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  $\varepsilon$  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  $\mu_E$  as an eigenvalue if and only if (i) holds true for  $\mu_E$  but not for  $\mu_E - 1$ , and this is equivalent to saying that (ii) holds true for  $\mu_E$  but not for  $\mu_E - 1$ , which exactly means that  $E \in \sigma_{\text{disc}}(\tilde{A})$  with multiplicity  $\mu_E$ . 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 17.* 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  $\mu_E$ . 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 18,  $(\lambda_0, \lambda_\infty) \cap \sigma_{\text{ess}}(\tilde{A})$  is empty hence  $\lambda_\infty \leq \underline{\lambda}$ , and the levels  $\lambda_k$  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  $(\lambda_k)$  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  $\lambda_\infty$  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 18, 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 17.  $\square$

*Proof of Theorem 1.* Propositions 12, 14 and 17 together imply Theorem 1.  $\square$

## 6. APPLICATIONS TO DIRAC-COULOMB OPERATORS

In this section, we consider the three-dimensional *Dirac-Coulomb operator*  $D_V = D + V$  mentioned in the Introduction. We assume that  $V$  is a linear combination of Coulomb potentials  $|x - x_j|^{-1}$  due to  $J$  distinct point-like charges located at  $x_1, \dots, x_J$ . If we define  $D_V$  on the minimal domain  $F = C_c^\infty(\mathbb{R}^3 \setminus \{x_1, \dots, x_J\}, \mathbb{C}^4)$ , it is obviously symmetric in the Hilbert space  $\mathcal{H} = L^2(\mathbb{R}^3, \mathbb{C}^4)$ . Thanks to Theorem 1 we are going to construct a distinguished self-adjoint realization of  $D_V$  and give a min-max principle for its eigenvalues,



under some conditions on the coefficients of the linear combination. In each case, Assumption (H3) will be checked by the method of Remark 4.

**6.1. The attractive case.** In this subsection we assume that  $V(x) = -\sum_{j=1}^J \frac{\nu_j}{|x-x_j|}$  is an attractive potential generated by  $J$  distinct point-like nuclei, each having  $Z_j$  protons with  $0 < Z_j \leq Z_* \approx 137.04$  so that  $0 < \nu_j = Z_j/Z_* \leq 1$  (we allow non-integer values of  $Z_j$ ).

We are going to use Talman's splitting  $\Lambda_+ \psi = \begin{pmatrix} \phi \\ 0 \end{pmatrix}$ ,  $\Lambda_- \psi = \begin{pmatrix} 0 \\ \chi \end{pmatrix}$  of four-spinors  $\psi = \begin{pmatrix} \phi \\ \chi \end{pmatrix}$  into upper and lower two-spinors, also called large and small two-components. Then  $\Lambda_+ F = \mathfrak{F} \times \{0\}$  and  $\Lambda_- F = \{0\} \times \mathfrak{F}$  with  $\mathfrak{F} := C_c^\infty(\mathbb{R}^3 \setminus \{x_1, \dots, x_J\}, \mathbb{C}^2)$ . With the standard notation  $\sigma = (\sigma_1, \sigma_2, \sigma_3)$  for the collection of Pauli matrices, we recall (see [30]) that

$$D_V \begin{pmatrix} \phi \\ \chi \end{pmatrix} = \begin{pmatrix} -i\sigma \cdot \nabla \chi + (1+V)\phi \\ -i\sigma \cdot \nabla \phi - (1-V)\chi \end{pmatrix}.$$

Assumptions (H1)-(H2) are easily checked with  $\lambda_0 = -1$ . It remains to check (H3). By Remark 4, it suffices to show that for some  $k_0 \geq 1$ ,  $\ell_{k_0}(0) \geq 0$ . Indeed, this inequality implies that  $\lambda_{k_0} \geq 0 > \lambda_0$ . So we are led to study the quadratic form  $q_0$ . For  $\phi \in \mathfrak{F}$  and  $\psi_+ = \begin{pmatrix} \phi \\ 0 \end{pmatrix}$ , the quantity  $q_0(\psi_+ + L_0 \psi_+)$  is a function of  $\phi$ ,  $V$  and in the rest of the subsection it is more convenient to denote it by  $q^V(\phi)$ . With this notation we have

$$q^V(\phi) = \int_{\mathbb{R}^3} \left\{ \frac{|\sigma \cdot \nabla \phi|^2}{1-V} + (1+V)|\phi|^2 \right\}, \quad \forall \phi \in \mathfrak{F}. \quad (6.1)$$

We start by the potential  $V(x) = -\nu|x|^{-1}$  with  $0 < \nu \leq 1$ , corresponding to a unique point-like nucleus. We recall the Hardy-Dirac inequality

$$q^{-|\cdot|^{-1}}(\phi) = \int_{\mathbb{R}^3} \left\{ \frac{|\sigma \cdot \nabla \phi|^2}{1+|x|^{-1}} + (1-|x|^{-1})|\phi|^2 \right\} \geq 0, \quad \forall \phi \in C_c^\infty(\mathbb{R}^3 \setminus \{0\}, \mathbb{C}^2) \quad (6.2)$$

proved in [4, 3]. Since  $q^{-\nu|\cdot|^{-1}} \geq q^{-|\cdot|^{-1}}$ , (6.2) implies that  $\ell_1(0) \geq 0$  and Assumption (H3) is satisfied with  $k_0 = 1$ . Then, using Theorem 1 we can define a distinguished self-adjoint extension of  $D_V$  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 (1.2). This is not a new result: see [4, 12, 10, 26], and it is known that  $V$  can be replaced by more general attractive potentials that are bounded from below by  $-|x|^{-1}$ .

We now assume that  $J \geq 2$ . In such a case, the distinguished self-adjoint extension was constructed in [24, 17] in the subcritical case  $\nu_i < 1$  ( $\forall i$ ) 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 [11], also in the subcritical case. But that paper appealed to the abstract result of [7] and as mentioned in the Introduction, the arguments in [7] suffered from the same closability issue as [4]. Theorem 1 solves this issue, moreover it provides a unified treatment: construction of the extension and justification of the min-max principle even in the critical case, *i.e.*, when some of the coefficients  $\nu_i$  are equal to 1. But of course, in order to apply this theorem we have to check (H3) and

this is more delicate than in the one-center case. Indeed, when the total number of protons  $\sum_j Z_j$  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  $\lambda_k$  should become equal to  $\lambda_0$ . To check Assumption (H3) in such a situation, let us prove by contradiction that for *some*  $k_0 \geq 1$ , the inequality  $\ell_{k_0}(0) \geq 0$  holds true.

Otherwise, there exists a sequence  $(G_k)_{k \geq 1}$  of  $k$ -dimensional subspaces of  $\mathfrak{F}$  such that  $q^V(\phi) < 0$  for all  $\phi \in G_k \setminus \{0\}$ . So one can construct by induction a sequence  $(\phi_k)$  of wave functions such that  $\phi_k \in G_k$  and  $\langle \phi_k, \phi_l \rangle_{L^2(\mathbb{R}^3, \mathbb{C}^2)} = \delta_{kl}$ . Then  $\phi_k$  converges weakly to 0 in  $L^2(\mathbb{R}^3, \mathbb{C}^2)$ . In order to derive a contradiction, one can try to prove that for  $k$  large enough,  $q^V(\phi_k) \geq 0$ . In the subcritical case  $v_i < 1$  ( $\forall i$ ) this has been done in [11, Section 6, Step 4, p. 1448-1449]. We give below a proof that is also valid in the critical case. In what follows, the constant  $C$  changes from line to line but we keep the same notation for the sake of simplicity.

With  $\delta := \frac{1}{2} \min_{1 \leq j < j' \leq K} |x_j - x_{j'}|$  one takes  $R > \delta + \max_{1 \leq j \leq J} |x_j|$  (to be chosen later) and a partition of unity  $(\theta_j)_{0 \leq j \leq J+1}$  consisting of smooth functions with values in  $[0, 1]$  such that  $\sum_{j=0}^{J+1} \theta_j^2 = 1$ ,  $\text{supp}(\theta_0) \subset B(0, 2R) \setminus \bigcup_{j=1}^J B(x_j, \delta/2)$ ,  $\text{supp}(\theta_j) \subset B(x_j, \delta)$  for  $1 \leq j \leq J$  and  $\text{supp}(\theta_{J+1}) \cap B(0, R) = \emptyset$ . The pointwise IMS formula [1, Lemma 4.1] for the Pauli operator gives

$$|\sigma \cdot \nabla \phi_k|^2 = \sum_{j=0}^{J+1} |\sigma \cdot \nabla (\theta_j \phi_k)|^2 - \left( \sum_{j=0}^{J+1} |\nabla \theta_j|^2 \right) |\phi_k|^2,$$

so, remembering that  $\|\phi_k\|_{L^2(\mathbb{R}^3)}^2 = 1$ , one gets

$$\begin{aligned} q^V(\phi_k) &= \sum_{j=0}^{J+1} q^V(\theta_j \phi_k) - \int_{\mathbb{R}^3} \left( \sum_{j=0}^{J+1} |\nabla \theta_j|^2 \right) \frac{|\phi_k|^2}{1-V} \\ &= \frac{1}{2} + \sum_{j=0}^J q^V(\theta_j \phi_k) + \left( q^V(\theta_{J+1} \phi_k) - \frac{1}{2} \|\theta_{J+1} \phi_k\|_{L^2(\mathbb{R}^3)}^2 \right) \\ &\quad - \int_{\mathbb{R}^3} \left( \frac{1 - \theta_{J+1}^2}{2} + \frac{1}{1-V} \sum_{j=0}^{J+1} |\nabla \theta_j|^2 \right) |\phi_k|^2 \\ &\geq \frac{1}{2} + \sum_{j=0}^J q^V(\theta_j \phi_k) + \left( q^V(\theta_{J+1} \phi_k) - \frac{1}{2} \|\theta_{J+1} \phi_k\|_{L^2(\mathbb{R}^3)}^2 \right) - C \int_{B(0, 2R)} |\phi_k|^2. \end{aligned}$$

From now on, we fix  $R$  such that  $-V \leq 1/4$  on  $\mathbb{R}^3 \setminus B(0, R)$ . Then one has

$$q^V(\theta_{J+1} \phi_k) - \frac{1}{2} \|\theta_{J+1} \phi_k\|_{L^2(\mathbb{R}^3)}^2 \geq \frac{1}{4} \|\theta_{J+1} \phi_k\|_{H^1(\mathbb{R}^3)}^2.$$

Let

$$M := 1 + \max \left\{ \sup_{x \in \text{supp}(\theta_0)} -V(x); \sup_{x \in \text{supp}(\theta_1)} (-V(x) - |x - x_1|^{-1}); \dots; \sup_{x \in \text{supp}(\theta_J)} (-V(x) - |x - x_J|^{-1}) \right\}.$$

Then

$$q^V(\theta_0 \phi_k) \geq \frac{1}{M} \|\theta_0 \phi_k\|_{H^1(\mathbb{R}^3)}^2 - C \int_{\mathbb{R}^3} |\theta_0 \phi_k|^2$$

and, introducing the rescaled functions  $\hat{\phi}_{j,k}(y) := (\theta_j \phi_k)(x_j + M^{-1}y)$  for  $1 \leq j \leq J$ , one finds

$$q^V(\theta_j \phi_k) \geq \frac{1}{M^2} q^{-|\cdot|^{-1}}(\hat{\phi}_{j,k}) - C \int_{\mathbb{R}^3} |\theta_j \phi_k|^2.$$

Gathering these estimates, one gets the lower bound

$$q^V(\phi_k) \geq \frac{1}{2} + \frac{1}{M^2} \sum_{j=1}^J q^{-|\cdot|^{-1}}(\hat{\phi}_{j,k}) + \frac{1}{M} \|\theta_0 \phi_k\|_{H^1(\mathbb{R}^3)}^2 + \frac{1}{4} \|\theta_{J+1} \phi_k\|_{H^1(\mathbb{R}^3)}^2 - C \int_{B(0,2R)} |\phi_k|^2. \quad (6.3)$$

From the Hardy-Dirac inequality (6.2), each of the terms  $q^{-|\cdot|^{-1}}(\hat{\phi}_{j,k})$  is nonnegative, so the assumptions that  $\|\phi_k\|_{L^2(\mathbb{R}^3)} = 1$  and  $q^V(\phi_k) < 0$  imply that the quantities  $q^{-|\cdot|^{-1}}(\hat{\phi}_{j,k})$ ,  $\|\theta_0 \phi_k\|_{H^1}$  and  $\|\theta_{J+1} \phi_k\|_{H^1}$  are uniformly bounded. But from [10, Theorem 1.9], for  $0 \leq s < 1/2$  there is a positive constant  $\kappa_s$  such that

$$q^{-|\cdot|^{-1}}(\phi) + \|\phi\|_{L^2(\mathbb{R}^3)}^2 \geq \kappa_s \|\phi\|_{H^s(\mathbb{R}^3)}^2, \quad \forall \phi \in \mathfrak{F}.$$

Applying this inequality to the functions  $\hat{\phi}_{j,k}$  ( $1 \leq j \leq J$ ), one easily finds that the sequence  $(\phi_k)_{k \geq 1}$  is bounded in  $H^s(\mathbb{R}^3)$ , hence precompact in  $L^2_{\text{loc}}(\mathbb{R}^3)$ . Since this sequence converges weakly to zero in  $L^2(\mathbb{R}^3)$ , one concludes that

$$\lim_{k \rightarrow \infty} \int_{B(0,2R)} |\phi_k|^2 = 0.$$

Combining this information with (6.3) one finds that for  $k$  large enough,  $q^V(\phi_k) \geq 0$  and this is a contradiction.

In conclusion, the assumptions of Theorem 1 are satisfied in our multi-center example, with  $k_0$  possibly larger than 1.

**6.2. The sign-changing case.** We now consider a potential of the form

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

The corresponding Dirac-Coulomb operator  $D_V$  is obviously symmetric if we define it on the ‘‘minimal’’ domain  $C_c^\infty(\mathbb{R}^3 \setminus \{0, x_0\}, \mathbb{C}^4)$ . But Talman’s decomposition in upper and lower spinors cannot be used: due the unbounded repulsive term  $\frac{\nu_2}{|x-x_0|}$ , (H2) would not be satisfied. Instead, for the splitting we choose the free-energy projectors

$$\Lambda_\pm = \mathbb{1}_{\mathbb{R}_\pm}(D).$$

We recall (see [30]) that

$$D\Lambda_\pm = \Lambda_\pm D = \pm \sqrt{1-\Delta} \Lambda_\pm = \pm \Lambda_\pm \sqrt{1-\Delta}.$$

In momentum space (*i.e.* after Fourier transform),  $\Lambda_\pm$  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 its derivatives. As a consequence, the multiplication by  $M_\pm$  preserves the Schwartz class  $\mathcal{S}(\mathbb{R}^3, \mathbb{C}^4)$ . So the same is true for  $\Lambda_\pm$  in position space. But this nonlocal operator does not preserve the

compact support property, so (H1) does not hold for the domain  $C_c^\infty(\mathbb{R}^3 \setminus \{0, x_0\}, \mathbb{C}^4)$ . Since  $\Lambda_+ C_c^\infty(\mathbb{R}^3 \setminus \{0, x_0\}, \mathbb{C}^4) \subset \mathcal{S}(\mathbb{R}^3, \mathbb{C}^4) \subset \mathcal{D}(\overline{D_V})$ , one can either replace the minimal domain by  $F = \Lambda_+ C_c^\infty(\mathbb{R}^3 \setminus \{0, x_0\}, \mathbb{C}^4) \oplus \Lambda_- C_c^\infty(\mathbb{R}^3 \setminus \{0, x_0\}, \mathbb{C}^4)$  as mentioned in the first comment after Theorem 1, or by  $F = \mathcal{S}(\mathbb{R}^3, \mathbb{C}^4)$ . In what follows,  $A$  is the restriction of  $\overline{D_V}$  to one of these two domains. We do not need to specify which one: the arguments proving (H2)-(H3) are the same in both cases.

By the upper bound on  $\nu_2$ , it follows from an inequality of Tix [32] that the Brown-Ravenhall operator  $-\Lambda_-(A + 1 - \nu_2) \upharpoonright_{F_-} = \Lambda_-(\sqrt{1 - \Delta} - V - 1 + \nu_2) \upharpoonright_{F_-}$  is non-negative, so (H2) holds true with  $\lambda_0 \leq -1 + \nu_2$ . In order to bound  $\lambda_1$  from below, we can use [4, inequality (38)]. This inequality involves a parameter  $\nu \in (0, 1)$  and is stated for all functions  $\psi_+ \in F_+$ . One easily passes to the limit  $\nu \rightarrow 1$  with  $\psi_+$  fixed and this gives us the inequality

$$\left\langle \psi_+, \sqrt{1 - \Delta} \psi_+ \right\rangle_{L^2(\mathbb{R}^3)} - \int_{\mathbb{R}^3} \frac{|\psi_+|^2}{|x|} + \left\langle \Lambda_- \frac{1}{|x|} \psi_+, (B_{-|x|^{-1}})^{-1} \Lambda_- \frac{1}{|x|} \psi_+ \right\rangle_{L^2(\mathbb{R}^3)} \geq 0 \quad (6.4)$$

for all  $\psi_+ \in F_+$ . Here, we denote by  $B_V$  the Friedrichs extension of the Brown-Ravenhall operator  $\Lambda_-(\sqrt{1 - \Delta} - V) \upharpoonright_{F_-}$ , for any electric potential  $V$  such that this operator is bounded from below. Inequality (6.4) exactly says that if one chooses  $(\nu_1, \nu_2) = (1, 0)$  then there holds  $q_0(\psi_+ + L_0 \psi_+) \geq 0$  for all  $\psi_+ \in F_+$ , so  $\ell_1(0) \geq 0$ , hence  $\lambda_1 \geq 0 > \lambda_0$ . This remains true for  $0 < \nu_1 \leq 1$  and  $0 < \nu_2 \leq \frac{2}{\pi/2 + 2/\pi}$ , since the min-max level  $\lambda_1$  is a non-decreasing function of  $V$ . Thus, Theorem 1 can be applied with  $k_0 = 1$  in order to find a distinguished self-adjoint extension of  $D_V$  and to characterize its eigenvalues by a min-max principle.

Note that by [31, Corollary 3], the operator  $-\Lambda_- A \upharpoonright_{F_-}$  is not essentially self-adjoint for  $\nu_2 > 3/4$ . So the abstract result [26, Theorem 1.1] cannot be applied in this case.

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