

 Open access • Journal Article • DOI:10.1007/S005260010321

Variational characterization for eigenvalues of Dirac operators — [Source link](#)

[Jean Dolbeault](#), [Maria J. Esteban](#), [Eric Séré](#)

Institutions: [Paris Dauphine University](#)

Published on: 01 Jun 2000 - [Calculus of Variations and Partial Differential Equations](#) (Springer-Verlag)

Topics: [Dirac operator](#), [Dirac \(software\)](#), [Rayleigh quotient](#), [Scalar potential](#) and [Eigenvalues and eigenvectors](#)

Related papers:

- [On the eigenvalues of operators with gaps. Application to Dirac operators.](#)
- [A minimax principle for eigenvalues in spectral gaps: Dirac operators with Coulomb potentials.](#)
- [A minimax principle for the eigenvalues in spectral gaps](#)
- [The Dirac Equation](#)
- [Minimax principle for the Dirac equation.](#)

Share this paper:    

View more about this paper here: <https://typeset.io/papers/variational-characterization-for-eigenvalues-of-dirac-2s8wulxmsq>

Variational characterization for eigenvalues of Dirac operators.

Jean Dolbeault & Maria J. Esteban

Ceremade (URA CNRS 749)
CNRS et Université Paris-Dauphine
Place Maréchal Lattre de Tassigny
F-75775 Paris Cedex 16

Eric Séré

Département de Mathématiques
Université de Cergy-Pontoise
2, Av. Adolphe Chauvin
F-95302 Cergy-Pontoise Cedex

Abstract. In this paper we give two different variational characterizations for the eigenvalues of $H + V$ where H denotes the free Dirac operator and V is a scalar potential. The first one is a min-max involving a Rayleigh quotient. The second one consists in minimizing an appropriate nonlinear functional. Both methods can be applied to potentials which have singularities as strong as the Coulomb potential.

AMS Subject Classification: 49 R 05, 49 R 10, 49 R 20, 49 S 05, 47 A 75, 81 Q 10, 35 P 05, 35 Q 75, 35 A 15.

Key Words : Dirac operators, relativistic quantum mechanics, eigenvalues, min-max, minimization, Rayleigh-Ritz technique.

1 - Introduction.

The Dirac operator is a first order operator which has the form

$$(1.1) \quad H = -ic\hbar \vec{\alpha} \cdot \vec{\nabla} + mc^2\beta$$

where c denotes the speed of light, $m > 0$ the mass of the electron, \hbar is Planck's constant, $\vec{\alpha} \cdot \vec{\nabla} = \sum_{k=1}^3 \alpha_k \partial_k$ and α_k are the Pauli-Dirac matrices,

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

The 2×2 matrices σ_k are the Pauli matrices :

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

All throughout this paper, we shall work with a system of physical units such that $m = c = \hbar = 1$.

In this paper we are interested in perturbed Dirac operators of the form $H + V$, V being a scalar potential. Our goal is to find variational characterizations for the eigenvalues of such operators. We hope that our results can be of some interest in *a priori* estimates, as well as practical computations of atomic energy levels. One expects the eigenvalues of $H + V$ to be critical points (in an appropriate sense) of the Rayleigh quotient

$$R_V(\varphi) := \frac{((H + V)\varphi, \varphi)}{(\varphi, \varphi)} ,$$

where (\cdot, \cdot) denotes the inner product in $L^2(\mathbb{R}^3)$. If $H + V$ were bounded below, like Schrödinger operators $-\Delta - Z/|x|$ for instance, minimizing the above quotient would give the least eigenvalue (ground state energy). This standard approach fails for Dirac operators: for physically relevant potentials V , the Rayleigh quotient is neither bounded from above nor from below (for instance, see [20]). This is the main difficulty we have to face.

Many efforts have been devoted to the characterization and computation of Dirac eigenvalues. Some works deal with approximate potentials acting on 2-spinors. The idea is to write Dirac's equation for the upper spinor in ψ by performing some adequate transformation. Then, different procedures have been produced to find approximate Hamiltonians, which "become exact" in the nonrelativistic limit. For references in this direction see, for instance, Durand [13], Durand-Malrieu [14], van Lenthe-Van Leeuwen-Baerends-Snijders [24].

Other approximate Hamiltonians are constructed by using projectors. One of the first attempts in this direction was made by Brown and Ravenhall. In [7], they proposed the following (usually called the Brown-Ravenhall "no-pair") Hamiltonian

$$(1.2) \quad B = \Lambda^+ (H + V) \Lambda^+$$

where $\Lambda^+ = \chi_{(0, \infty)}(H)$ denotes the projection on the positive spectral subspace of the free Dirac operator.

The projected Hamiltonian B has received a lot of attention concerning the question of the "stability of matter" for relativistic multi-particle systems (see Lieb-Siedentop-Solovej [26]).

If 0 is not in the spectrum of $H + V$, then instead of defining B as above, one can use the exact positive projector corresponding to $H + V$, denoted by Λ_V^+ . The new operator

$$(1.3) \quad \tilde{B}_V = \Lambda_V^+ (H + V) \Lambda_V^+$$

coincides with $H + V$ in its positive spectral subspace. For attractive potentials V that are not “too strong”, minimizing the Rayleigh quotient for \tilde{B}_V yields the smallest positive eigenvalue of $H + V$. This eigenvalue may be interpreted as the ground state energy. Unfortunately, the exact projector Λ_V^+ is not known *a priori*. This makes its use difficult in numerical computations. On the contrary, the approximate Brown-Ravenhall Hamiltonian B is known explicitly.

Several recent papers have been devoted to the mathematical study of the Brown-Ravenhall Hamiltonian for one-electron atoms with nuclear charge $Z > 0$. Its precise form is

$$(1.4) \quad B^Z := \Lambda_+ (H - \frac{Z\alpha}{|x|}) \Lambda_+$$

where α is the fine structure constant ($\alpha^{-1} = 137.037\dots$). Hardekopf and Sucher [18], on the basis of numerical computations, conjectured that the operator B^Z is strictly positive for $Z < Z_c = 2\alpha^{-1}/(\pi/2 + 2/\pi)$, that its first eigenvalue vanishes for $Z = Z_c$, and that B_Z is unbounded from below for $Z > Z_c$. Evans, Perry and Siedentop [16] proved that the operator B^Z is bounded from below if and only if $Z \leq Z_c$, as predicted in [18]. Tix [32, 33] proved that the operator B^Z is strictly positive for $Z \leq Z_c$ (see also Burenkov-Evans [8]). Note that the integer part of Z_c is 124, strictly below the critical value $Z_* = 137$, for which the first eigenvalue of the Dirac-Coulomb Hamiltonian $H - Z\alpha/|x|$ vanishes (see for instance [28, 31]).

One the most important properties of the free Dirac operator H is that

$$(1.5) \quad H^2 = -\Delta + 1$$

Another Hamiltonian having the same property is :

$$(1.6) \quad \sqrt{-\Delta + 1}$$

This Hamiltonian is positive definite, and so, it does not pose the problems related to the unboundedness of the Dirac operator. But it is nonlocal, which contradicts the Causality Principle in special relativity and does not preserve

the symmetry in the t and x variables for the evolution problem (covariance of the equation under the action of Lorentz boosts). Nevertheless, the study of the spectrum of

$$(1.7) \quad \sqrt{-\Delta + 1} + V$$

and its use as an approximation model for multi-particle systems is interesting. For references in this direction, let us mention [10, 19, 23, 25] and references therein.

In 1994, Hill and Krauthauser proposed a variational characterization of eigenvalues of $H + V$ based on maximization of quotients like

$$\frac{(\psi, (H + V)\psi)}{(\psi, (H + V)^2\psi)}.$$

This method works when the spectrum of $H + V$ has a gap around 0. The mathematical study of this approach has still to be done.

The characterization of the stable eigenvalues of $H + V$ by a minimax method is a quite natural idea and it has been attempted both analytically and numerically : in 1986, Talman [30] proposed a minimax procedure to find the first eigenvalue of $H + V$ for negative potentials V (see also [9]). His proposal consisted in first maximizing in the lower component of the spinor ψ , and then minimizing over the upper spinor.

In 1995, in a PDE conference in Toronto (see its proceedings [15]), Esteban and Séré presented a minimax technique (without approximation) inspired of critical point theory. This same result was also presented in the ICDEMP in Atlanta in March 1997. A sequence of min-max levels was introduced in [15]:

$$(1.8) \quad \lambda_k = \inf_{\substack{F \subset Y^+ \\ F \text{ vector space} \\ \dim F = k}} \sup_{\substack{\varphi \in F \oplus Y^- \\ \varphi \neq 0}} \frac{((H + V)\varphi, \varphi)}{(\varphi, \varphi)}.$$

Here, Y^\pm are the spaces $\Lambda^\pm(H^{1/2}(\mathbb{R}^3))$. The following result was announced: for a class of potentials that includes the Coulomb potentials $-a|x|^{-1}$ ($0 < a < 1/2$), λ_k is the k 'th positive eigenvalue of $H + V$ (counted with multiplicity). These values of a correspond to one-electron atoms of atomic charge $Z \leq 68$.

Recently, Griesemer and Siedentop ([17]) proved a general minimax theorem on the eigenvalues in a spectral gap of an abstract operator. As an application, they prove that under appropriate conditions on V , the sequence

λ_k defined in (1.8) coincides with the sequence of positive eigenvalues μ_k of $H + V$. The method of proof in [17], as well as the class of potentials V to which their theorem applies, seems to be quite different from ours: in the case of Coulomb potentials, they only prove that $\lambda_k \leq \mu_k$. Another interesting result in [17], is that Talman's approach, slightly modified, is indeed mathematically correct for a large class of bounded potentials.

In Section 2 of the present paper, we state and prove some technical results on the Dirac operator. Sections 3 and 4 deal with two variational characterizations of the eigenvalues.

Section 3 is devoted to the study of the minimax procedure (1.8). We give a detailed proof of the results announced in Toronto (see [15]) and in Atlanta. In [15], we could not treat "strong" Coulomb potentials $-a|x|^{-1}$, for $a \geq 1/2$, because we were using estimates based on Hardy's inequality

$$\int \frac{|u|^2}{|x|^2} \leq 4 \int |\nabla u|^2 .$$

We are now able to treat all $a < 2/(\pi/2 + 2/\pi) \approx 0.9$. This corresponds to an atomic charge Z up to 124. The proof is almost the same for these strong fields, we simply replace Hardy's inequality by the very precise estimates of Tix [32, 33] and Burenkov-Evans [8].

The minimization method introduced in Section 4, follows a completely different idea. It comes from the reduction of the Hamiltonian to a 2-spinor function space. The reduced energy functional J^+ is nonlinear, but semi-bounded. For a large family of operators V , the minimization of J^+ provides us with the smallest eigenvalue of $H + V$ (and an associated eigenfunction) as long as it is positive. This yields an optimal result for the Coulomb potential $-Z\alpha/|x|$: our minimization method works for all $Z < 137$, the best condition under which $H - Z\alpha/|x|$ possesses a ground state in $L^2(\mathbb{R}^3)$. In a sense, J^+ seems to contain information related to the exact projector Λ_V^+ in an implicit way. Note that the idea to build a semibounded energy functional had already been introduced by Bayliss and Peel [1] in another context.

Acknowledgement. The authors wish to thank H. Siedentop for his interest in this work. His bibliographical remarks have been very useful.

2 - Generalities on the Dirac operator and auxiliary results.

In the Fourier domain, the Dirac operator is a multiplication operator

(by a 4×4 hermitian matrix) :

$$(2.1) \quad \hat{H}(\xi) = \xi \cdot \alpha + \beta,$$

and it satisfies

$$(2.2) \quad \hat{H}^2 = |\xi|^2 + 1.$$

For every $\xi \in \mathbb{R}^3$, $\hat{H}(\xi)$ has two eigenvalues, $\pm\sqrt{|\xi|^2 + 1}$ and one has the following properties :

Lemma 2.1.

(P1) H is a self-adjoint operator on $L^2(\mathbb{R}^3, \mathbb{C}^4)$, with domain $\mathcal{D}(H) = H^1(\mathbb{R}^3, \mathbb{C}^4)$. Its spectrum is $(-\infty, -1] \cup [1, +\infty)$. There are two orthogonal projectors on $L^2(\mathbb{R}^3, \mathbb{C}^4)$, Λ^+ and $\Lambda^- = 1_{L^2} - \Lambda^+$, both with infinite rank, and such that

$$(2.3) \quad \begin{cases} H\Lambda^+ = \Lambda^+H = \sqrt{1-\Delta} \Lambda^+ = \Lambda^+ \sqrt{1-\Delta} \\ H\Lambda^- = \Lambda^-H = -\sqrt{1-\Delta} \Lambda^- = -\Lambda^- \sqrt{1-\Delta} \end{cases}.$$

(P2) The Coulomb potential $W(x) = \frac{1}{|x|}$ satisfies the following Hardy-type inequalities :

$$(2.4) \quad (\varphi, W(x)\varphi)_{L^2} \leq \frac{\pi}{2}(\varphi, \sqrt{-\Delta} \varphi)_{L^2} \leq \frac{\pi}{2}(\varphi, |H|\varphi)_{L^2}, \forall \varphi \in H^{1/2}(\mathbb{R}^3, \mathbb{C}^4)$$

$$(2.5) \quad (\varphi, W(x)\varphi)_{L^2} \leq \frac{1}{2}\left(\frac{\pi}{2} + \frac{2}{\pi}\right)(\varphi, |H|\varphi)_{L^2}, \forall \varphi \in \Lambda^+(H^{1/2}) \cup \Lambda^-(H^{1/2})$$

$$(2.6) \quad \|W(x)\varphi\|_{L^2} \leq 2\|\nabla\varphi\|_{L^2} \leq 2\|H\varphi\|_{L^2}, \quad \forall \varphi \in H^1(\mathbb{R}^3, \mathbb{C}^4).$$

Remark. Equalities (2.3) are a consequence of the following fact : in Fourier variables, the projectors Λ^\pm are multiplication operators given by the following expressions:

$$(2.7) \quad \hat{\Lambda}^\pm(\xi) = \frac{\pm\hat{H} + \sqrt{|\xi|^2 + 1}}{2\sqrt{|\xi|^2 + 1}}.$$

Inequalities (P2) are classical, except for (2.5), whose proof, based on a method of Evans-Perry-Siedentop [16], is contained in the recent papers [8], [32] and [33]. For the proof of (2.4), see [19] and [21].

Part (P1) of the above lemma enables us to decompose the space $Y = H^{1/2}(\mathbb{R}^3, \mathbb{C}^4)$ as the direct sum of two infinite dimensional Hilbert spaces Y^\pm which are stable under the action of H . Furthermore, a norm in Y is given by

$$(2.8) \quad \|\varphi\|_Y = \left(\varphi, (H\Lambda^+ - H\Lambda^-)\varphi \right)_{Y \times Y'}^{1/2} = \left(\varphi, |H|\varphi \right)^{1/2}$$

This norm is the usual $H^{1/2}$ -norm and for $\|\cdot\|_Y$, Y^+ and Y^- are orthogonal, as well as for $\|\cdot\|_{L^2}$. In the sequel, $\|\cdot\|$ will denote the $L^2(\mathbb{R}^3, \mathbb{C}^4)$ -norm and $\|\cdot\|_Y$ the $H^{1/2}$ -norm defined in (2.8).

Based on Lemma 2.1, we define now the class of scalar potentials V to be considered all throughout this section. In the following, we will need to introduce the Marcinkiewicz space $M^3(\mathbb{R}^3)$ (see [2]).

Definition 2.2 . We say that a scalar potential V defined a.e. in \mathbb{R}^3 satisfies assumption (H1) if it belongs to $M^3(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ and if there is a positive constant δ such that

$$(2.9) \quad \Lambda^+(H + V)\Lambda^+ \geq \delta\sqrt{1 - \Delta}, \quad \Lambda^-(H + V)\Lambda^- \leq -\delta\sqrt{1 - \Delta} \text{ in } Y.$$

Remark 1. If V belongs to $M^3(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$, then V is $|H|$ -bounded. In particular, any $|V| \leq a|x|^{-\beta} + C$ is $|H|$ -bounded for all $a, C > 0$, $\beta \in (0, 1]$. If $|V| \leq a|x|^{-1}$, then, by (2.5), V satisfies (H1) if and only if $a < (\pi/4 + 1/\pi)^{-1} \approx 0.9$. Moreover, any $V \in L^\infty(\mathbb{R}^3)$ satisfies (H1) if $\|V\|_\infty < 1$.

Remark 2. Assumption (H1) implies that for all constants $\kappa > 1$ close to 1, there is a positive constant $\delta(\kappa) > 0$ such that :

$$\Lambda^+(H + \kappa V)\Lambda^+ \geq \delta(\kappa)\Lambda^+, \quad \Lambda^-(H + \kappa V)\Lambda^- \leq -\delta(\kappa)\Lambda^- \quad \text{on } Y,$$

In the sequel, we consider potentials V satisfying (H1) and for those, we will look for eigenvalues of $H + V$ in the spectral gap of H . Before starting this program, let us recall some well-known results on the spectrum of $(H + V)$. For precise references and proofs, see [31].

Remark 3. Using the Friedrichs extension theorem, inequality (2.9) implies that $\Lambda^+(H + V)\Lambda^+$ (resp. $\Lambda^-(H + V)\Lambda^-$) can be defined, in a unique way, as a self-adjoint operator with domain contained in Y^+ (resp. Y^-).

Theorem 2.3 (see e.g. [31]; Theorems 4.5, 4.6, 4.7) *Let V be a scalar potential which is H -bounded and such that $V(x) \rightarrow 0$ as $|x| \rightarrow +\infty$ and the operator $H + V$ is essentially self-adjoint. Then*

$$\sigma_{ess}(H + V) = \sigma_{ess}(H).$$

Eigenvalues belonging to the essential spectrum are not stable. So, stable Dirac states will be represented by eigenvalues lying in the gap of the

essential spectrum of H , *i.e.* in the interval $(-1, 1)$. There are a number of results concerning the nonexistence of eigenvalues lying in the essential spectrum of Dirac operators. Let us mention the work of A. Berthier and V. Georgescu (see [4, 5]), where it is proven that if the scalar potential V satisfies very general decay conditions at infinity, there is no eigenvalue of the operator $H + V$ in the essential spectrum. In the particular case of the Coulomb potential, an elementary method based on the virial theorem implies the same result (see [31]). There are also results about the number of eigenvalues lying in the gap of the essential spectrum of H . More precisely, these results give conditions for the existence of an infinity of eigenvalues in the gap $(-1, 1)$. In the case of only a finite number of eigenvalues in this interval, there are estimates about their number. For more details, see the exhaustive reference list in [31].

3 - Minimax characterization of Dirac eigenvalues

This section is devoted to the proof of a minimax characterization for the positive eigenvalues of $H + V$. More precisely, let us define the nondecreasing sequence $\{\lambda_k\}$ by

$$(3.1) \quad \lambda_k(V) = \inf_{\substack{F \subset Y^+ \\ F \text{ vector space} \\ \dim F = k}} \sup_{\substack{\varphi \in F \oplus Y^- \\ \varphi \neq 0}} \frac{((H + V)\varphi, \varphi)}{(\varphi, \varphi)}.$$

Then, we have the following :

Theorem 3.1. *Let V be a scalar potential satisfying assumption (H1). Assume also that $V \in L^\infty(\mathbb{R}^3 \setminus \overline{B}_{R_0})$ for some $R_0 > 0$ and that we have :*

$$(H2) \quad \lim_{R \rightarrow +\infty} \|V\|_{L^\infty(|x| > R)} = 0, \quad \lim_{R \rightarrow +\infty} \sup \operatorname{ess}_{|x| > R} V(x)|x|^2 = -\infty.$$

Then, λ_k is an eigenvalue of $H + V$, $\{\lambda_k\}_{k \geq 1}$ is the non-decreasing sequence of eigenvalues of $H + V$ in the interval $[0, 1)$, counted with multiplicity, and

$$(3.2) \quad 0 < \delta \leq \lambda_1 \leq \lambda_k < 1, \quad \lim_{k \rightarrow +\infty} \lambda_k = 1$$

Remark. As it is clear from (3.1), all the eigenfunctions of $H + V$ corresponding to the eigenvalues λ_k have Morse index equal to $+\infty$ as critical points of the Rayleigh quotient.

The proof of Theorem 3.1 will be carried out after we prove some technical auxiliary results.

Lemma 3.2. *Let V satisfy (H1). Assume that there are at least k eigenvalues of $H + V$ in $(0, 1)$, counted with multiplicity, $\mu_1 \leq \dots \leq \mu_k$. Then, $\lambda_k \leq \mu_k$.*

Proof.

Let e_1, \dots, e_k be an orthonormal family of eigenvectors, associated to the eigenvalues μ_1, \dots, μ_k . Let $F = \text{span}(\Lambda^+ e_1, \dots, \Lambda^+ e_k)$. This space has dimension k , otherwise there would be a linear combination φ of e_1, \dots, e_k with $\varphi \in Y^-$, hence $(\varphi, (H + V)\varphi) < 0$ by (H1): this is impossible, since $\mu_k \geq \dots \geq \mu_1 \geq 0$. If Π denotes the projector on $F + Y^-$, then the operator $-\Pi(H + V)\Pi$ is self-adjoint and bounded below, and its smallest eigenvalue is $-\mu_k$, by the standard theory of Rayleigh quotients (see [29], vol 4). This theory also gives

$$\mu_k = \sup_{\substack{\varphi \in F \oplus Y^- \\ \varphi \neq 0}} \frac{((H + V)\varphi, \varphi)}{(\varphi, \varphi)}$$

hence $\mu_k \geq \lambda_k$.

□

Remark. Let S be the 4×4 matrix $\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$. S is a self-adjoint involution which anticommutes with H . So, if ψ is an eigenvector of $H + V$ with associated eigenvalue λ , then $S\psi$ is an eigenvector of $H - V$ with eigenvalue $-\lambda$. As a consequence, Lemma 3.2 implies the following result:

Corollary 3.3. *Let V satisfy (H1). Then, there is no eigenvalue of $H + V$ in the interval $(-\lambda_1(-V), \lambda_1(V))$. If, moreover, $V \leq 0$ a.e., then, $-\lambda_1(-V) = -1$ and there is no eigenvalue of $H + V$ in the interval $(-1, \lambda_1(V))$.*

Let us now begin the study of the non-decreasing sequence $\{\lambda_k\}$ defined by (3.1). It is straightforward to see that $\lambda_1 \geq \delta > 0$, from (H1). The next lemma tells us that the supremum $\sup_{\substack{\varphi \in F \oplus Y^- \\ \varphi \neq 0}} \frac{((H + V)\varphi, \varphi)}{(\varphi, \varphi)}$ is in fact a maximum.

Lemma 3.4. *Let V satisfy (H1). Then, for all $k \geq 1$, and F a k -dimensional subspace of Y^+ , there is an orthonormal family $\varphi_1, \dots, \varphi_k$ of eigenvectors of $\Pi(H + V)\Pi$ in $F + Y^-$, with eigenvalues $\gamma_k \geq \dots \geq \gamma_1 > 0$ (Π is the projector on $F + Y^-$). Moreover, $(\psi, \Pi(H + V)\Pi\psi) \leq 0$ for any ψ in the orthogonal space of $\text{span}(\varphi_1, \dots, \varphi_k)$ for the L^2 scalar product in*

$F + Y^-$ and

$$\gamma_k = \sup_{\substack{\varphi \in F \oplus Y^- \\ \varphi \neq 0}} \frac{((H + V)\varphi, \varphi)}{(\varphi, \varphi)},$$

so φ_k is a maximum point.

Proof. Once again, this follows immediately from the standard theory of Rayleigh quotients (see [29], vol 4), applied to the semibounded self-adjoint operator $-\Pi(H + V)\Pi$ in the Hilbert space $F + Y^-$, defined as a Friedrichs extension of the corresponding minimal operator. \square

Now we proceed to obtain upper bounds for the λ_k 's. This will be crucial to prove that the λ_k 's are achieved.

Lemma 3.5. *Let V a scalar potential satisfying (H1)-(H2). Then, for all $k \geq 1$, there exists a k -dimensional subspace of Y^+ , F_k , such that*

$$(3.3) \quad \sup_{\substack{\varphi \in F_k \oplus Y^- \\ \varphi \neq 0}} \frac{((H + V)\varphi, \varphi)}{(\varphi, \varphi)} < 1$$

Corollary 3.6. *If V satisfies (H1)-(H2), then for all $k \geq 1$,*

$$(3.4) \quad \lambda_k < 1$$

The proof of the corollary is immediate.

Proof of Lemma 3.5. Let G be the Hilbert subspace of Y of the functions $e(x)$ whose Fourier transform can be written as $\hat{e}(\xi) = \theta(|\xi|) \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$, $\theta \in C^\infty([0, 1], \mathbb{R})$, $\text{supp } \theta \subset (0, 1)$.

We note that for such functions e , $(\alpha_k \partial_k e, e) = 0$. Let us now choose any $e_1 \in G$ such that $\|e_1\| = 1$. We define $e_\lambda(x) = \lambda^{-3/2} e_1(\frac{x}{\lambda})$ for $\lambda > 0$. Consider now any $\varphi^- \in Y^-$ satisfying $\|\varphi^-\| \leq 1$ and take $\mu = \mu(\lambda) \geq 0$ such that $\|\varphi^- + \mu e_\lambda\| = 1$. From the properties of G and of the operator H , we have

$$(3.5) \quad \begin{cases} A_\lambda(e_1) : & = ((H + V)(\varphi^- + \mu e_\lambda), \varphi^- + \mu e_\lambda) \\ & = \mu^2 \left(\int_{\mathbb{R}^3} |e_1(x)|^2 dx + \int_{\mathbb{R}^3} V(\lambda x) |e_1(x)|^2 dx \right) \\ & \quad + ((H + V)\varphi^-, \varphi^-) + 2\mu \text{Re}((H + V)e_\lambda, \varphi^-). \end{cases}$$

Now, from (H1) we find that

$$(3.6) \quad ((H + V)\varphi^-, \varphi^-) \leq -\delta \|\varphi^-\|^2, \quad \text{for some } \delta > 0.$$

Moreover, by applying Cauchy-Schwarz inequality,

$$(3.7) \quad |(He_\lambda, \varphi^-)| \leq \lambda^{-1} \|\vec{\alpha} \cdot \vec{\nabla} e_1\| \|\varphi^-\| + \|\Lambda^- e_\lambda\| \|\varphi^-\|,$$

$$(3.8) \quad |(Ve_\lambda, \varphi^-)| \leq \left(\int |V(\lambda x)|^2 |e_1(x)|^2 dx \right)^{1/2} \|\varphi^-\|$$

Now, let us prove that $\|\Lambda^- e_\lambda\| = O(\lambda^{-1})$. Indeed,

$$\|\Lambda^- e_\lambda\|_{L^2}^2 = (\Lambda^- e_\lambda, \Lambda^- e_\lambda) = (\Lambda^- e_\lambda, e_\lambda),$$

since Λ^- is a projection operator. By (2.7),

$$\begin{aligned} \|\Lambda^- e_\lambda\|_{L^2}^2 &= \int_{\mathbb{R}^3} \frac{\sqrt{1+|\xi|^2}-1}{2\sqrt{1+|\xi|^2}} |\hat{e}_\lambda(\xi)|^2 d\xi \\ &\leq \frac{1}{4} \int_{\mathbb{R}^3} |\xi|^2 |\hat{e}_\lambda(\xi)|^2 d\xi = \frac{1}{4\lambda^2} \int_{\mathbb{R}^3} |\xi|^2 |\hat{e}_+(\xi)|^2 d\xi. \end{aligned}$$

Thus, $\|\Lambda^- e_\lambda\|_{L^2}^2 \leq \frac{C_1^2}{\lambda^2}$ with $C_1^2 = \frac{1}{4} \int_{\mathbb{R}^3} |\xi|^2 |\hat{e}_+(\xi)|^2 d\xi$.

Moreover, we can use assumption (H2) to obtain

$$(3.9) \quad \overline{\lim}_{\lambda \rightarrow +\infty} \lambda^2 \int_{\mathbb{R}^3} V(\lambda x) |e_1(x)|^2 dx = -\infty$$

$$(3.10) \quad \int_{\mathbb{R}^3} |V(\lambda x)|^2 |e_1(x)|^2 dx \leq \frac{\delta}{4} \int_{\mathbb{R}^3} |V(\lambda x)| |e_1(x)|^2 dx,$$

for λ large enough. Now, for e_1 and φ^- given, μ depends on λ . Indeed, $\|\varphi^- + \mu e_\lambda\| = 1$ implies that $\mu \|\Lambda^+ e_\lambda\| \leq 1$ and again from (2.7), it is easy to see that for λ large,

$$(3.11) \quad \|\Lambda^+ e_\lambda\|_{L^2}^2 = 1 - \|\Lambda^- e_\lambda\|_{L^2}^2 \geq 1 - \frac{C_1^2}{\lambda^2}, \quad \text{i.e., } \mu \leq 1 + \frac{C_1^2}{2\lambda^2},$$

Estimates (3.5) to (3.11) and an optimization w.r.t. $\|\varphi^-\|$ imply that

$$\begin{aligned} A_\lambda(e_1) &\leq \mu^2 \left(1 + \int_{\mathbb{R}^3} V(\lambda x) |e_1(x)|^2 dx \right) - \delta \|\varphi^-\|^2 \\ &\quad + 2\mu \left(\frac{\|\vec{\alpha} \cdot \vec{\nabla} e_1\|}{\lambda} + \frac{C_1}{\lambda} + \left(\int |V(\lambda x)|^2 |e_1(x)|^2 dx \right)^{1/2} \right) \|\varphi^-\| \\ &\leq \mu^2 \left(1 + \int_{\mathbb{R}^3} V(\lambda x) |e_1(x)|^2 dx + \frac{2}{\delta} \int_{\mathbb{R}^3} |V(\lambda x)|^2 |e_1(x)|^2 dx + O\left(\frac{1}{\lambda^2}\right) \right) \\ &\leq 1 + O\left(\frac{1}{\lambda^2}\right) + \frac{1}{2} \int_{\mathbb{R}^3} V(\lambda x) |e_1(x)|^2 dx < 1 \quad \text{for } \lambda \text{ large.} \end{aligned} \tag{3.12}$$

To end the proof, we consider a k -dimensional subspace of G , G_k and define F_k^λ as

$$(3.13) \quad F_k^\lambda = \left\{ \lambda^{-\frac{3}{2}} e_1 \left(\frac{\cdot}{\lambda} \right) \mid e_1 \in G_k \right\}.$$

Inequality (3.12) can be made uniform for $e_1 \in G_k$ in such a way that there exists $A_\lambda > 0$ such that

$$A_\lambda(e_1) \underset{\lambda \sim +\infty}{<} 1 \text{ uniformly for all } e_1 \in G_k, \lambda > 0 \text{ large.}$$

Then, it is sufficient to define

$$(3.14) \quad F_k := F_k^\lambda, \quad \lambda \text{ large}$$

and the lemma is proved. \square

Proof of Theorem 3.1.

From Lemma 3.4, the supremum appearing in the definition of λ_k is achieved for every k -dimensional subspace F of Y^+ .

Let us now prove that the min-max is also achieved. We begin with the case $k = 1$. Let us consider a minimizing sequence $\{\varphi_1^n\}$ such that $\|\varphi_{1,n}\| = 1$, $\Lambda^+ \varphi_{1,n} \neq 0$,

$$(3.15) \quad \lambda_{1,n} := \sup_{\substack{\varphi \in \mathbb{C}\varphi_{1,n} + Y^- \\ \varphi \neq 0}} \frac{((H + V)\varphi, \varphi)}{(\varphi, \varphi)},$$

is achieved by $\varphi_{1,n}$ and

$$\lim_n \lambda_{1,n} = \lambda_1.$$

The Euler-Lagrange equation satisfied by $\varphi_{1,n}$ reads

$$(3.16) \quad (H + V) \varphi_{1,n} = \lambda_{1,n} \varphi_{1,n} + f_n,$$

for some f_n which is orthogonal to $Y^- \oplus \mathbb{C}\varphi_{1,n}$ for the duality product in $H^{-1/2} \times H^{1/2}$. Multiplying both sides of this equation by $\varphi_{1,n}^+ - \varphi_{1,n}^-$, where $\varphi_{1,n}^\pm := \Lambda^\pm \varphi_{1,n}$ we obtain

$$(3.17) \quad \left((H + V)\varphi_{1,n}^+, \varphi_{1,n}^+ \right) - \left((H + V)\varphi_{1,n}^-, \varphi_{1,n}^- \right) \leq \lambda_{1,n}.$$

Hence, by hypothesis (H1), the sequence $\{\varphi_{1,n}\}_n$ is uniformly bounded in Y and therefore, relatively compact for the Y -weak and $L_{\text{loc}}^q(\mathbb{R}^3)$ -strong topologies, $1 \leq q < 3$. Up to subsequences, we may assume that $\varphi_1 \in Y$ is the limit of $\{\varphi_{1,n}\}_n$ in those topologies. Finally, assume that the sequence

of Lagrange multipliers $\{f_n\}$ converges to 0 in $H^{-1/2}(\mathbb{R}^3)$. If this holds, we have

$$(H + V)\varphi_1 = \lambda_1 \varphi_1.$$

Thus, under the above assumption on f_n , Theorem 3.1 will be proved (in the case $k = 1$) if we show that $\varphi_1 \not\equiv 0$. Assume the contrary. Since $V \xrightarrow{|x| \rightarrow +\infty} 0$ and $V \in L^r_{\text{loc}}(\mathbb{R}^3)$ for $r \in (2, 3)$, $V\varphi_{1,n} \xrightarrow{n \rightarrow +\infty} 0$ in $L^2(\mathbb{R}^3) + L^s(\mathbb{R}^3)$ for $s \in (\frac{6}{5}, \frac{3}{2})$. But then, for n large we can write

$$(3.18) \quad \varphi_{1,n} = (H - \lambda_1^n)^{-1} (f_n - V\varphi_{1,n})$$

The operators $(H - \lambda_1^n)^{-1}$ are uniformly bounded, since $\lambda_1 \in (0, 1)$. So, if $f_n \xrightarrow{n \rightarrow +\infty} 0$ in $H^{-1/2}(\mathbb{R}^3)$ and $\varphi_1 \equiv 0$,

$$\varphi_{1,n} \xrightarrow{n \rightarrow +\infty} 0 \quad \text{in } L^2(\mathbb{R}^3) + H^1(\mathbb{R}^3) + W^{1,s}(\mathbb{R}^3),$$

which contradicts the normalization $\|\varphi_{1,n}\| = 1$.

Let us finally prove that the sequence $\{f_n\}$ has to converge to 0 in $H^{-1/2}(\mathbb{R}^3)$. If this were not the case, up to subsequences, we would find $\chi_n \in Y^+$, $(\chi_n, \varphi_{1,n}) = 0$ such that $\|\chi_n\|_Y = 1$ and

$$(3.19) \quad \text{Re}((H + V)\varphi_{1,n}, \chi_n) = \text{Re}(f_n, \chi_n) \geq \sigma > 0$$

for some σ independent of n . Since V is $|H|$ -bounded, there exists a constant C_1 such that for all n , $|((H + V)\chi_n, \chi_n)| \leq C_1$. Then, for any $t > 0$, let us consider the space $G_t = \text{span}\{\varphi_{1,n}^+ - t\chi_n\} \oplus Y^-$. Let us now take any $\psi \in G_t$ of the form $\psi = \varphi_{1,n} - t\chi_n + \varphi^-$, $\varphi^- \in Y^-$. We obtain :

$$(3.20) \quad \begin{aligned} ((H + V)\psi, \psi) &= \lambda_1^n \|\varphi_n\|^2 + 2\lambda_1^n \text{Re}(\varphi_n, \varphi^-) \\ &+ ((H + V)\varphi^-, \varphi^-) - 2t \text{Re}(f_n, \chi_n) \\ &+ t^2((H + V)\chi_n, \chi_n) - 2t \text{Re}((H + V)\varphi^-, \chi_n) \end{aligned}$$

Since V satisfies assumption (H1), $((H + V)\psi, \psi) \leq 0$ for $\|\varphi^-\|_Y$ large. Hence, there exists a constant M such that $((H + V)\psi, \psi) \geq 0$ implies $\|\varphi^-\|_Y \leq M$. This, (3.20) and our assumptions imply that for $\|\varphi^-\|_Y \leq M$,

$$\begin{aligned} ((H + V)\psi, \psi) &\leq \lambda_{1,n} \|\varphi_{1,n}\|^2 + 2\lambda_{1,n} \text{Re}(\varphi_{1,n}, \varphi^-) \\ &\quad - \delta \|\varphi^-\|_Y^2 - 2t\sigma + C_1 t^2 + 2Ct \|\varphi^-\|_Y \\ &\leq \lambda_{1,n} \|\varphi_{1,n} - t\chi_n + \varphi^-\|^2 - 2t\sigma + C_1 t^2 + 2Ct \|\varphi^-\|_Y - \delta \|\varphi^-\|_Y^2 \end{aligned}$$

with C independent of n . Then, we optimize the above inequality in $\|\varphi^-\|_Y$ to obtain

$$(3.21) \quad ((H + V)\psi, \psi) \leq \lambda_{1,n} \|\varphi_{1,n} - t\chi_n + \varphi^-\|^2 - 2t\sigma + \left(C_1 + \frac{C^2}{\delta}\right) t^2$$

and hence, for t small enough,

$$(3.22) \quad \sup_{\psi \in G_t} \frac{((H + V)\psi, \psi)}{(\psi, \psi)} \leq \lambda_{1,n} - \frac{t\sigma}{\|\psi\|^2} < \lambda_1 - \varepsilon$$

for some $\varepsilon > 0$, because $\|\psi\|$ is uniformly bounded. Indeed, in the second step of the proof, we obtained an estimate for $\{\varphi_{1,n}\}$ in Y and by assumption, $\|\varphi^-\| \leq M$, $\|\chi_n\| \leq 1$. The contradiction in (3.22) ends the proof in the case $k = 1$.

Case $k > 1$: Assume that we have already solved the min-max problem corresponding to λ_i , $1 \leq i \leq k - 1$ and let φ_i be the corresponding eigenfunction. If F_n is a minimizing sequence for λ_k and $\varphi_{k,n}$ the corresponding maximizer given by Lemma 3.4, we normalize it to have $\|\varphi_{k,n}\| = 1$ and as above, the Euler-Lagrange equation satisfied by $\varphi_{k,n}$ is

$$(3.23) \quad (H + V)\varphi_{k,n} = \lambda_{k,n} \varphi_{k,n} + f_n,$$

for some f_n which is orthogonal to $Y^- \oplus F_n$ for the duality product in $H^{-1/2} \times H^{1/2}$ and

$$\lim_n \lambda_{k,n} = \lambda_k.$$

If $\lambda_{k-1} < \lambda_k$, then we follow the same steps as in the case $k = 1$ to conclude that the weak limit in Y of $\varphi_{k,n}$ is a function φ_k satisfying

$$(H + V)\varphi_k = \lambda_k \varphi_k, \quad \varphi_k \neq 0,$$

and therefore, φ_k is a solution for the min-max problem defining λ_k . Note that the only important change that we make here is to replace G_t with a similar subspace $\tilde{G}_t := \text{span}\{\varphi_{1,n}, \dots, \varphi_{k,n} - t\chi_n\}$.

If, on the contrary, $\lambda_{k-1} = \lambda_k$, let us then define ℓ as the largest integer in the set $\{1, \dots, k\}$ such that $\lambda_\ell < \lambda_k$. Hence, $\lambda_{\ell+1} = \lambda_{k-1} = \lambda_k$ and we can find a subspace G_n of $F_n \cap \{\varphi_{\ell+1}, \dots, \varphi_{k-1}\}^\perp$, of dimension $\ell + 1$, which is minimizing for $\lambda_{\ell+1}$. So, as in the preceding case, we find a function φ , solution of

$$(H + V)\varphi = \lambda_{\ell+1} \varphi = \lambda_k \varphi, \quad \varphi \neq 0,$$

and by construction, $(\varphi, \varphi_i) = 0$ for all $i \in \{\ell + 1, \dots, k - 1\}$. We define $\varphi_k := \varphi$, and by induction, this ends the proof. \square

4 - A minimization procedure providing an eigenstate of Dirac operators : the ground state.

In this section, we introduce a minimization method which, under appropriate assumptions on the potential V , yields the eigenvalues of $H + V$ lying in the spectral gap as well as the corresponding eigenfunctions.

The Dirac equation is originally written for 4-spinors. Here, we begin by making a reduction to an equivalent equation for 2-spinors. Of course, this requires some conditions on V .

For any ψ with values in \mathbb{C}^4 , let us write $\psi = \begin{pmatrix} \varphi \\ \chi \end{pmatrix}$, with φ, χ taking values in \mathbb{C}^2 . Then, the equation

$$(4.1) \quad (H + V) \psi = \lambda \psi \quad \text{in } \mathbb{R}^3$$

is equivalent to the system

$$(4.2) \quad \begin{cases} L\chi = (E - V) \varphi & \text{in } \mathbb{R}^3 \\ L\varphi = (E + 2 - V) \chi \end{cases}$$

with $E = \lambda - 1$ and $L = i(\vec{\sigma} \cdot \vec{\nabla}) = \sum_{k=1}^3 i\sigma_k \partial_k$.

If $V \leq 0$ a.e. in \mathbb{R}^3 and $E > -2$ (which is the case for stable eigenvalues, see Section 2), the system (4.2) can be written as

$$(4.3) \quad L\left(\frac{L\varphi}{g_E}\right) + V\varphi = E\varphi, \quad \chi = \frac{L\varphi}{g_E} \quad \text{in } \mathbb{R}^3$$

where $g_E = E + 2 - V$. Now, we make the following change of function :

$$\varphi = \sqrt{g_E} \phi$$

which is well defined (for $V \leq 0$ and $E > -2$). From (4.3) we obtain

$$(4.4) \quad H_E \phi := \sqrt{g_E} L\left(\frac{1}{g_E} L(\sqrt{g_E} \phi)\right) = (E - V)(E + 2 - V)\phi \quad \text{in } \mathbb{R}^3$$

and we notice that the operator acting on ϕ in the left-hand side of (4.4) is formally symmetric. If ϕ is a solution of (4.4), we have

$$(4.5) \quad (\phi, \phi) E^2 + 2(\phi, (1 - V)\phi)E - (\phi, (2 - V)V\phi) - (\phi, H_E \phi) = 0$$

and we notice that (4.5) holds if and only if

$$(4.6) \quad E = J^\pm(E, \phi) := \frac{1}{(\phi, \phi)} \left(\pm \sqrt{\Delta(E, \phi)} - (\phi, (1 - V)\phi) \right)$$

where $\Delta(E, \phi) := |(\phi, V\phi)|^2 + (\phi, \phi) \left[(\phi, \phi) + (\phi, H_E\phi) - (\phi, V^2\phi) \right]$. Thus, we have obtained that if $E > -2$ is an eigenvalue of $\varphi \mapsto L \left(\frac{L\varphi}{g_E} \right) + V\varphi$, there exists an associated eigenfunction $\phi \neq 0$ such that (4.6) holds. The main idea of Section 4 is to prove conversely that under appropriate conditions, critical points of $J^+(E, \phi)$ are solutions of equation (4.4). In fact, for a given potential W , we will prove this for the operators $H + aW$ with a less than some constant A_W , depending only on the potential W .

In order to proceed further, let us define

$$T(E, \phi) := (\phi, \phi) + (\phi, H_E\phi) - (\phi, V^2\phi) = \tilde{T}(E, \varphi) := \int_{\mathbb{R}^3} \frac{|L\varphi|^2 + |\varphi|^2 - V^2|\varphi|^2}{g_E}$$

so that $\Delta(E, \phi) = (\phi, V\phi)^2 + (\phi, \phi)T(E, \phi)$, provided $\varphi = \sqrt{g_E}\phi$.

We notice that since E has to be real, $\Delta(E, \phi)$ must be nonnegative for all the functions ϕ which we will be considering. Also, for $\phi \neq 0$,

$$(4.7) \quad T(E, \phi) \geq 0$$

if and only if $\Delta(E, \phi) \geq |(\phi, V\phi)|^2 \geq 0$. Then, if $\phi \neq 0$, $J^+(E, \phi) \geq \frac{|(\phi, V\phi)| + (\phi, V\phi)}{(\phi, \phi)} - 1 \geq -1$ and $J^-(E, \phi) \leq \frac{(\phi, V\phi) - |(\phi, V\phi)|}{(\phi, \phi)} - 1 \leq -1$, with equality if and only if $T(E, \phi) = 0$.

Thus, if $V \neq 0$ is a nonpositive potential and if (4.7) holds for all (E, ϕ) in some adapted set X , with strict inequality, the only functional yielding positive stable eigenvalues of $H + V$ is J^+ .

In this section, we will prove that critical points of J^+ in a well chosen but natural class of functions solve equation (4.4). At a formal level, critical points (E, ϕ) of the functional $J^+(E, \phi)$, satisfying the constraint $E = J^+(E, \phi)$, are indeed solutions of (4.4) (for more details, see step 4 in the proof of Theorem 4.3 below). Moreover, under adequate assumptions on V , we will find the ‘‘ground state energy’’ of $H + V$ as the minimum value of J^+ .

Let X_0 be defined by

$$X_0 := \left\{ \varphi \in L^2(\mathbb{R}^3) ; \int_{\mathbb{R}^3} \frac{|L\varphi|^2 + |\varphi|^2}{1 + |V|} dx < +\infty \right\}$$

and

$$X := \left\{ \phi \in L^2(\mathbb{R}^3) ; \varphi := \sqrt{g_E} \phi \in X_0 \text{ for some } E \in (-1, 0) \right\}.$$

Note that for all $\phi \in X$, $E \in (-1, 0)$,

$$\|\phi\|_E^2 := (H_E \phi, \phi) + (\phi, \phi) = \int_{\mathbb{R}^3} \frac{|L\varphi|^2 + |\varphi|^2}{g_E} dx < +\infty$$

Note also that if V is a nonpositive scalar potential and $\psi = \begin{pmatrix} \varphi \\ \chi \end{pmatrix} \in L^2 \setminus \{0\}$ is an eigenfunction of $H + V$, associated with an eigenvalue $\lambda > -1$, then the corresponding ϕ is in X whenever $V\chi^2 \in L^1(\mathbb{R}^3)$. This last condition is automatically satisfied if V satisfies assumption (H1) of Section 3.

Now, assume that the scalar potential W satisfies

$$(J1) \quad W \in L_{loc}^\infty(\mathbb{R}^3 \setminus \{0\}) \text{ and either } W \in L^\infty(\mathbb{R}^3) \text{ or } W \xrightarrow{|x| \rightarrow 0} -\infty$$

$$(J2) \quad W \leq 0 \text{ a.e. in } \mathbb{R}^3, \quad \lim_{R \rightarrow +\infty} \|W\|_{L^\infty(|x| > R)} = 0,$$

$$(J3) \quad M_W := \min \left(\inf_{\varphi \in X_0} \frac{\int_{\mathbb{R}^3} |W|^{-1} (|L\varphi|^2 + |\varphi|^2)}{\int_{\mathbb{R}^3} |W| |\varphi|^2}, \inf_{\varphi \in X_0} \frac{\int_{\mathbb{R}^3} |\nabla \varphi|^2 + |\varphi|^2}{\int_{\mathbb{R}^3} W^2 |\varphi|^2} \right) > 0.$$

Remarks. Assumptions (J1) to (J3) are invariant by multiplication by a positive constant, i.e. if W satisfies (J1) to (J3), then the same holds for $V = aW$ for all $a > 0$. However, assumption (H1) (stated in Section 3) for $V = aW$ may strongly depend on the value of a .

If $W_\beta = -|x|^{-\beta}$, $\beta \in (0, 1]$, it is easy to check that W_β satisfies assumptions (J1) to (J3). To do so, one has to use classical Hardy-type inequalities.

It is also possible to replace a single singularity of V at the origin by several isolated singularities.

Let us now derive some implications of assumptions (J1)-(J3) which will be useful in the sequel of the paper.

Proposition 4.1. *Let W a potential satisfying (J1) to (J3). For any $a_0 > 0$, we have*

$$(4.8) \quad l(a_0) := \inf_{0 < a < a_0} \inf_{(E, \varphi) \in (-1, 0) \times X_0} \frac{\int_{\mathbb{R}^3} \frac{|L\varphi|^2 + |\varphi|^2}{E + 2 + a|W|}}{\int_{\mathbb{R}^3} \frac{aW^2 |\varphi|^2}{E + 2 + a|W|}} > 0.$$

Proof of Proposition 4.1.

If W is bounded, the proof immediately follows. If, on the contrary, W tends to $-\infty$ at 0, then, if $l(a_0) = 0$, there must exist a sequence $\{(E_n, \phi_n)\} \in (-1, 0) \times X$ and $a_n \in (0, a_0]$ such that

$$(4.9) \quad \int_{\mathbb{R}^3} \frac{W^2 |\varphi_n|^2}{E_n + 2 + a_n |W|} = 1, \quad \frac{1}{a_n} \int_{\mathbb{R}^3} \frac{|L\varphi_n|^2 + |\varphi_n|^2}{E_n + 2 + a_n |W|} \xrightarrow{n \rightarrow +\infty} 0.$$

Let us choose $\beta > 0$ such that $2 \leq |W|$ a.e. in the set $\{x \in \mathbb{R}^3; 0 < |x| \leq 2\beta\}$ and define $\ell := \max_{|x| \geq \beta} |W(x)|$. Finally, we consider a function $\xi \in C^1(\mathbb{R}^3)$, with values in the interval $[0, 1]$, such that $\xi \equiv 1$ on the ball of radius β , B_β , $\text{supp } \xi \subset B_{2\beta}$ and $\nabla \sqrt{1 - \xi^2} \in L^\infty$. Then,

$$(4.10) \quad \int_{\mathbb{R}^3} \frac{|L\varphi_n|^2 + |\varphi_n|^2}{E_n + 2 + a_n |W|} \geq \int_{\mathbb{R}^3} \frac{|L(\xi\varphi_n)|^2 + |\xi\varphi_n|^2}{(a_n + 1)|W|} + \frac{|L(\sqrt{1 - \xi^2}\varphi_n)|^2 + (1 - \xi^2)|\varphi_n|^2}{2 + a_n \ell} + r_n a_n$$

with $\lim_{n \rightarrow +\infty} r_n = 0$. By using (J3) we find :

$$(4.11) \quad \begin{aligned} \int_{\mathbb{R}^3} \frac{|L\varphi_n|^2 + |\varphi_n|^2}{E_n + 2 + a_n |W|} &\geq \frac{M_W}{a_n + 1} \int_{\mathbb{R}^3} |W| \varphi_n^2 \xi^2 + M_W \int_{\mathbb{R}^3} \frac{W^2 \varphi_n^2 (1 - \xi^2)}{2 + a_n \ell} + r_n a_n \\ &\geq \frac{M_W a_n}{a_n + 1} \int_{\mathbb{R}^3} \frac{W^2 \varphi_n^2 \xi^2}{E_n + 2 + a_n |W|} + \frac{M_W}{2 + a_n \ell} \int_{\mathbb{R}^3} \frac{W^2 \varphi_n^2 (1 - \xi^2)}{E_n + 2 + a_n |W|} + r_n a_n \\ &\geq M_W \min\left(\frac{a_n}{a_n + 1}, \frac{1}{2 + a_n \ell}\right) + r_n a_n \end{aligned}$$

and this shows that (4.9) cannot hold, what ends the proof.

A straightforward corollary of the above proposition is the following

Corollary 4.2. *If a potential W satisfies (J1) to (J3), then for $a > 0$ small enough, $V = aW$ satisfies*

$$(4.12) \quad I_V := \inf_{\substack{(E, \varphi) \in (-1, 0) \times X_0 \\ J^+(E, \phi) \leq E}} \frac{\int_{\mathbb{R}^3} \frac{|L\varphi|^2 + |\varphi|^2}{E + 2 + |V|}}{\int_{\mathbb{R}^3} \frac{V^2 |\varphi|^2}{E + 2 + |V|}} > 1.$$

Proof. Since the function l is nonincreasing and strictly positive on \mathbb{R}^+ , $l(a)/a > 1$ for $a > 0$ small enough. Finally, $I_{aW} \geq (l(a)/a)$, since the extra constraint $J^+(E, \phi) \leq E$ only increases the value of the infimum. \square

Remark. Note that

$$\begin{aligned} I_V > 1 &\Rightarrow \int_{\mathbb{R}^3} \frac{V^2(x)|\varphi(x)|^2}{g_E(x)} dx < \int_{\mathbb{R}^3} \frac{|L\varphi|^2 + |\varphi|^2}{g_E(x)} dx \\ &\Leftrightarrow T(E, \phi) = (\phi, H_E\phi) + (\phi, \phi) - (\phi, V^2\phi) > 0 \\ &\Leftrightarrow J^+(E, \phi) > -1 \end{aligned}$$

for all $(E, \phi = \frac{\varphi}{\sqrt{g_E}}) \in [-1, 0] \times X$, such that $J^+(E, \phi) \leq E$.

In order to find the minimal ‘‘eigenvalue’’ E of (4.4), we would like to minimize $J^+(E, \phi)$ over the set $\{(E, \phi) ; \phi \neq 0, J^+(E, \phi) = E\}$. Let us introduce a relaxed minimization problem over the set

$$(4.13) \quad D_V := \{(E, \phi) \in (-2, 0) \times X ; \phi \neq 0, J^+(E, \phi) \leq E\}.$$

Now we are ready to state the main theorem of this section.

Theorem 4.3. *Assume that V is a scalar potential satisfying (J1) to (J3) such that*

$$(4.14) \quad I_V > 1$$

and

$$(4.15) \quad D_V \neq \emptyset.$$

Then, the following infimum

$$(4.16) \quad E_0 := \inf \{E \in (-2, 0); \exists \phi \in X \text{ with } (E, \phi) \in D_V\}$$

is achieved in D_V by some (E_0, ϕ_0) . Moreover,

$$\phi_0 \neq 0, J^+(E_0, \phi_0) = E_0 \in (-1, 0)$$

and $\phi \equiv \phi_0$ is a solution of (4.4) with $E = E_0$.

Remark. By Corollary 4.2 and Theorem 4.3, if W satisfies (J1) to (J3) and $a > 0$ is small enough, then the ‘‘ground state’’ of the operator $H + aW$ is given by the minimization of J^+ over the set D_{aW} . So, Theorem 4.3 applies to $V = -a|x|^{-\beta}$, $\beta \in (0, 1]$, $a > 0$ small. Moreover, as shown below (see Proposition 4.6), this theorem is optimal for the Coulomb potential: in the case $\beta = 1$, one can take any $a < 1$.

Corollary 4.4. *Under the assumptions of Theorem 4.3, the function $\psi_0 = \begin{pmatrix} \varphi_0 \\ \chi_0 \end{pmatrix}$, with $\varphi_0 = \sqrt{g_{E_0}} \phi_0$, $\chi_0 = L\varphi_0/g_{E_0}$ satisfies*

$$(4.17) \quad H\psi_0 + V\psi_0 = (E_0 + 1)\psi_0 \quad \text{in } \mathbb{R}^3, \psi_0 \neq 0.$$

Moreover, $E_0 + 1$ is the smallest eigenvalue of $(H + V)$ in $(0, 1)$ corresponding to an eigenfunction $\psi = \begin{pmatrix} \varphi \\ \chi \end{pmatrix}$ such that $\varphi \in X_0$.

Proof of Corollary 4.4. The first assertion follows immediately from Theorem 4.3 and the introduction of this section. As for the fact that $E_0 + 1$ is the smallest eigenvalue of $H + V$ in $(0, 1)$ such that $\varphi \in X_0$, we just invoke the fact that J^- maps X into $(-\infty, -1)$. \square

Proof of Theorem 4.3.

Step 1 : $E_0 \in (-1, 0)$.

Since the set D_V is not empty, we have : $E_0 < 0$. Also, from the definition of J^+ and (4.14), $E_0 \geq -1$. Assume by contradiction that $E_0 = -1$. Then, since the functional J^+ is homogeneous of degree 0, there exists a sequence $\{(E_n, \phi_n)\}$ in D_V such that

$$(4.18) \quad \int_{\mathbb{R}^3} h_{E_n} |\phi_n|^2 = 1, \quad -1 < J^+(E_n, \phi_n) \leq E_n \xrightarrow{n \rightarrow +\infty} -1,$$

a contradiction with the following lemma :

Lemma 4.5. *Assume that V satisfies (J1)-(J3) and that $I_V > 1$. If $E > -1$ and $\phi \in X$ satisfy*

$$(i) \quad \int_{\mathbb{R}^3} (E + 1 - V)|\phi|^2 dx = 1 \quad (\text{normalization condition})$$

and

$$(ii) \quad J^+(E, \phi) \leq E$$

then,

$$E + 1 > \min \left\{ \sqrt{\frac{\zeta}{2(1 + \zeta)}}, \frac{1}{\sqrt{1 + \zeta}}, \frac{\zeta}{1 + 2\sqrt{1 + \zeta} + \sqrt{5 + 4(\zeta + \sqrt{1 + \zeta})}} \right\}$$

with $\zeta = I_V - 1$.

Proof of Lemma 4.5.

By (ii), $\theta := E + 1 \geq J^+(E, \phi) + 1 = \|\phi\|^{-2} \left\{ \sqrt{\Delta(E, \phi)} + \int_{\mathbb{R}^3} V|\phi|^2 dx \right\}$. Now, combining (i) and (ii) we obtain

$$(4.19) \quad \Delta(E, \phi) = \|\phi\|^2 T(E, \phi) + (\phi, V\phi)^2 \leq 1.$$

By (i) again,

$$(4.20) \quad \|\phi\|^2 T(E, \phi) \leq 1 - (1 - \theta \|\phi\|^2)^2$$

and then

$$(4.21) \quad T(E, \phi) \leq \theta(2 - \theta \|\phi\|^2) \leq 2\theta.$$

On the other hand, since $I_V > 1$, by definition of ζ , we have

$$(4.22) \quad \frac{(\phi, H_E \phi) + (\phi, \phi)}{1 + \zeta} \geq (\phi, V^2 \phi)$$

Hence,

$$(4.23) \quad T(E, \phi) = (\phi, H_E \phi) + (\phi, \phi) - (\phi, V^2 \phi) \geq \frac{\zeta}{1 + \zeta} \left(\|\phi\|^2 + (\phi, H_E \phi) \right),$$

and then

$$(4.24) \quad \|\phi\|^2 \leq (\phi, H_E \phi) + \|\phi\|^2 \leq \frac{(1 + \zeta)T(E, \phi)}{\zeta},$$

$$(4.25) \quad \int_{\mathbb{R}^3} g_E(x) |\phi|^2 dx = 1 + \|\phi\|^2 \leq 1 + \frac{(1 + \zeta)T(E, \phi)}{\zeta}.$$

By using Cauchy-Schwarz's inequality and (4.25) we also have

$$(4.26) \quad \left(\int_{\mathbb{R}^3} V |\phi|^2 dx \right)^2 \leq \left(1 + \frac{(1 + \zeta)T(E, \phi)}{\zeta} \right) \int_{\mathbb{R}^3} \frac{V^2 |\phi|^2}{g_E} dx.$$

Clearly, for any $a, b > 0$, we have $\frac{a}{b} \geq I_V$ if and only if $b \leq \frac{a-b}{I_V-1} = \zeta^{-1}(a-b)$. Taking $a = \int_{\mathbb{R}^3} \frac{|L\phi|^2 + |\phi|^2}{g_E} dx$ and $b = \int_{\mathbb{R}^3} \frac{V^2 |\phi|^2}{g_E} dx$, we have $a - b = T(E, \phi)$ and

$$(4.27) \quad \left(\int_{\mathbb{R}^3} V |\phi|^2 dx \right)^2 \leq \frac{T(E, \phi)}{\zeta} \left(1 + \frac{(1 + \zeta)T(E, \phi)}{\zeta} \right)$$

Using (4.24) and then (4.27) we have

$$(4.28) \quad \begin{aligned} \frac{\theta(1+\zeta)}{\zeta} T(E, \phi) &\geq \theta \|\phi\|^2 = 1 + \int_{\mathbb{R}^3} V |\phi|^2 dx \\ &\geq 1 - \sqrt{\frac{T(E, \phi)}{\zeta} \left(1 + \frac{1+\zeta}{\zeta} T(E, \phi) \right)} \end{aligned}$$

If $\theta \leq \sqrt{\frac{\zeta}{2(1+\zeta)}}$, $\left(1 - \frac{\theta(1+\zeta)T(E, \phi)}{\zeta} \right) \geq 1 - \frac{2(1+\zeta)\theta^2}{\zeta} \geq 0$, because of (4.21), and then

$$(4.29) \quad T(E, \phi) \left(1 + \frac{(1 + \zeta)T(E, \phi)}{\zeta} \right) \geq \zeta \left(1 - \theta \frac{(1 + \zeta)}{\zeta} T(E, \phi) \right)^2,$$

or what is equivalent

$$(4.30) \quad \left(\frac{1+\zeta}{\zeta} - \frac{(1+\zeta)^2\theta^2}{\zeta} \right) T(E, \phi)^2 + (1 + 2(1+\zeta)\theta) T(E, \phi) - \zeta \geq 0.$$

Thus, since by assumption, $T(E, \phi) > 0$, either $\theta \geq \frac{1}{\sqrt{1+\zeta}}$ or $\theta < \frac{1}{\sqrt{1+\zeta}}$ and

$$(4.31) \quad \begin{aligned} 2\theta \geq T(E, \phi) &\geq \frac{-(1+2\theta(1+\zeta)) + \sqrt{1+4(1+\theta)(1+\zeta)}}{\frac{2(1+\zeta)}{\zeta}(1-(1+\zeta)\theta^2)} \\ &= \frac{2\zeta}{1+2\theta(1+\zeta) + \sqrt{1+4(1+\theta)(1+\zeta)}} \geq \frac{2\zeta}{1+2\sqrt{1+\zeta} + \sqrt{5+4(\zeta + \sqrt{1+\zeta})}} \end{aligned}$$

on the interval $\left(0, \frac{1}{\sqrt{1+\zeta}}\right]$. \square

Step 2 : E_0 is achieved.

Let $\{(E_n, \phi_n)\}$ be a minimizing sequence for E_0 . Since $I_V = 1 + \zeta > 1$, by (4.23), $\zeta \|\phi_n\|_{E_n}^2 \leq (1 + \zeta)T(E_n, \phi_n)$ for all n . Then, by the same arguments as in the proof of Lemma 4.5, we have

$$(4.32) \quad \begin{aligned} (1 + \zeta) \int_{\mathbb{R}^3} V^2 |\phi_n|^2 dx &\leq \|\phi_n\|_{E_n}^2 \leq \frac{(1+\zeta)T(E_n, \phi_n)}{\zeta} \\ &\leq \frac{2(1+\zeta)(E_n+1)}{\zeta} < \frac{2(1+\zeta)}{\zeta} \end{aligned}$$

This implies that

$$(4.33) \quad \int_{\mathbb{R}^3} V^2 |\phi_n|^2 dx + \|\phi_n\|_{E_n} \leq \frac{2(2+\zeta)}{\zeta}$$

Therefore, up to subsequences, we can find $\phi_0 \in L^2(\mathbb{R}^3)$ such that $\phi_n \rightharpoonup \phi_0$ weakly in $L^2(\mathbb{R}^3)$. Moreover, for all $\varepsilon > 0$, there exists $R(\varepsilon) > 0$ such that $\lim_{\varepsilon \rightarrow 0} R(\varepsilon) = +\infty$ and $\|\phi_0\|_{L^2(|x|>R(\varepsilon))} \leq \frac{\varepsilon}{2}$.

From (4.33), $\int_{\mathbb{R}^3} g_{E_n}^{-1} |L\varphi_n|^2 dx \leq C$ for some constant $C > 0$ independent of n . If V is in $L^\infty(\mathbb{R}^3)$, this implies that $\{\varphi_n\}$ is bounded in $H^1(\mathbb{R}^3)$ and relatively compact in $L^q_{loc}(\mathbb{R}^3)$ if $2 \leq q < 6$. If on the contrary, $V(x)$ tends to $-\infty$ when x approaches 0, then $\{\varphi_n\}$ is only bounded in $H^1_{loc}(\mathbb{R}^3 \setminus \{0\})$ and relatively compact in $L^q_{loc}(\mathbb{R}^3 \setminus \{0\})$, $2 \leq q < 6$. In all cases, $\{\phi_n\}$ is relatively bounded in $L^q_{loc}(\mathbb{R}^3 \setminus \{0\})$, $2 \leq q < 6$. Finally, one can use (4.33) to prove that $\{\phi_n\}$ is relatively compact in $L^2_{loc}(\mathbb{R}^3)$ and that

$$(4.34) \quad \int_{\mathbb{R}^3} V|\phi_n|^2 dx \xrightarrow{n \rightarrow \infty} \int_{\mathbb{R}^3} V|\phi_0|^2 dx$$

Up to subsequences, we may consider now that $\lim_n \|\phi_n\|^2$ exists and we define

$$(4.35) \quad M = \lim_n \|\phi_n\|^2 - \|\phi_0\|^2.$$

Let us now prove that

$$(4.36) \quad \phi_n \xrightarrow{n \rightarrow \infty} \phi_0 \text{ in } L^2(\mathbb{R}^3).$$

If $M = 0$, (4.36) holds. Assume, by contradiction, that $M > 0$. By definition of J^+ we have

$$(\phi_n, \phi_n) J_n^2 + 2(\phi_n, (1-V)\phi_n) J_n - (\phi_n, (2-V)V\phi_n) - (\phi_n, H_{E_0}\phi_n) = 0$$

where by J_n we denote $J^+(E_n, \phi_n)$. Now we consider a function $\chi_\varepsilon \in C^2(\mathbb{R}^3)$ such that $\chi_\varepsilon \equiv 1$ on $B(0, \varepsilon^{-1})$, $\text{supp } \chi_\varepsilon \subset B(0, 2\varepsilon^{-1})$ and $\|\nabla \chi_\varepsilon\|_{L^\infty} \leq 2\varepsilon$ and define $\phi_n^\varepsilon = \phi_n \chi_\varepsilon$. Obviously, the weak limit of ϕ_n^ε in $L^2(\mathbb{R}^3)$ is $\phi_0^\varepsilon := \phi_0 \chi_\varepsilon$. For ε small enough, we obtain:

$$(\phi_n, \phi_n)(J_n^2 + 2J_n) - 2(J_n + 1)(\phi_n^\varepsilon, V\phi_n^\varepsilon) + (\phi_n^\varepsilon, V^2\phi_n^\varepsilon) - (\phi_n^\varepsilon, H_{E_0}\phi_n^\varepsilon) > C\varepsilon$$

where C is a negative constant independent of n and ε . Then, we use the lower semicontinuity in X of the quadratic form

$$\phi \mapsto (\phi, H_{E_0}\phi) + (\phi, \phi) - (\phi, V^2\phi)$$

and (4.34)-(4.35) to obtain, as $n \rightarrow +\infty$ and then as $\varepsilon \rightarrow 0$:

$$\begin{aligned} ((\phi_0, \phi_0) + M)(\bar{J}^2 + 2\bar{J}) - 2(\bar{J} + 1)(\phi_0, V\phi_0) \\ + (\phi_0, V^2\phi_0) - (\phi_0, H_{E_0}\phi_0) \geq 0, \end{aligned}$$

where $\bar{J} = \limsup_n J_n$.

Now, since $-1 < \bar{J} < 0$, if $M > 0$ one has:

$$M(\bar{J}^2 + 2\bar{J}) < 0.$$

Hence,

$$(4.37) \quad (\phi_0, \phi_0)\bar{J}^2 + 2(\phi_0, (1-V)\phi_0)\bar{J} - (\phi_0, (2-V)V\phi_0) - (\phi_0, H_{E_0}\phi_0) > \alpha > 0$$

which implies that for large n , either $J_n < J^-(E_0, \phi_0) \leq -1$, which is impossible, or $\underline{\lim}_n J_n > J^+(E_0, \phi_0)$, which contradicts the definition of $E_0 := \lim_n E_n \geq \underline{\lim}_n J_n$. Therefore, necessarily $M = 0$ and $\phi_n \xrightarrow{n \rightarrow \infty} \phi_0$ in $L^2(\mathbb{R}^3)$. This, together with our assumptions on V and lower semi-continuity implies that

$$(4.38) \quad \begin{aligned} & (\phi_0, H_{E_0} \phi_0) + (\phi_0, \phi_0) - (\phi_0, V^2 \phi_0) \leq \\ & \leq \underline{\lim}_n ((\phi_n, H_{E_n} \phi_n) + (\phi_n, \phi_n) - (\phi_n, V^2 \phi_n)), \end{aligned}$$

$$(4.39) \quad \Delta(E_0, \phi_0) \leq \underline{\lim}_n \Delta(E_n, \phi_n) \leq 1,$$

and therefore,

$$(4.40) \quad J^+(E_0, \phi_0) \leq E_0$$

and (E_0, ϕ_0) is a minimizer for E_0 .

Step 3 : Constraint saturation.

Under our assumptions, it is straightforward to see that if (E_0, ϕ_0) is a minimum of problem (4.16), then $J^+(E_0, \phi_0) = E_0$, by definition of E_0 and because the map $E \mapsto J^+(E, \phi_0)$ is continuous. This also shows that

$$(4.41) \quad E_0 = \inf\{J^+(E, \phi) ; \phi \neq 0, (E, \phi) \in (-1, 0) \times X, J^+(E, \phi) = E\}.$$

Step 4 : Euler-Lagrange equations.

By classical computations, there is a Lagrange multiplier $\mu \in \mathbb{R}$ such that (E_0, ϕ_0) is a critical point of the functional $(1 - \mu)E + \mu J^+$, i. e.,

$$(1 - \mu) + \mu \partial_E J^+(E_0, \phi_0) = 0 = \mu \partial_\phi J^+(E_0, \phi_0).$$

These two equalities show that $\partial_\phi J^+(E_0, \phi_0) = 0$, or equivalently

$$H_{E_0} \phi_0 = (E_0 - V)(E_0 + 2 - V)\phi_0 \quad \text{in } \mathcal{D}'(\mathbb{R}^3)$$

i.e., (E_0, ϕ_0) is a solution of (4.4). □

It seems difficult to find a characterization of all potentials V such that the assumptions of Theorem 4.3 hold. But, in order to fix our ideas about the validity range of this result, let us look at Coulomb potentials $-a|x|^{-1}$, $a > 0$.

Proposition 4.6 . *Let us consider $W_1(x) := -|x|^{-1}$. Then, for all $a \in (0, 1)$, $D_{aW_1} \neq \emptyset$ and there is a constant $\zeta_a > 0$ such that*

$$(4.42) \quad I_{aW_1} = 1 + \zeta_a > 1,$$

and therefore, for all $a < 1$ the smallest eigenvalue of $H - \frac{a}{|x|}$ in the interval $(-1, 1)$ is given by the infimum of E over the set D_{aW_1} .

Proof of Proposition 4.6.

It is well known that for all $a < 1$ there exists a smallest eigenvalue of $H - \frac{a}{|x|}$ in the gap of the essential spectrum, $\lambda_1^a > 0$. Moreover, when a approaches 1, λ_1^a converges to 0. This implies the existence of a minimal $E_a = \lambda_1^a - 1$ in $(-1, 0)$ (given by the minimization method of Theorem 4.3) and $\phi_a \in X \setminus \{0\}$ such that (E_a, ϕ_a) is a solution of equation (4.4).

The map $a \mapsto I_{aW_1}$ is continuous. Assume, by contradiction, that $I_{A_1W_1} = 1$ for some $A_1 < 1$. Then, there exist $E_n \in (-1, 0)$, $a_n \rightarrow A_1$ and ϕ_n in X_0 such that $J^+(E_n, \phi_n) \leq E_n$ and

$$(4.43) \quad \int_{\mathbb{R}^3} \frac{|L\varphi_n|^2 + |\varphi_n|^2}{E_n + 2 + a_n|W_1|} = \left(1 + \frac{1}{n}\right) \int_{\mathbb{R}^3} \frac{a_n^2 W_1^2 |\varphi_n|^2}{E_n + 2 + a_n|W_1|}$$

By homogeneity, we can choose the sequence $\{\varphi_n\}$ to satisfy

$$\int_{\mathbb{R}^3} \frac{W_1^2 |\varphi_n|^2}{E_n + 2 + a_n|W_1|} = 1 \quad \text{for all } n.$$

Then, by the definition of J^+ we have

$$(4.44) \quad \begin{aligned} -1 < J^+(E_n, \phi_n) &= -1 + \frac{a_n(\phi_n, W_1\phi_n) + \sqrt{a_n^2(\phi_n, W_1\phi_n)^2 + \frac{a_n^2}{n}\|\phi_n\|^2}}{\|\phi_n\|^2} \\ &\leq -1 + \frac{a_n}{\sqrt{n}\sqrt{(\phi_n, \phi_n)}}. \end{aligned}$$

Now, if $\liminf_n(\phi_n, \phi_n) > 0$, (4.44) implies that $\lim_n J^+(E_n, \phi_n) = -1$, and then for n large, the minimization of J^+ on $D_{a_nW_1}$ provides us with an eigenvalue of $H - a_nW_1$ smaller than the minimum eigenvalue of this operator, λ_1^a . So, up to subsequences one must have

$$(4.45) \quad \lim_n(\phi_n, \phi_n) = 0.$$

Let us show that this is also impossible and so we will have proved that $A_1 = 1$.

If (4.45) holds, we can take a cut-off function $\chi_r \in C^1(\mathbb{R}^3)$, $\chi_r \equiv 1$ on $B(0, r)$, $\text{supp } \chi_r \subset B(0, 2r)$ such that for r small and n large, we have

$$(4.46) \quad \int_{\mathbb{R}^3} \frac{|L(\varphi_n\chi_r)|^2}{|W_1|} dx \leq \beta A_1 \int_{\mathbb{R}^3} |W_1| |\varphi_n\chi_r|^2 dx$$

for some $\beta \in (1, A_1^{-1})$, which is impossible, because for the Coulomb potential one has

$$\inf_{\varphi \in H^{1/2}(\mathbb{R}^3)} \left(\int_{\mathbb{R}^3} |x| |L\varphi|^2 \right) \left(\int_{\mathbb{R}^3} |x|^{-1} |\varphi|^2 \right)^{-1} = 1$$

and A_1 was supposed to be strictly less than 1. □

References

- [1] W.E. Bayliss, S. J. Peel. Stable variational calculations with the Dirac Hamiltonian. *Physical Review A*, **28** (4) (1983), p. 2552-2554.
- [2] C. Bennet, R. Sharpley. *Interpolation of Operators*. Academic Press, 1988.
- [3] A. Berthier, V. Georgescu. Sur la propriété de prolongement unique pour l'opérateur de Dirac. *C. R. Acad. Sci. Paris, Sér. A* **291** (1980), p. 603-606.
- [4] A. Berthier, V. Georgescu. Sur le spectre ponctuel de l'opérateur de Dirac. *C. R. Acad. Sci. Paris, Sér. A* **297** (1983), p. 335-338.
- [5] A. Berthier, V. Georgescu. On the point spectrum for Dirac operators. *J. Func. Anal.* **71** (1987), p. 309-338.
- [6] J.D. Bjorken-S.D. Drell. *Relativistic quantum fields*. McGraw-Hill (1965).
- [7] G.E. Brown, D.G. Ravenhall. On the interaction of two electrons. *Proc. Roy. Soc. London A* **208** (A 1095) (1951), p. 552-559.
- [8] V.I. Burenkov, W.D. Evans. On the evaluation of the norm of an integral operator associated with the stability of one-electron atoms. *Math. Phys. Preprint archive mp-arc* (97-247) (1997).
- [9] S.N. Datta, G. Deviah. The minimax technique in relativistic Hartree-Fock calculations. *Pramana* **30**(5) (1988), p. 393-416.
- [10] I. Daubechies, E.H. Lieb. One-electron relativistic molecules with Coulomb interaction. *Comm. Math. Phys.* **90**(4) (1983), p. 497-510.

- [11] I. Daubechies, E.H. Lieb. Relativistic molecules with Coulomb interaction, in *Differential equations* , I. Knowles and R. Lewis ed., p. 143–148, North-Holland Math. Stud., 92, North-Holland, Amsterdam-New York, 1984.
- [12] G.W.F. Drake, S.P. Goldman. Relativistic sturmian and finite basis set methods in atomic physics. *Adv. Atomic Molecular Phys.* **23**(1988), p. 23-29.
- [13] Ph. Durand. Transformation du Hamiltonien de Dirac en Hamiltoniens variationnels de type Pauli. Application à des atomes hydrogénéoïdes. *C. R. Acad. Sc. Paris* **303** , série II, numéro 2 (1986), p. 119-124.
- [14] Ph. Durand, J.-P. Malrieu. Effective Hamiltonians and pseudo potentials as tools for rigorous modelling. In *Ab initio methods in Quantum Chemistry I*. K.P. Lawley ed.. J. Wiley and sons, 1987.
- [15] M.J. Esteban, E. Séré. Existence and multiplicity of solutions for linear and nonlinear Dirac problems. *Partial Differential Equations and Their Applications*. CRM Proceedings and Lecture Notes, volume 12. Eds. P.C. Greiner, V. Ivrii, L.A. Seco and C. Sulem. AMS, 1997.
- [16] W.D. Evans, P. Perry, H. Siedentop. The spectrum of relativistic one-electron atoms according to Bethe and Salpeter. *Comm. Math. Phys.* **178(3)** (1996), p. 733-746.
- [17] M. Griesemer, H. Siedentop. A minimax principle for the eigenvalues in spectral gaps. To appear in *J. London Math. Soc.*
- [18] G. Hardekopf, J. Sucher. Critical coupling constants for relativistic wave equations and vacuum breakdown in quantum electrodynamics. *Phys. Rev. A* **31(4)** (1985), p. 2020-2029.
- [19] I.W. Herbst. Spectral theory of the operator $(p^2 + m^2)^{1/2} - Ze^2/r$. *Comm. Math. Phys.* **53** (1977), p. 285-294.
- [20] R.N. Hill, C. Krauthauser. *A solution to the problem of variational collapse for the one-particle Dirac equation*. *Phys. Rev. Lett.* **72(14)** (1994), p. 2151-2154.
- [21] T. Kato. *Perturbation theory for linear operators*. Springer, 1966.
- [22] W. Kutzelnigg. Relativistic one-electron Hamiltonians for electrons only' and the variational treatment of the Dirac equation. *Chem. Phys.* (1997).

- [23] A. Le Yaouanc, L. Oliver, J.-C. Raynal. The Hamiltonian $(p^2+m^2)^{1/2}-\alpha/r$ near the critical value $\alpha_c = 2/\pi$. J. Math. Phys. **38(8)** (1997), p. 3397-4012.
- [24] E. van Lenthe, R. van Leeuwen, E.J. Baerends, J.G. Snijders. Relativistic regular two-component Hamiltonians. In *New challenges in computational Quantum Chemistry*. R. Broek et al ed.. Publications Dept. Chem. Phys. and Material sciences. University of Groningen, 1994.
- [25] Selecta of E. H. Lieb. *The stability of matter: from atoms to stars*. Edited by W. Thirring (second edition), Springer.
- [26] E.H. Lieb, H. Siedentop, J.P. Solovej. Stability and instability of relativistic electrons in classical electromagnetic fields. J. Stat. Phys. (1997).
- [27] E.H. Lieb, H. Siedentop, J.P. Solovej. Stability of relativistic matter with magnetic fields. Phys. Rev. Lett. **79(10)** (1997), p. 1755-1758.
- [28] A. Messiah. *Mécanique quantique II*. Masson, Paris, 1960.
- [29] M. Reed, B. Simon. *Methods of Modern Mathematical Physics*. Academic Press, New York, 1978.
- [30] J.D. Talman. Minimax principle for the Dirac equation. Phys. Rev. Lett. **57(9)** (1986), p. 1091-1094.
- [31] B. Thaller. *The Dirac equation*. Springer-Verlag, 1992.
- [32] C. Tix. Strict positivity of a relativistic Hamiltonian due to Brown and Ravenhall. Bull. London Math. Soc. (1998).
- [33] C. Tix. Lower bound for the ground state energy of the no-pair Hamiltonian. Physics Letters B **405** (1997), p. 293-296.