Variational methods in relativistic quantum mechanics: new approach to the computation of Dirac eigenvalues

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1 Abstract.

The main goal of this paper is to describe some new variational methods for the characterization and computation of the eigenvalues and the eigenstates of Dirac operators. Our methods are all based on exact variational principles, both of min-max and of minimization types. The minimization procedure that we introduce is done in a particular set of functions satisfying a nonlinear constraint. Finally, we present several numerical methods that we have implemented in particular cases, in order to construct approximate solutions of that minimization problem.

2 Introduction.

The free Dirac operator has been successfully used in the description of the kinematics of the electron. It is a first order operator which, in the appropriate units, has the form

$$H_0 = i\,\vec{\alpha}\cdot\vec{\nabla} + \beta \tag{1}$$

where $\vec{\alpha}\cdot\vec{\nabla} = \sum_{k=1}^{3} \alpha_k \partial_k$ and α_k are the Pauli-Dirac matrices,

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

σ_k being the well-known 2×2 matrices Pauli matrices :

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

The spectrum of the free Dirac operator is only continuous and we have :

$$\sigma(H_0) = (-\infty, -1] \cup [1, +\infty) .$$

The total unboudedness of $\sigma(H_0)$ creates many difficulties which are not present in its nonrelativistic limit, the Schrödinger operator, which is semi-bounded. The difficulties associated with the numerical computation of Dirac eigenvalues are known under the generic name of *variational collapse* .

The basic equation describing an electron evolving in an exterior scalar potential V is

$$i\,\partial_t\,\Psi = (H_0 + V)\Psi \quad \text{in} \quad \mathbb{R} \times \mathbb{R}^3 . \tag{2}$$

When looking for stationary states of (2) of the form $\Psi(t,x) = e^{-i\lambda t}\,\psi(x)$, one checks that the wave function ψ has to satisfy the following stationnary equation:

$$(H_0 + V)\,\psi = \lambda\,\psi \quad \text{in} \quad \mathbb{R}^3 . \tag{3}$$

Equality (3) is an eigenvalue equation which corresponds to bound states of the electron if ψ is square integrable in $\mathbb{R}^3$. For those states to be stable, the eigenvalue λ has to be in the gap of the spectrum of H_0, *i.e.* in $(-1, 1)$. In particular, if it exists, the smallest eigenvalue (or the smallest positive eigenvalue) of $H_0 + V$ in the gap $(-1, 1)$, corresponds to the ground-state level of the electron in the potential V (in the sense that its nonrelativistic limit is the ground-state level of the limiting Schrödinger equation).

In the case of a semibounded operator H like the Schrödinger operator, finding the ground-state corresponds to minimizing the Rayleigh quotient

$$R(\psi) := \frac{((H + V)\psi, \psi)}{(\psi, \psi)} , \tag{4}$$

where by $(\cdot, \cdot)$ we denote either the $L^2(\mathbb{R}^3)$- inner product or, when necessary, a duality product. There are many practical ways of tackling the problem of minimizing a function like $R(\psi)$.

In the case of the Dirac potential H_0, and for standard potentials V, minimizing $R(\psi)$ is useless, because it takes us to $-\infty$. On the other hand, the solutions of (3) correspond to critical points of $R(\psi)$. Hence, one has to find ways of characterizing non-minimization variational problems to find the eigenvalues of $H_0 + V$ in the interval $(-1, 1)$. Many works have been devoted to this question. W. Kutzelnigg has written two excellent reviews on this subject, where many relevant references can be found : [14, 15]. The main approaches to this problem can be classified in three groups:

1) Use of approximate Hamiltonians: the first idea is to replace equation (3) by another one in which the main operator is semibounded. In general this

is done by reducing equation (3) to a system of two equations for the upper and lower spinors in ψ. Then, one eliminates the lower spinor and shows that this system is equivalent to an equation for the upper spinor which involves a semibounded Hamiltonian. For instance, the above reduction can be done via the Foldy-Wouthuysen transformation. Finally, approximate Hamiltonians are constructed by considering different expansions of the exact Hamiltonian in powers of $1/c^2$ or other small quantities. This method yields models which are perturbations of the nonrelativistic one. To this category of works belong for instance [8, 9, 16, 17, 15].

2) Using appropriate finite "basis", with the right asymptotic (or other) behavior and thus avoiding to fall into the negative continuum $(-\infty, -1)$. This is equivalent to projecting the equation onto a well chosen space. For instance, this has been done in [7, 14].

3) Finding variational approaches other than simple minimization like minimization of Rayleigh quotients for the squared Hamiltonian $(H_0 + V)^2$ (see [20, 1]) or later on, maximization of the Rayleigh quotients for the "inverse Hamiltonian" $((H_0 + V)\psi, \psi)/((H_0 + V)^2\psi, \psi)$ (see [13]).

Actually, it is rather easy to see that the eingenstates of $(H_0 + V)$ should be obtained by defining appropriate min-max procedures for the Rayleigh quotient. This idea was first put forward by Talman [18]. Then other proposals followed : [10, 11, 4, 12, 5]. In these papers, various min-max and constrained minimization procedures were described and justified for some families of potentials.

Our work places itself in the third direction, but still uses the idea of eliminating the lower spinor in terms of the upper one, without any further approximation. In this paper, we present three different alternatives for the characterization and computation of all the eigenvalues of $H_0 + V$ in the gap of the essential spectrum of $H_0 + V$. Of course, in order to define these variational procedures, one has to choose a class of potentials V for which the operator $H_0 + V$ is well defined. In some sense, V has to be not "too strong" with respect to H_0. The class of potentials for which our methods work include sums of powers $-\gamma_i |x|^{-\beta_i}$, β_i being positive, but satisfying $\beta_i \leq 1$. Hence, sums of Coulomb potentials are admissible. Even if it is not always necessary, our presentation will be simplified if we make the assumption that V is an attractive potential, *i.e.* V is nonpositive everywhere in $\mathbb{R}^3$. For more details about the precise assumptions which are necessary on V see below and [4, 5].

3 Min-max approaches.

As far as the Dirac operator is concerned, the first works in this direction are those of Talman [18] and Datta-Deviah [3]. In [18] Talman proposed the following strategy : if any 4-spinor $\psi \in \mathbb{C}^4$ is seen as a pair $\psi = \binom{\varphi}{\chi}$, with φ, χ taking

values in $\mathbb{C}^2$, let us compute the following min-max

$$\inf_{\varphi \neq 0} \sup_{\chi} \frac{(\psi, (H_0 + V)\psi)}{(\psi, \psi)} \ . \tag{5}$$

Talman claimed that the above min-max yields in fact the ground-state energy of the operator $H_0 + V$. This assertion is very interesting, since the decomposition of any spinor ψ into its upper and lower components, φ and χ, is indeed much easier to implement than projections based on spectral decomposition of H_0. The dificulty here is to give appropriate conditions on the potential for the approach to be valid.

In [10] another min-max strategy was proposed. This was the first rigorous approach to the variational solution of the problem under study and we present an improved version of it below. Then, the first abstract min-max characterization for the eigenvalues of operators with gaps was given by Griesemer and Siedentop in [11]. In [11], we also find the first mathematical justification of the correctness of Talman's min-max for a class of bounded potentials V. Other results in this direction have been proved in [4, 12].

The min-max approach which seems to apply to the largest class of potentials is described in [5]. In that paper, we use an abstract variational method together with an appropriate continuation argument which allows us to treat all potentials V which are not too singular at the origin and which, being self-adjoint, have a smallest eigenvalue in the interval $(-1, 1)$ which "comes from the positive continuum", that is, which is close to 1 for small values of the coupling constant γ. In particular, this method is applicable to the Coulomb potentials $-\gamma\,|x|^{-1}$, in the optimal class $\gamma \in (0, 1)$.

The main result concerning the min-max in [5] is the following. Let us consider an operator $H_0 + \gamma V_1$, where V_1 is a given scalar potential and $\gamma > 0$ is a coupling constant. Assume that there is an orthogonal decomposition of $\mathcal{H} = L^2(\mathbb{R}^3, \mathbb{C}^4)$ as $\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_-$ and let us denote by $\Lambda_\pm$ the projectors associated to this decomposition.

Assume moreover that

(i) there exists a dense subspace F of $H^1(\mathbb{R}^3, \mathbb{C}^4)$, such that $F_\pm := \Lambda_\pm F$ are two subspaces of $H^{1/2}(\mathbb{R}^3, \mathbb{C}^4)$.

(ii) $a := \sup_{\psi \in F_- \setminus \{0\}} \dfrac{(\psi, H_0\,\psi)}{\|\psi\|^2_{\mathcal{H}}} < +\infty$.

Then, we define the min-max levels :

$$\lambda_{k,\gamma}(V_1) := \inf_{\substack{W \text{ subspace of } F_+ \\ \dim W = k}} \sup_{\psi \in (W \oplus F_-)\setminus\{0\}} \frac{(\psi, (H_0 + \gamma V_1)\,\psi)}{||\psi||^2_{\mathcal{H}}} \ , \quad k \geq 1 \, , \tag{6}$$

and we assume that

(iii) $\lambda_{1,0}(V_1) > a$.

On V_1 we make the hypothesis:

(iv) $V_1(x) \underset{|x|\to+\infty}{\longrightarrow} 0$,

Then, if we define $b := \inf\{\sigma_{ess}(H_0 + \gamma V_1) \cap [a, +\infty)\}$, we can state the following result (see [5]) :

Under the above assumptions (i)-(iv), for all $\gamma > 0$ such that $H_0 + \gamma V_1$ can be defined as a self-adjoint operator with domain included in $H^{1/2}(\mathbb{R}^3, \mathbb{C}^4)$ and such that $\lambda_{1,\gamma}(V_1) > a + \gamma \sup_{\mathbb{R}^3} V_1$, all the eigenvalues of $H_0 + \gamma V_1$ in the interval (a, b) are given by the sequence $\lambda_{k,\gamma}(V_1)$. In particular, the energy of the ground-state is equal to $\lambda_{1,\gamma}(V_1)$. Note that if there is no eigenvalue of $H_0 + \gamma V_1$ in the interval (a, b) then all the min-max values $\lambda_{k,\gamma}$ are equal to b.

So, in this result it is not necessary to assume that the potentials are attractive. In this particular case, the assumption $\lambda_{1,\gamma}(V_1) > a + \gamma \sup_{\mathbb{R}^3} V_1$ is of course replaced by $\lambda_{1,\gamma}(V_1) > a$.

Let us notice that a simple case in which are satisfied all the assumptions for the above result to hold is given by γ and V_1 satisfying:

$$-\frac{\nu}{|x|} - c_1 \leq V_1 \leq c_2 = \sup_{\mathbb{R}^3} V_1 < +\infty\,,$$

$$c_1, c_2 \geq 0\,,\ \gamma(c_1 + c_2) < 1 + \sqrt{1 - \gamma^2 \nu^2}\,,$$

and $a = -1$.

The above result can be particularized to various cases in which different decompositions of $\mathcal{H}$ are considered. A possible decomposition corresponds to the projectors associated with the free Dirac operator, that is, $\Lambda_+ = \chi_{(0,+\infty)}(H_0)$ and $\Lambda_- = \chi_{(-\infty,0)}(H_0)$. Another decomposition which seems simpler for actual computations corresponds to considering the upper and the lower spinors separately, *i. e.* :

$$\text{for } \psi = \begin{pmatrix} \varphi \\ \chi \end{pmatrix}, \quad \Lambda_+\psi = \begin{pmatrix} \varphi \\ 0 \end{pmatrix}\,,\ \Lambda_-\psi = \begin{pmatrix} 0 \\ \chi \end{pmatrix}\,. \tag{7}$$

Let us also notice that with the above decomposition (7), $\lambda_{1,\gamma}(V_1)$ is the min-max proposed by Talman. In particular, the above result proves that Talman's min-max yields indeed the first eigenvalue of $H_0 + \gamma V_1$ for all potentials V_1 and all constants γ such that the above properties are satisfied. In the particular case of the Coulomb potentials $-\gamma |x|^{-1}$, this means being able to consider any γ between 0 and 1, the optimal range of self-adjointness. Note also that less singular potentials like $\gamma|x|^{-\beta}$ can be dealt with as long as $\beta \in (0, 1)$ and γ is such that $\lambda_{1,\gamma}(V_1) > -1$.

4 Minimization method and corresponding min-max approaches.

4.1 A constrained minimization method.

In [4] we reduced the computation of the first eigenvalue of a large family of Dirac operators to the consideration of a minimization problem in a class of functions described by a nonlinear constraint. Below we describe this method, since we believe that it can be useful in numerical computations or at least in understanding the positivity properties of constrained problems.

First, one reduces the eigenvalue for the 4-spinor $\psi = \binom{\varphi}{\chi}$ to a system of two equations for the 2-spinors φ and χ. This is a common procedure when trying to construct approximate semibounded Hamiltonians, as was described in the Introduction.

Let us introduce a shift of length -1 in the eigenvalues: $E = \lambda - 1$, so that for λ to be in the spectral gap $(-1, 1)$, E has to be in the interval $(-2, 0)$. Next, notice that the equation $(H_0 + V)\,\psi = \lambda\,\psi = (E+1)\,\lambda$ is equivalent to the system

$$\left\{ \begin{array}{rcl} L\chi & = & (E - V)\,\varphi \\ L\varphi & = & (E + 2 - V)\,\chi \end{array} \right. \tag{8}$$

with $L = i(\vec{\sigma}\cdot\vec{\nabla}) = \sum_{k=1}^{3} i\sigma_k \partial/\partial x_k$. As long as $E + 2 - V \neq 0$, the system (8) can be written as

$$L\Big(\frac{L\varphi}{g_{_E}}\Big) + V\varphi \;=\; E\varphi\;, \quad \chi = \frac{L\varphi}{g_{_E}} \tag{9}$$

with $g_{_E} = E + 2 - V$. Note that for attractive potentials V ($V \leq 0$ a. e.), $g_E \neq 0$ for all E in the gap $(-2, 0)$.

Then, we consider $\phi = \varphi/\sqrt{g_{_E}}$ which solves the equation

$$H_E\phi := \sqrt{g_{_E}}\; L\Big(\frac{1}{g_{_E}} L(\sqrt{g_{_E}}\;\phi)\Big) = (E - V)(E + 2 - V)\phi \tag{10}$$

where the operator H_E defined in (10) is symmetric.

Thus, any $E \in (-2, 0)$, eigenvalue of the operator $H_0 + V - 1$, with associated eigenfunction $\varphi = \sqrt{g_E}\,\phi$, is a solution of the equation

$$(\phi, \phi)\,E^2 + 2(\phi, (1 - V)\phi)E - (\phi, (2 - V)V\phi) - (\phi, H_E\phi) = 0\,, \tag{11}$$

which is quadratic in E if we forget the dependence of H_E on E. So, E is necessarily solution of one of the following equations :

$$E = J^{\pm}(E, \phi) := \frac{1}{(\phi, \phi)}\Big(\pm\,\sqrt{\Delta(E, \phi)} - \Big(\phi, (1 - V)\phi\Big)\Big) \tag{12}$$

where $\Delta(E,\phi) := |(\phi, V\phi)|^2 + (\phi,\phi)[(\phi,\phi)+(\phi, H_E\phi)-(\phi, V^2\phi)]$.

Note that if $T(E,\phi) := [(\phi,\phi)[(\phi,\phi) + (\phi, H_E\phi) - (\phi, V^2\phi)]$ is nonnegative, then the range of J^- (resp. J^+) is contained in the interval $(-\infty, -1]$ (resp. $[-1, +\infty)$). Hence, eigenvalues E corresponding to positive energies λ necessarily satisfy the equation $E = J^+(E,\phi)$.

By a simple continuation argument, one can see that for a large family of potentials, the inequality $T(E,\phi) \geq 0$ is equivalent to the existence of a gap around 0 in the spectrum of $H_0 + V$. Hence, one can try to compute the smallest positive eigenvalue of $H_0 + V$ by just minimizing the functional $J^+(E,\phi)$ in the set $\{(E,\phi)\,;\, J^+(E,\phi) = E\}$. And indeed, we prove in [4] that under appropriate assumptions, the solution of this minimization problem is a ground-state for $H_0 + V - 1$ (at this level, we do not discuss the regularity conditions required on the functions ϕ). The class of potentials $-\gamma|x|^{-\beta}$ is again admissible for all $\beta \in (0,1]$ and $\gamma > 0$ not too large. In the case $\beta = 1$, the condition on γ is again optimal : $0 < \gamma < 1$.

4.2 Relationship with Talman's min-max.

In Section 3, we introduced a general class of min-max problems yielding the eigenvalues of $H_0 + V$ in the interval $(-1, 1)$. Here, the same has been achieved for the positive ground state of the electron moving in the potential V. Actually, it is not difficult to see that there is a strong relationship between the two methods, specially in the case in which the decomposition of the 4-spinors is the one which corresponds to the consideration of the upper and lower 2-spinors separately. As pointed out above, this was actually the proposal made by Talman. Let us come back to that min-max for potentials γV_1, $\gamma > 0$:

$$\lambda_1^\gamma = \inf_{\varphi \neq 0} \sup_\chi \frac{(\psi, (H_0 + \gamma V_1)\psi)}{(\psi,\psi)} \quad , \quad \psi = \begin{pmatrix} \varphi \\ \chi \end{pmatrix}. \tag{13}$$

If one tries to apply the result of Section 3, one sees that a can be chosen to be equal to -1. Moreover, one can explicitly solve the maximization problem in χ as follows : for every φ, the supremum

$$\lambda^\gamma(\varphi) := \sup_\chi \frac{(\psi, (H_0 + \gamma V_1)\psi)}{(\psi,\psi)} \quad , \quad \psi = \begin{pmatrix} \varphi \\ \chi \end{pmatrix} \tag{14}$$

is achieved by

$$\chi^\gamma(\varphi) := \frac{L\varphi}{1 - \gamma V_1 + \lambda^\gamma(\varphi)}, \tag{15}$$

and $\lambda^\gamma(\varphi)$ is the unique number in $(-1, +\infty)$ such that

$$\lambda^\gamma(\varphi) \int_{\mathbb{R}^3} |\varphi|^2 dx = \int_{\mathbb{R}^3} \Big(\frac{|L\varphi|^2}{1 - \gamma V_1 + \lambda^\gamma(\varphi)} + (1 + \gamma V_1)|\varphi|^2 \Big) dx\,, \tag{16}$$

So, finally, λ_1^γ can be defined as the minimum (in φ) of all $\lambda^\gamma(\varphi)$. This is again a minimization problem with a nonlinear constraint.

This minimization method is actually equivalent to the one described in Section 4.1 and they are both rigorously justified for the same class of potentials.

5 Some related numerical computations.

In this section we present recent numerical results that have been obtained for the very particular class of potentials $-\gamma|x|^{-\beta}$, with $\gamma > 0$, $0 < \beta \leq 1$ and in some specific cases (see [6]). Our aim has been to show that these new variational techniques could help to better understand how to perform computations in relativistic quantum mechanics, without having to care about variational collapse, boundary conditions, choice of good special basis of functions, etc.

More precisely, we have implemented three methods, one based on shooting arguments and the other two, on variational ones. The first one is used as a comparison test for the variational method. Note that for $\beta = 1$, the exact eigenvalues are explicitly known, wich provides us with a good test for the computations.

Let V be a radial attractive scalar potential and let us try compute the first positive eigenvalue of $H_0 + V$. Since V is radial (see for instance [19, 2]) the eigenfunctions of $H_0 + V$ can be expressed in terms of the spherical harmonics according to the decomposition

$$\begin{aligned} L^2(\mathbb{R}^3;\mathbb{C}^4) = \quad & L^2(]0,+\infty[, r^2dr;\mathbb{C}) \\ & \bigotimes \left(\bigoplus_{j=\frac{1}{2},\frac{3}{2},\ldots}^{+\infty} \bigoplus_{m_j=-j}^{+j} \bigoplus_{\kappa_j=\pm(j+\frac{1}{2})} \mathcal{K}_{m_j,\kappa_j} \right). \end{aligned}$$

of the set of the square integrable functions defined on $\mathbb{R}^3$ with values in $\mathbb{C}^4$. Any spinor $\psi \in L^2(\mathbb{R}^3\ \mathbb{C}^4)$ can therefore be written as

$$\psi(x) = \sum_{\substack{j,m_j,\kappa_j \\ \epsilon=\pm}} \frac{1}{|x|} f^\epsilon_{m_j,\kappa_j}(|x|)\Phi^\epsilon_{m_j,\kappa_j}(\frac{x}{|x|}) \tag{17}$$

where

$$\Phi^+_{m_j,\mp(j+1/2)} = \begin{pmatrix} i\Psi^{m_j}_{j\mp1/2} \\ 0 \end{pmatrix}, \quad \Phi^-_{m_j,\mp(j+1/2)} = \begin{pmatrix} 0 \\ \Psi^{m_j}_{j\pm1/2} \end{pmatrix} \tag{18}$$

generate the space $\mathcal{K}_{m_j,\kappa_j}$ and can be expressed in terms of the spherical harmonics as follows :

$$\Psi^{m_j}_{j-1/2} = \frac{1}{\sqrt{2j}} \begin{pmatrix} \sqrt{j+m_j}\, Y^{m_j-1/2}_{j-1/2} \\ \sqrt{j-m_j}\, Y^{m_j+1/2}_{j-1/2} \end{pmatrix}, \tag{19}$$

$$\Psi^{m_j}_{j+1/2} = \frac{1}{\sqrt{2j+2}} \begin{pmatrix} \sqrt{j+1-m_j}\, Y^{m_j-1/2}_{j+1/2} \\ -\sqrt{j+1+m_j}\, Y^{m_j+1/2}_{j+1/2} \end{pmatrix} , \tag{20}$$

where $(Y^m_l)^{m=-l,-l+1,...l}_{l=0,1,2...}$ are the usual spherical harmonics. The radial Dirac operator acting on the set of the square integrable real functions on $(0,+\infty)$, $L^2(0,+\infty)$, is

$$h_\kappa = \begin{pmatrix} 1+V & -\frac{d}{dr}+\frac{\kappa}{r} \\ \frac{d}{dr}+\frac{\kappa}{r} & -1+V \end{pmatrix} \quad \kappa = \pm 1,\ \pm 2, ... \tag{21}$$

and the eigenvalue problem takes the form

$$\begin{cases} u' = (1+\lambda)v - (Vv + \frac{\kappa}{r}u) \\ v' = (1-\lambda)u + (Vu + \frac{\kappa}{r}v) \end{cases} \tag{22}$$

The solutions of this system are characterized by two parameters, λ and $\delta = v(1)/u(1)$ for instance, and we shall denote by X the set of the solutions of (22) such that $u(1) = 1$ when λ and δ vary in $\mathbb{R}$. However, the condition that u and v are in $L^2(0,+\infty)$ determines uniquely λ and δ. One can show that this integrability condition is equivalent to assuming that

$$\begin{array}{c} \lim_{r\to 0_+} r(|u(r)|^2 + |v(r)|^2) = 0 , \\ \lim_{r\to+\infty}(|u(r)|^2 + |v(r)|^2) = 0 , \end{array} \tag{23}$$

thus providing a simple numerical ("shooting") method to determine λ and δ (we shall refer to this method by the letter "s" and use it to compare the numerical results with the numerical minimization method given below).

Let us describe now a first numerical minimization method, which uses the special form (22) of the eigenvalue problem and goes along the main lines of the method described in Section 4.1. Similarly to (9), in (22) v can be eliminated in terms of u:

$$\frac{v}{r^\kappa} = (r^{2\kappa}(1+\lambda-V))^{-1}\frac{d}{dr}(r^\kappa u) . \tag{24}$$

For many central potentials, the ground-state of $H_0 + V$ is a solution of (22), with $\kappa = -1$. For instance, in the case of Coulomb potentials, there is no square integrable solution of (22) when $\kappa = 1$ and the ground-state is achieved for $\kappa = -1$. The eigenvalue problem (22) for $\kappa = -1$ is now equivalent to solving

$$h^\lambda\phi = (1+\lambda-V)(1-\lambda+V)\phi \tag{25}$$

where h^λ is a symmetric operator

$$h^\lambda\phi = \sqrt{1+\lambda-V}\,\frac{d}{dr}\left[\frac{r^2}{1+\lambda-V}\frac{d}{dr}(\sqrt{1+\lambda-V}\phi)\right] \tag{26}$$

and $\phi(r) = r^{-1}u(r)/\sqrt{1+\lambda-V}$ is now a function defined on $(0,+\infty)$. Equation (10) is then equivalent to

$$(\phi,\phi)\lambda^2 - 2(\phi,V\phi)\lambda + (\phi,V^2\phi) - [(\phi,\phi) + (\phi,h_\lambda\phi)] = 0 \tag{27}$$

where $(\cdot,\cdot)$ is the usual scalar product in $L^2(0,+\infty)$ (and $\|\cdot\|$ the corresponding norm). The eigenvalue problem is then reduced to finding a critical point of $J^+(\lambda-1,\cdot)$ with $\lambda - 1 = J^+(\lambda-1,\phi)$ and

$$J^+(\lambda-1,\phi)+1 = \frac{\sqrt{\Delta(\lambda-1,\phi)} + (\phi,V\phi)}{\|\phi\|^2}\ , \tag{28}$$

$$\Delta(\lambda-1,\phi) = (\phi,V\phi)^2 + \|\phi\|^2[(\phi,h_\lambda\phi) + \|\phi\|^2 - (\phi,V^2\phi)]\ . \tag{29}$$

To solve this constrained problem numerically, the natural idea is to introduce a penalization method and to minimize

$$J^+(\lambda-1,\phi) + A|(\lambda-1) - J^+(\lambda-1,\phi)|^2$$

in the limit $A \to +\infty$. In practical computations, one has to consider positive constants A large enough to ensure that the constraint is "almost" satisfied. Actually if we assume that ϕ is given by (26) with (u,v) in X, the condition that u and v are in $L^2(0,+\infty)$ is equivalent to assuming that the integrals involved in the expression (28) are finite. Of course these integrals are numerically computed on an interval (ϵ,R), because there is a singularity at $r=0$ and one wants to compute the integral in a finite interval. So, the approximate value $J^+_{\epsilon,R}$ of J^+ is finite even if the constraint is not satisfied, but we observe that $\lim_{(\epsilon,R)\to(0,+\infty)} J^+_{\epsilon,R}(\lambda-1,\phi) = +\infty$ unless $\lambda - 1 = J^+(\lambda-1,\phi)$. Hence, a minimization of J^+ (numerically of $J^+_{\epsilon,R}$) on the set X takes care of the constraint $\lambda - 1 = J^+(\lambda-1,\phi)$ automatically. This method will be referred by the letter "m" in Tables 1 and 2. Note that from a mathematical point of view, this is also a shooting method in (λ,δ).

In Table 1 below we present a comparison of the shooting (s) and the minimization (m) methods for $\kappa = -1$, $V(r) = -\gamma r^{-\beta}$, $\gamma = 0.5$ and $\beta \in (0,1)$. The system (22) is numerically solved with a stepsize adaptative Runge-Kutta method on the interval $(\epsilon = 10^{-4}, R = 15)$. For the shooting method we minimize the quantity $\epsilon(|u(\epsilon)|^2 + |v(\epsilon)|^2) + \theta(|u(R)|^2 + |v(R)|^2) = \Delta_{\rm s}$ for some scale parameter $\theta > 0$, while for the minimization method, the quantity $J^+(\lambda-1,\phi)$ is directly minimized, the quantity $CEr := |J^+(\lambda-1,\phi) - (\lambda-1)|^2$ being computed *a posteriori*. The parameter θ is chosen in order that the terms $\epsilon(|u(\epsilon)|^2 + |v(\epsilon)|^2)$ and $\theta(|u(R)|^2 + |v(R)|^2)$ have the same maximum value on the boundary of the domain of minimization. For $\beta = 1$, the result is known explicitly: $\lambda_1 = [1-\gamma^2]^{1/2} = 0.866025...$, $\delta_1 = -[(1-\lambda)/(1+\lambda)]^{1/2} = -0.267949...$. For practical reasons, the results given here correspond to parameters taken in a neighborhood of (δ_1,λ_1). The results correspond therefore to the branch $(\delta_\beta,\lambda_\beta)$ starting from (δ_1,λ_1) at $\beta = 1$ and parametrized by β.

Table 1:

β	$\delta_{\rm s}$	$\delta_{\rm m}$	$\lambda_{\rm s}$	$\lambda_{\rm m}$	J^+	CEr	$\Delta_{\rm s}$
1	-0.267954	-0.267943	0.866034	0.866013	0.866014	$1.8\ 10^{-12}$	0.00029
0.9	-0.235187	-0.235174	0.856725	0.856698	0.856698	$2.1\ 10^{-14}$	0.00053
0.8	-0.207802	-0.207788	0.843181	0.843146	0.843146	$5.2\ 10^{-14}$	0.00063
0.7	-0.183397	-0.183379	0.825877	0.825832	0.825831	$4.3\ 10^{-13}$	0.00076
0.6	-0.160651	-0.160627	0.804699	0.804639	0.804639	$4.1\ 10^{-13}$	0.00094
0.5	-0.138654	-0.138619	0.779161	0.779071	0.779070	$3.4\ 10^{-13}$	0.0012
0.4	-0.116645	-0.116584	0.748381	0.748221	0.748220	$3.8\ 10^{-13}$	0.0018
0.3	-0.0938375	-0.0937016	0.710904	0.710537	0.710536	$3.5\ 10^{-13}$	0.0049
0.2	-0.069224	-0.068798	0.664252	0.663067	0.663067	$2.4\ 10^{-13}$	0.0097
0.1	-0.0412322	-0.0392963	0.60391	0.59833	0.59833	$1.4\ 10^{-13}$	0.018

The main advantage of the minimizing approach is that it can be extended to the case of nonsymmetric (non central) potentials, but of course for a minimizing set which is larger than X.

We will now assume that the potential is radial, but consider a general basis of $L^2(0,+\infty)$ (of course well chosen). For that purpose, we introduce a third formulation, which is intermediate between the abstract min-max theory and the minimization of J^+, and goes as follows. Its main advantage is that the constraint $E = J^+(E,\phi)$ will then be automatically satisfied. We will therefore call this method the "direct minimisation method".

As in Equation (9) we may rewrite system (8) as

$$L\Big(\frac{L\varphi}{\lambda+1-V}\Big)+V\varphi \;=\; (\lambda-1)\varphi\;,\quad \chi=\frac{L\varphi}{\lambda+1-V}\,, \tag{30}$$

at least if $\lambda\in(-1,1)$ and if V is nonpositive almost everywhere. Multiplying the equation (30) by φ and integrating with respect to $x\in\mathbb{R}^3$, we obtain :

$$\begin{aligned} f_\varphi(\lambda) := \quad & \int_{\mathbb{R}^3}\frac{|L\varphi|^2}{\lambda+mc^2-V}\,dx \\ = \quad & (\lambda-1)\int_{\mathbb{R}^3}|\varphi|^2\,dx-\int_{\mathbb{R}^3}V|\varphi|^2\,dx =: g_\varphi(\lambda)\;. \end{aligned} \tag{31}$$

Since for a given φ, $f_\varphi(\lambda)$ is decreasing and $g_\varphi(\lambda)$ is increasing in λ, if there exits a $\lambda=\lambda(\varphi)$ such that (31) is satisfied, then it is unique (the existence of such a λ for all φ depends on the properties of the potential V). According to Section 4.2, for those V's, the ground state is such that

$$\lambda_1=\min_\varphi\lambda(\varphi)\;. \tag{32}$$

One can solve (32) by any numerical minimization method. A possible way to do it to consider a finite basis $\{\varphi_1, \ldots, \varphi_n\}$ and define $\lambda(x_1, \ldots, x_n)$ by :

$$\ell(x_1, \ldots, x_n) := \lambda\big(\sum_{i=1}^{n} x_i\, \varphi_i\big).$$

Then,

$$\lambda_1^n := \inf_{(x_1,\ldots,x_n)\in \mathbb{R}^n} \ell(x_1, \ldots, x_n)$$

is an approximation of $\lambda_1(V)$ which can be found by any well suited minimization algorithm.

In order ot simplify the presentation, we come back to the radially symmetric situation in which the potential V is central and we can decompose the whole problem by using spherical spinors. This is not necessary, but has the advantage of being easier to describe.

For a radial potential we may use the radial Dirac equation and consider (22) instead of (8). Define $\lambda = \lambda_r(u)$ as the unique solution of

$$\begin{aligned} f(\lambda) = &\quad \int_0^{+\infty} \frac{|(r^\kappa u)'|^2}{r^{2\kappa}(1+\lambda-V(r))}\, dr \qquad (33)\\ = &\quad (\lambda-1)\int_0^{+\infty} |u(r)|^2\, dr - \int_0^{+\infty} V(r)|u(r)|^2\, dr := g(\lambda)\,. \end{aligned}$$

(Notice that the existence of $\lambda_r(u)$ depends on the assumptions made on the potential V). Then, λ_1 is given by :

$$\lambda_1 = \inf_u \lambda_r(u)\,.$$

To solve equation (33) numerically it is more convenient to rewrite $f(\lambda)$ as an alternated series :

$$f(\lambda) = \sum_{k=0}^{+\infty}\Big[(-1)^k \int_0^{+\infty} \frac{r^{-2\kappa}|(r^\kappa u)'|^2}{(1-V(r))^{k+1}}\, dr\Big]\lambda^k\,. \qquad (34)$$

¿From a numerical point of view, the solution (with $\kappa = -1$) is approximated on a finite basis of $L^2(0,\infty)$, $(u_i)_{i=1,2,\ldots n}$: $u = \sum_{i=1}^n x_i u_i$. If

$$f_{ijk} = (-1)^{k-1}\int_0^{+\infty} \frac{r^2(u_i/r)'(u_j/r)'}{(1-V(r))^k}\, dr \qquad (35)$$

and

$$V_{ij} = \int_0^{+\infty} u_i(r)u_j(r)V(r)\, dr\,, \qquad (36)$$

the approximating equation for λ corresponding to (33) is then

$$\sum_{i,j=1}^{n} \left((\sum_{k=1}^{m} f_{ijk} \lambda^{k-1}) + V_{ij} \right) x_i x_j + (1-\lambda) \sum_{i=1}^{n} x_i^2 = 0 \,, \tag{37}$$

where the series in λ has been truncated at order m. It is actually more convenient to define

$$A^{n,m}(\lambda) = \left((\sum_{k=1}^{m} f_{ijk} \lambda^{k-1}) + (1-\lambda)\delta_{ij} + V_{ij} \right)_{i,j=1,2,\ldots n}$$

and to approximate λ_1 by $\lambda_1^{n,m}$ defined as the first positive root of $\lambda \mapsto \mu_1(\lambda) := \mu(A^{n,m}(\lambda))$ where $\mu(A)$ denotes the first eigenvalue of the matrix A. The function $\lambda \mapsto \mu_1(\lambda)$ is indeed continuous, nonincreasing in λ and such that $\mu_1(0) > 0$ when we make the right assumptions on the potential V, *i.e.* when V is not too strong with respect to H_0 (this corresponds to the hypothesis made in Section 3). Moreover, if there exist $x_1, \ldots, x_m$ such that (37) holds, then $\mu_1(\lambda) \leq 0$. Hence, indeed $\lambda_1^{n,m} = inf\{\lambda > 0 \,;\, \mu_1(\lambda) \leq 0\}$.

Note that $(\lambda_1^{n,m} - \lim_m \lambda_1^{n,m})_{m \geq 1}$ is an alternating sequence (essentially converging at a geometric rate): consider indeed $u = \sum_{i=1}^{n} x_i \, u_i$.

$$\sigma_m^n(\lambda) = \sum_{\substack{i,j=1,\ldots n \\ k=1,\ldots m}} x_i x_j f_{ijk} \lambda^{k-1} = \sum_{k=1}^{m} \int_0^{+\infty} (-1)^{k-1} \frac{r^2 |(u/r)'|^2}{(1-V)^k} \lambda^{k-1} \, dr$$

$$= \int_0^{+\infty} \frac{r^2}{1-V} \, |(u/r)'|^2 \, \frac{1 - \left(\frac{-\lambda}{1-V}\right)^m}{1 + \frac{\lambda}{1-V}} \, dr.$$

If $V \leq 0$ a.e., $(1-V) \geq 1$, so that the series $(\sigma_m^n(\lambda))_{m \in I\!N}$ is an alternating sequence (and $(\lambda/(1-V))^m$ converges at a geometric rate).

The results in Table 2 have been obtained by taking an orthonormal basis generated by the ground state of the hydrogen atom and $n-1$ Hermite functions, with $n = 10$. Our purpose in this numerical computation was not to provide very accurate results but just to prove the feasibility of such a numerical approach. Clearly, depending on the specific properties of the potential, the choice of a well suited basis should greatly improve the accuracy of the computation. More precisely, we have considered $V(r) = -\gamma r^{-\beta}$, $\gamma = 0.5$ and β close to 1. The approximating space is of dimension $n = 10$ and the series are truncated at $m = 14$ or $m = 15$ (the corresponding values $\lambda_1^{10,14}$ and $\lambda_1^{10,15}$ are respectively a lower and an upper bound of $\lim_{m \to +\infty} \lambda_1^{10,m}$). As in Table 1, J^+ is obtained through a minimization procedure on the set X, and $\Delta_{\rm m}$ measures the error (in the L^2-norm) when the corresponding solution is approximated on the basis (with $n = 10$ elements) used for the direct minimisation method.

Table 2:

β	0.90	0.93	0.95	0.97	0.99	1.00
$\lambda_1^{10,14}$	0.855681	0.858516	0.860228	0.861792	0.863200	0.863843
$\lambda_1^{10,15}$	0.858012	0.861112	0.863004	0.864749	0.866338	0.867071
J^+	0.856698	0.859984	0.861954	0.863735	0.865310	0.866014
$\Delta_{\rm m}$	0.0082	0.0058	0.0046	0.0033	0.0020	0.0022

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