Spectral results and open problems for Dirac-Coulomb operators with general charge distributions

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The free Dirac Hamiltonian

$$\mathbf{H} = \mathbf{H_0} = -i\,\alpha\cdot\nabla + \beta\,, \qquad \alpha_1,\ \alpha_2,\ \alpha_3,\ \beta \in \mathcal{M}_{4\times4}(\mathbb{C}) \qquad (c = m = \hbar = 1)$$

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

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

Two of the main properties of H are :

$$\mathbf{H_0}^2 = -\Delta + 1\,, \qquad \sigma(\mathbf{H_0}) = (-\infty, -1] \cup [1, +\infty)$$

Remark. acts on functions $\psi : \mathbb{R}^3 \to \mathbb{C}^4$

Eigenvalues below / in the middle of the essential spectrum

Spectrum of a self-adjoint operator A ($-\Delta + V$, $\mathbf{H_0} + V$) :

Eigenvalues below / in the middle of the essential spectrum

Spectrum of a self-adjoint operator $A\,(-\Delta + V\,,\quad \mathbf{H_0} + V\,)$:

In the first case, $\lambda_1 = \min\limits_{x \neq 0} \dfrac{(Ax, x)}{||x||^2}$, $\lambda_2 = \min\ \max\ \dfrac{(Ax, x)}{||x||^2}$, etc ...

In the second case, $\lambda_1 = \min\limits_{?}\ \max\limits_{?}\ \dfrac{(Ax, x)}{||x||^2}$, ...

Abstract min-max theorem (with Jean Dolbeault and Eric Séré, 2000)

Let $\mathcal{H}$ be a Hilbert space and $A : D(A) \subset \mathcal{H} \to \mathcal{H}$ a self-adjoint operator. Let F be a core for A, that is, a subset of $D(A)$, dense in $D(A)$ for the $D(A)$-topology. Let $\mathcal{H}_+$, $\mathcal{H}_-$ be two orthogonal Hilbert subspaces of $\mathcal{H}$ such that $\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_-$. Define $F_\pm := P_\pm F$.

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(i) $a_- := \sup_{x_- \in F_- \setminus \{0\}} \frac{(x_-, Ax_-)}{\|x_-\|^2_{\mathcal{H}}} < +\infty$.

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Let
$$c_k = \inf_{\substack{V \text{ subspace of } F_+ \\ \dim V = k}} \ \sup_{x \in (V \oplus F_-)\setminus\{0\}} \frac{(x, Ax)}{||x||^2_{\mathcal{H}}}, \qquad k \geq 1.$$

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If (ii) $c_1 > a_-$,

then c_k is the k-th eigenvalue of A in the interval (a_-, b), where $b = \inf\left(\sigma_{\text{ess}}(A) \cap (a_-, +\infty)\right)$.

NOTE : See also related results by Griesemer and Siedentop, and very recent ones by L. Schimmer, J. P. Solovej, and S. Tokus (2019).

Application to Dirac operators I (Talman's decomposition)

$$\psi:\mathbb{R}^3\to\mathbb{C}^4\,,\quad \psi=\begin{pmatrix}\varphi\\ \chi\end{pmatrix}=\begin{pmatrix}\varphi\\ 0\end{pmatrix}+\begin{pmatrix}0\\ \chi\end{pmatrix}\,,\quad \varphi,\chi:\mathbb{R}^3\to\mathbb{C}^2$$

Assume also that the potential V satisfies

$$\lim_{|x|\to+\infty} V(x)\;=\;0\,,\quad -\frac{\nu}{|x|}\le V\le 0\,,\quad (0<\nu\le 1)$$

Then, for all $k\ge 1$,

$$\lambda_k(\mathbf{H_0}+V)=\inf_{\substack{Y \text{ subspace of } C_o^\infty(\mathbb{R}^3,\mathbb{C}^2)\\ \dim Y=k}}\ \sup_{\varphi\in Y\setminus\{0\}}\ \sup_{\substack{\psi=\begin{pmatrix}\varphi\\ \chi\end{pmatrix}\\ \chi\in C_0^\infty(\mathbb{R}^3,\mathbb{C}^2)}}\frac{(\psi,(\mathbf{H_0}+V)\psi)}{(\psi,\psi)}$$

Application to Dirac operators II (Talman's decomposition)

In particular, the first eigenvalue of $\mathbf{H_0} + V$ in the gap $(-1, 1)$ is given by

$$\lambda_1(\mathbf{H_0} + V) := \inf_{\varphi \neq 0} \sup_{\chi} \frac{(\psi, (\mathbf{H_0} + V)\psi)}{(\psi, \psi)}, \qquad \psi = \begin{pmatrix} \varphi \\ \chi \end{pmatrix}$$

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$$\lambda(\varphi) := \sup_{\substack{\psi = \begin{pmatrix} \varphi \\ \chi \end{pmatrix} \\ \chi \in C_0^\infty(\mathbb{R}^3, \mathbb{C}^2)}} \frac{(\psi, (\mathbf{H_0} + V)\psi)}{(\psi, \psi)}$$

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is the unique number λ such that

$$\lambda \int_{\mathbb{R}^3} |\varphi|^2 dx = \int_{\mathbb{R}^3} \Big(\frac{|\sigma \cdot \nabla \varphi|^2}{1 - V + \lambda} + (1 + V)|\varphi|^2 \Big) dx .$$

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AND

$$\lambda_1(\mathbf{H_0} + V) = \inf_{\varphi \neq 0} \lambda(\varphi) \text{ with } \int_{\mathbb{R}^3} \Big(\frac{|\sigma \cdot \nabla \varphi|^2}{\lambda(\varphi) + 1 - V} + (V + 1 - \lambda(\varphi)) |\varphi|^2 \Big) dx = 0 .$$

Consequence I : towards easy to implement algorithms

We want to find the minimum of all $\lambda(\varphi)$ over all possible φ in :

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Let $A(\lambda)$ be the operator defined via the quadratic form which acts on 2-spinors :

$$(\varphi, A(\lambda)\varphi) := \int_{\mathbb{R}^3} \left(\frac{|\sigma \cdot \nabla \varphi|^2}{\lambda + 1 - V} + (V + 1 - \lambda)\, |\varphi|^2 \right) dx$$

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Since $A(\lambda)$ is monotone decreasing with respect to λ, there exists a unique λ such that $\mu_1(\lambda) = 0$.

THEOREM : The unique root of $\mu_1(\lambda) = 0$ is the first eigenvalue of $\mathbf{H_0} + V$ in the gap $(-1, 1)$.

Discretisation

Consider an n-dimensional space of functions from $\mathbb{R}^3$ to $\mathbb{C}^2$ and generated by $\varphi_1, \varphi_2, \ldots, \varphi_n$

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Let $A_n(\lambda)$ the $n \times n$ matrix whose elements are given by

$$A_n^{i,j}(\lambda) = \int_{\mathbb{R}^3} \left(\frac{(\sigma \cdot \nabla \varphi_i, \sigma \cdot \nabla \varphi_j)}{\lambda + 1 - V} + (V + 1 - \lambda)(\varphi_i, \varphi_j) \right) dx$$

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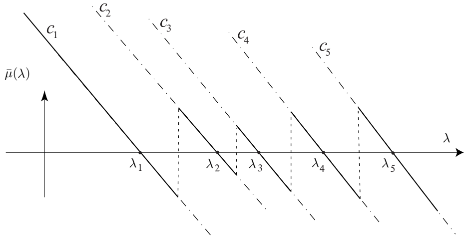
Let $\mu_1^n(\lambda)$ the smallest eigenvalue of $A_n(\lambda)$

Then, the unique zero of the map $\lambda \mapsto \mu_1^n(\lambda)$, λ_1^n, is an approximation of the first eigenvalue of $\mathbf{H_0} + V$ in the gap $(-1, 1)$.

Idea of how the algorithm works



Each curve $\mathcal{C}_i$ corresponds to the set $\{\,(\lambda, \mu_i(\lambda)\,\}$ where $\mu_i(\lambda)$ is the i-th eigenvalue of the matrix $A_n(\lambda)$ or the operator $A(\lambda)$.

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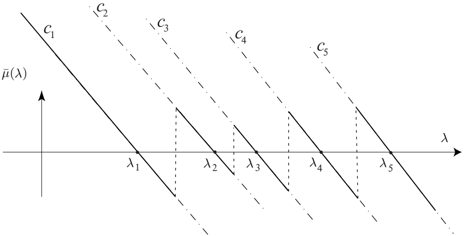

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The value λ_i such that $\mu_i(\lambda_i) = 0$ is the i-th eigenvalue of $\mathbf{H_0} + V$ in the spectral "gap" $(-1, 1)$.

Some computations

We have used this algorithm to make

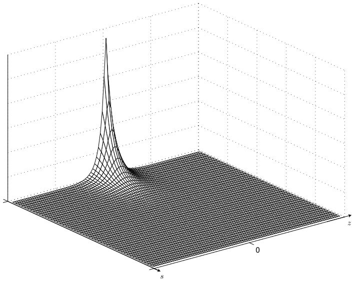
– **atomic computations** (basically a $1d$ problem) for H, He^+, Cr^{23+} and Th^{89+}

Basis formed by Hermite polynomials or B-splines

– **Diatomic molecular computations** (2-d problem in cylindrical coordinates), for H_2^+ and Th_2^{179+}

B-splines

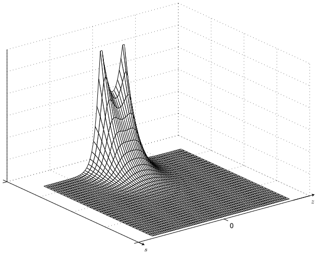
Some figures I (Dolbeault-E.-Séré-Vanbreugel, 2000)



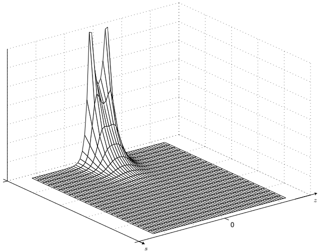
Fundamental state of Th^{89+} corresponding to $Z = 90$, one atom

J. Dolbeault, M.J. Esteban, E. Séré, M. Vanbreugel. *Phys. Rev. Letters* (2000)

Some figures II (Dolbeault-E.-Séré, 2003)



Fundamental state of H_2^+ corresponding to $Z = 1$, two atoms.



Fundamental state of Th_2^{179+} corresponding to $Z = 90$, two atoms

J. Dolbeault, M.J. Esteban, E. Séré. *Int. J. Quant. Chem.* (2003)

The limitations of this approach and solutions

– In which basis sets can we implement our numerical computations ?

– What are the domains of these operators ?

Self-adjoint extensions of the minimal operator $D_V := \mathbf{H_0} + V$ defined on $C_c^\infty(\mathbb{R}^3 \setminus \{0\}, \mathbb{C}^2)$

– Si $V = -\nu/|x|$, $0 < \nu < \sqrt{3}/2$, the minimal operator is essentially self-adjoint, and $\mathcal{D} = H^1(\mathbb{R}^3, \mathbb{C}^4)$ (Rellich, 1953)

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– For $\sqrt{3}/2 \leq \nu < 1$, Nenciu (see also Klaus and Wüst ; 1973-1979) gave a definition of a self-adjoint extension with domain $H^1(\mathbb{R}^3, \mathbb{C}^4) \subset \mathcal{D} \subset H^{1/2}(\mathbb{R}^3, \mathbb{C}^4)$.

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– For $\sqrt{3}/2 \leq \nu \leq 1$, E.-Loss (2008) found another definition of the self-adjoint extension with domain

$$\mathcal{D} := \left\{ \psi = \begin{pmatrix} \varphi \\ \chi \end{pmatrix} \in \mathcal{H}_{+1} \times L^2(\mathbb{R}^3, \mathbb{C}^2) \ : \ D_V^* \psi \in L^2(\mathbb{R}^3, \mathbb{C}^4) \right\} .$$

where $\mathcal{H}_{+1}$ is the closure of $C_c^\infty(\mathbb{R}^3 \setminus \{0\}, \mathbb{C}^2)$ for the norm $q_E^{1/2}$, with

$$q_E(\varphi) := \int_{\mathbb{R}^3} \frac{|\sigma \cdot \nabla \varphi(x)|^2}{1 - V(x) + E} \, dx + \int_{\mathbb{R}^3} (1 + V(x) - E) |\varphi(x)|^2 \, dx \, .$$

Subcritical case $0 < \nu < 1$ (Lewin - E. - Séré 2017)

THEOREM : Assume that $V(x) \geq -\frac{\nu}{|x|}$, $0 < \nu < 1$, $\sup(V) < 2$ and let

$$\mathcal{V} := \Big\{ \varphi \in L^2(\mathbb{R}^3, \mathbb{C}^2) \cap H^1_{\rm loc}(\mathbb{R}^3 \setminus \{0\}, \mathbb{C}^2) \ : (2 - V)^{-1/2}\, \sigma \cdot \nabla \varphi \in L^2(\mathbb{R}^3, \mathbb{C}^2) \Big\}.$$

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Then $C^\infty_c(\mathbb{R}^3 \setminus \{0\}, \mathbb{C}^2)$ is dense in $\mathcal{V}$ for the norm

$$\|\varphi\|_{\mathcal{V}} := \|(2 - V)^{-1/2} \sigma \cdot \nabla \varphi\|_{L^2} + \|\varphi\|_{L^2} \,.$$

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In addition, we have the continuous embedding $\mathcal{V} \subset H^{1/2}(\mathbb{R}^3, \mathbb{C}^2)$.

Then the distinguished self-adjoint extension of the minimal operator D_V is also the unique extension with domain included in

$$\left\{\psi = \begin{pmatrix}\varphi\\ \chi\end{pmatrix} \in L^2(\mathbb{R}^3, \mathbb{C}^4) \ : \ \varphi \in \mathcal{V}\right\}.$$

More precisely, the domain of this extension is

$$\mathcal{D} = \left\{\psi = \begin{pmatrix}\varphi\\ \chi\end{pmatrix} \in L^2(\mathbb{R}^3, \mathbb{C}^4) \ : \ \varphi \in \mathcal{V},\ D_V^*\psi \in L^2(\mathbb{R}^3, \mathbb{C}^4)\right\}.$$

Critical case $\nu = 1$ (Lewin - E. - Séré 2017)

In the Coulomb case $V(x) = -|x|^{-1}$ we introduce

$$\mathcal{W}_{\rm C} = \left\{ \varphi \in L^2(\mathbb{R}^3, \mathbb{C}^2) \ : \ \frac{\sigma \cdot \nabla |x| \varphi}{|x|^{1/2}(1+|x|)^{1/2}} \in L^2(\mathbb{R}^3, \mathbb{C}^2) \right\}. \tag{1}$$

Then we assume that $V(x) \geq -|x|^{-1}$ and that $\sup(V) < 1$ and we introduce the space

$$\mathcal{W} = \left\{ \varphi \in \mathcal{W}_{\rm C} \ : \ \left(\frac{1}{1 - V(x)} - \frac{|x|}{1+|x|} \right)^{1/2} \sigma \cdot \nabla \varphi \in L^2(\mathbb{R}^3, \mathbb{C}^2), \right.$$
$$\left. \left(V(x) + \frac{1}{|x|} \right)^{1/2} \varphi \in L^2(\mathbb{R}^3, \mathbb{C}^2) \right\}. \tag{2}$$

Critical case $\nu = 1$ (II)

THEOREM : We assume that

$$V(x) \geq -\frac{1}{|x|} \qquad \text{and} \qquad \sup(V) < 1.$$

Then the space $C_c^\infty(\mathbb{R}^3 \setminus \{0\}, \mathbb{C}^2)$ is dense in $\mathcal{W}_{\mathrm{C}}$ and in $\mathcal{W}$ for their respective norms. Also, we have the continuous embeddings

$$\mathcal{W} \subset \mathcal{W}_{\mathrm{C}} \subset H^s(\mathbb{R}^3, \mathbb{C}^2)$$

for every $0 \leq s < 1/2$.

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Moreover, the minimal operator D_V has a unique self-adjoint extension with domain $\mathcal{D}$ satisfying $\mathcal{D} \subset \left\{\psi = \begin{pmatrix}\varphi \\ \chi\end{pmatrix} \in L^2(\mathbb{R}^3, \mathbb{C}^4) \ : \ \varphi \in \mathcal{W}\right\}$ and we have

$$\mathcal{D} = \left\{\psi = \begin{pmatrix}\varphi \\ \chi\end{pmatrix} \in L^2(\mathbb{R}^3, \mathbb{C}^4) \ : \ \varphi \in \mathcal{W},\ D_V^*\psi \in L^2(\mathbb{R}^3, \mathbb{C}^4)\right\}.$$

Consequences for the min-maxes (MJE - M. Lewin - E. Séré 2017)

MAIN THEOREM : Assume that $0 < \nu \leq 1$ and

$$V(x) \geq -\frac{\nu}{|x|}\,, \quad \sup(V) < 1 + \sqrt{1-\nu^2}$$

Take any space F such that $C_c^\infty(\mathbb{R}^3 \setminus \{0\}, \mathbb{C}^4) \subseteq F \subseteq H^{1/2}(\mathbb{R}^3, \mathbb{C}^4)$.

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Then, the number λ_k defined via the min-max of the abstract theorem, for the Talman decomposition, is independent of the subspace F.

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Take any space F such that $C_c^\infty(\mathbb{R}^3 \setminus \{0\}, \mathbb{C}^4) \subseteq F \subseteq H^{1/2}(\mathbb{R}^3, \mathbb{C}^4)$.

Then, the number λ_k defined via the min-max of the abstract theorem, for the Talman decomposition, is independent of the subspace F.

Corollary.- We are extremely free when computing eigenvalues by discretizing the min-max formula ! And this for all $0 < \nu \leq 1$!

Consequences for the min-maxes (MJE - M. Lewin - E. Séré 2017)

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Morozov and Müller (2015) : min-max in $H^{1/2}$, $\nu < 1$ (spectral decomposition for the free Dirac operator), $\nu < 2/(\frac{2}{\pi} + \frac{\pi}{2})$ (Talman decomposition).

Schimmer-Solovej-Tolkus (2018) : min-max in C^∞, $\nu \leq 1$, for Talman decomposition, alternative min-max.

The (extended) molecular case :
(MJE - M. Lewin - E. Séré, 2 articles, 2021)

1) The molecular case : $\mathbf{H}_0 - \sum_{m=1}^{M} \frac{\nu_m}{|x-R_m|}$ is a particular case of the more general one $\mathbf{H}_0 - \mu \star \frac{1}{|x|}$, where μ is any finite (sometimes nonnegative) Borel measure.

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(ii) All the eigenvalues of $\mathbf{H}_0 - \mu \star \frac{1}{|x|}$ in the gap $(-1, 1)$ are given by the min-maxes defined by the abstract min-max procedure presented before.

Comments on the eigenvalues

For all positive Borel measures μ, we can define the min-maxes λ_k as in the abstract theorem. And it is easy to see that $a_- = -1$.

So, only if $\lambda_1 > -1$, all the λ_k, $k \geq 1$ will be the eigenvalues of $\mathbf{H}_0 - \mu \star \frac{1}{|x|}$ in the spectral gap $(-1, 1)$.

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For general measures μ as above, if $t > 0$ is small enough,

$$\lambda_1(\mathbf{H}_0 - t\,\mu \star \frac{1}{|x|}) > -1 \quad \text{(stability)}$$

and there exists $t_\mu > 0$ such that as $t \uparrow t_\mu$

$$\lambda_1(\mathbf{H}_0 - t\,\mu \star \frac{1}{|x|}) \longrightarrow -1$$

Open questions and conjectures I

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THM.- ν_1 is the **best constant in the Hardy-type inequality**

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for every $\phi \in C_c^\infty(\mathbb{R}^3, \mathbb{C}^2)$ and every finite non-negative measure $\mu \geq 0$.

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Conjecture 1.- The optimal $\nu_1 = 1$.

Open questions and conjectures II

If $\sum_{m=1}^{M} \nu_m$ is small enough, we have proved that

$$\lim_{R_m \to 0,\ \forall m} \lambda_1 \left(\mathbf{H}_0 - \sum_{m=1}^{M} \frac{\nu_m}{|x - R_m|} \right) = \lambda_1 \left(\mathbf{H}_0 - \frac{\sum_{m=1}^{M} \nu_m}{|x|} \right) = \sqrt{1 - \left(\sum_{m=1}^{M} \nu_m \right)^2}$$

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When $M = 2$ the conjecture is supported numerically : [McConnell, 2013] and [Artemyev-Surzhykov-Indelicato-Plunien-Stöhlker, 2010].

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In the nonrelativistic case, the result is known to be true. In this case λ_1 is defined by a minimization problem, which yields the result without much effort by using some **concavity argument.** Lieb, Simon and Hoffman-Ostenhof have generalized this to the multi-electron case.

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The above conjecture holds true is a μ is a **radially symmetric measure**, because by Newton's theorem, we have the *pointwise* bound

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This is the only known case where we have a definite answer for the conjecture.

THANK YOU

FOR

YOUR ATTENTION !