Hardy inequalities and Dirac Operators

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Standard Hardy inequality

Let $u \in H^1(\mathbb{R}^N)$ and consider

$$\int_{\mathbb{R}^N} \left| \nabla u + \tfrac{N-2}{2} \frac{x}{|x|^2} u \right|^2 dx \geq 0 \ .$$

Develop this square and integrate by parts using the identity $\nabla \cdot \left(\frac{x}{|x|^2}\right) = \frac{N-2}{|x|^2}$

$$\boxed{\int_{\mathbb{R}^N} |\nabla u|^2 \, dx \geq \frac{1}{4}(N-2)^2 \int_{\mathbb{R}^N} \frac{|u|^2}{|x|^2} \, dx}$$

It is *optimal* (take appropriate truncations of $x \mapsto |x|^{-(N-2)/2}$): the operator $-\Delta - \frac{A}{|x|^2}$ is nonnegative if and only if $A \leq \frac{1}{4}(N-2)^2$. Optimality has to be taken with care: improvements with l.o.t. in L^2 by Brezis-Vazquez, in $W^{1,q}$ with $q < 2$ by Vazquez-Zuazua, and logarithmic terms by Adimurthi & al. $N = 3$ from now on.

Some notations

Free Dirac operator:

$$H_0 = -i\,\alpha\cdot\nabla + \beta\,, \quad \text{with } \alpha_1,\ \alpha_2,\ \alpha_3,\ \beta \in \mathcal{M}_{4\times 4}(\mathbb{C})$$

$$\beta = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & -\mathbb{1} \end{pmatrix}\,,\ \alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix}$$

Pauli matrices:

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

Decomposition into upper / lower component: $\Psi = \begin{pmatrix} \varphi \\ \chi \end{pmatrix}$

$$H_0\Psi = \begin{pmatrix} R\chi + \varphi \\ R\varphi - \chi \end{pmatrix}\,, \quad \text{with } R = -i\,\sigma\cdot\nabla$$

Two of the main properties of H_0 are:

$$H_0^2 = -\Delta + 1$$

and

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

Denote by $Y^{\pm}$ the spaces $\Lambda^{\pm}(H^{1/2}(\mathbb{R}^3, \mathbb{C}^4))$, where $\Lambda^{\pm}$ are the positive and negative spectral projectors on $L^2(\mathbb{R}^3, \mathbb{C}^4)$ corresponding to the free Dirac operator: Λ^+ and $\Lambda^- = \mathbb{1}_{L^2} - \Lambda^+$ have both infinite rank and satisfy

$$H_0\,\Lambda^+ \;=\; \Lambda^+ H_0 \;=\; \sqrt{1-\Delta}\;\;\Lambda^+ \;=\; \Lambda^+\,\sqrt{1-\Delta}\,,$$

$$H_0\,\Lambda^- \;=\; \Lambda^- H_0 \;=\; -\sqrt{1-\Delta}\;\;\Lambda^- \;=\; -\Lambda^-\,\sqrt{1-\Delta}\,.$$

With $R = -i\,\sigma \cdot \nabla$, $\quad R^2 = -\Delta$.

Hardy inequality for the operator R

Proposition 1 *With the above notations, for any* $\varphi \in H^{1/2}(\mathbb{R}^3, \mathbb{C}^2)$,

$$\int_{\mathbb{R}^3} \frac{|(\sigma \cdot \nabla)\varphi|^2}{1 + \frac{1}{|x|}}\, dx + \int_{\mathbb{R}^3} |\varphi|^2\, dx \;\geq\; \int_{\mathbb{R}^3} \frac{|\varphi|^2}{|x|}\, dx$$

This is a consequence of the following inequality, which is slightly more general: for all $\varphi \in H^{1/2}(\mathbb{R}^3, \mathbb{C}^2)$ and all $\nu \in (0, 1]$,

$$\nu \int_{\mathbb{R}^3} \frac{|\varphi|^2}{|x|} + \sqrt{1 - \nu^2} \int_{\mathbb{R}^3} |\varphi|^2 \leq \int_{\mathbb{R}^3} \frac{|(\sigma \cdot \nabla)\varphi|^2}{\frac{\nu}{|x|} + 1 + \sqrt{1 - \nu^2}} + \int_{\mathbb{R}^3} |\varphi|^2$$

Replace $\varphi(x)$ by $\varphi\left(\frac{x}{\mu}\right)$ and let $\mu \to 0$.

$$\int_{\mathbb{R}^3} \frac{|\varphi|^2}{|x|}\, dx \le \int_{\mathbb{R}^3} |x||(\sigma\cdot\nabla)\varphi|^2\, dx \quad \text{for all} \quad \varphi \in H^{1/2}(\mathbb{R}^3, \mathbb{C}^2)$$

Actually, taking $\phi = |x|^{1/2}\varphi$, this inequality has to be directly related to the standard Hardy inequality

$$\int_{\mathbb{R}^3} \frac{|\varphi|^2}{|x|} = \int_{\mathbb{R}^3} \frac{|\phi|^2}{|x|^2} \le 4\int_{\mathbb{R}^3} |\nabla\phi|^2 = 4\int_{\mathbb{R}^3} \left| |x|^{1/2}\nabla\phi + \frac{1}{2}\frac{x}{|x|^{3/2}}\phi \right|^2$$

$$\int_{\mathbb{R}^3} \frac{|\varphi|^2}{|x|}\, dx \le \int_{\mathbb{R}^3} |x|\, |\nabla\varphi|^2\, dx$$

Connection with the spectrum of the Dirac operator

Let $\lambda_1(V)$ be the lowest eigenvalue of H_0+V in the gap $(-1,1)$ of the continuous spectrum of H_0+V (under appropriate assumptions on V). Let $\Psi = \begin{pmatrix} \varphi \\ \chi \end{pmatrix}$ be the corresponding eigenfunction.

$$(H_0+V)\Psi = \lambda_1(V)\Psi$$

means, for $R = -i\,c\,(\sigma\cdot\nabla)$

$$\begin{cases} R\,\chi &= (\lambda_1(V) - c^2 - V)\varphi \\ R\,\varphi &= (\lambda_1(V) + c^2 - V)\,\chi \end{cases}$$

which can be solved by

$$\begin{cases} \chi = (\lambda_1(V) + c^2 - V)^{-1} R\,\varphi \\ R\left(\frac{R\,\varphi}{\lambda_1(V)+c^2-V}\right) = (\lambda_1(V) - c^2 - V)\,\varphi \end{cases}$$

Multiplying by φ and integrating with respect to $x \in \mathbb{R}^3$, we get :

$$\int_{\mathbb{R}^3} \frac{|R\,\varphi|^2}{\lambda_1(V) + c^2 - V}\, dx + \int_{\mathbb{R}^3} V|\varphi|^2\, dx + (c^2 - \lambda_1(V)) \int_{\mathbb{R}^3} |\varphi|^2\, dx = 0$$

Note that for any fixed ϕ

$$\lambda \mapsto \int_{\mathbb{R}^3} \frac{|R\,\phi|^2}{\lambda + c^2 - V}\, dx + \int_{\mathbb{R}^3} V|\phi|^2\ dx\ + (c^2 - \lambda) \int_{\mathbb{R}^3} |\phi|^2\ dx$$

is monotone decreasing. We shall see that $\lambda_1(V)$ and ϕ can be characterized as follows

$\lambda_1(V)$ is the smallest λ for which

$$\int_{\mathbb{R}^3} \frac{|R\,\phi|^2}{\lambda + c^2 - V}\, dx + \int_{\mathbb{R}^3} V|\phi|^2\ dx\ + (c^2 - \lambda) \int_{\mathbb{R}^3} |\phi|^2\ dx \geq 0\ \forall\, \phi$$

and φ is the corresponding optimal function.

The generalized Hardy inequality is recovered with $\lambda = \sqrt{1 - \nu^2}$.

Other standard Hardy type inequalities

Define the spectral projectors:

$$\Lambda^+ = \chi_{(0,+\infty)}(H_0) \quad \text{and} \quad \Lambda^- = \chi_{(-\infty,0)}(H_0)$$

Using the Fourier transform $u(x) \mapsto \widehat{u}(\xi)$, we get

$$\widehat{H}_0 = i\,\alpha \cdot \xi + \beta\,, \quad \widehat{H}_0^2 = |\xi|^2 + 1\,,$$

$$H_0^2 = -\Delta + 1\,.$$

1) Using $-\Delta \geq \frac{1}{4}\frac{1}{|x|^2}$ (Hardy inequality), $|H_0| = \Lambda^+ H_0 \Lambda^+ - \Lambda^- H_0 \Lambda^-$ satisfies

$$\boxed{|H_0| \geq \frac{\kappa}{|x|} \quad \kappa = \frac{1}{2}}$$

$Z\,\alpha \leq \kappa$ with $\alpha^{-1} = 137.037...$ means $Z \leq 68$.

2) *Kato's inequality.*

$$|H_0| \geq \frac{\kappa}{|x|} \qquad \kappa = \frac{2}{\pi} = 0.63662...$$

$Z\alpha \leq \kappa$ means $Z \leq 87$. Optimal [Herbst].

3) An inequality for the Brown & Ravenhall operator [Burenkov, Evans, Perry, Siedentop, Tix]:

$$B := \Lambda^+ \left(H_0 - \frac{\kappa}{|x|} \right) \Lambda^+ \geq 0 \qquad \kappa = \frac{2}{\frac{2}{\pi} + \frac{\pi}{2}} = 0.906037...$$

B was introduced by Bethe and Salpeter. κ is sharp. $Z\alpha \leq \kappa$ means $Z \leq 124$.

Min-max characterization of the discrete spectrum

Kato's inequality and related inequalities have no evident relation with the spectrum of H_0: $\nu = \frac{2}{\pi}$ or $\nu = \frac{2}{2/\pi+\pi/2}$ are not critical for the (point) spectrum of $H_0 - \frac{\nu}{|x|}$. The operator

$$H_\nu := H_0 - \frac{\nu}{|x|}\,, \quad 0 < \nu < 1$$

has a self-adjoint extension with domain included in $H^{1/2}(\mathbb{R}^3, \mathbb{C}^4)$ and its spectrum is given by

$$\sigma(H_\nu) = (-\infty, -1] \cup \{\lambda_1^\nu, \lambda_2^\nu, \ldots\} \cup [1, \infty)\,, \quad \lim_{\nu \to 1} \lambda_1^\nu = 0\,.$$

H_ν is self-adjoint only for $\nu < 1$. The notion of "first eigenvalue" in $(-1, 1)$ does not make sense for $\nu \geq 1$.

Assume that $V \in M^3(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ and $\exists\, \delta > 0$ such that

$$(H) \qquad \pm\, \Lambda^\pm\, (H_0 + V)\, \Lambda^\pm \geq \delta\, \Lambda^\pm \sqrt{1 - \Delta}\, \Lambda^\pm \quad \text{in } H^{1/2}(\mathbb{R}^3, \mathbb{C}^4)$$

With $Y^\pm = \Lambda^\pm H^{1/2}(\mathbb{R}^3, \mathbb{C}^4)$, define

$$c_k(V) = \inf_{\substack{F \subset Y^+ \\ F \text{ vector space} \\ \dim F = k}} \ \sup_{\substack{\psi \in F \oplus Y^- \\ \psi \neq 0}} \frac{((H_0 + V)\psi, \psi)}{(\psi, \psi)}$$

Theorem 1 *[J.D., Esteban, Séré] Under assumption (H), if* $V \in L^\infty(\mathbb{R}^3 \setminus \overline{B}_{R_0})$ *for some* $R_0 > 0$ *is such that*
$\lim_{R \to +\infty} \|V\|_{L^\infty(|x|>R)} = 0$, $\lim_{R \to +\infty} \text{supess}_{|x|>R} V(x)|x|^2 = -\infty$,
then $\{c_k(V)\}_{k \geq 1}$ *is the non-decreasing sequence of eigenvalues of* $H_0 + V$ *in the interval* $[0, 1)$, *counted with multiplicity, and*

$$0 < \delta \leq c_1(V) = \lambda_1(V) \leq \ldots c_k(V) = \lambda_k(V) \leq \ldots \leq 1\ , \ \lim_{k \to +\infty} c_k(V) = 1$$

Griesemer and Siedentop proved an abstract result which implies the above min-max characterization for the eigenvalues of $H_0 + V$ for a certain class of potentials V (which does not include singularities close to the Coulombic ones). This has

Remark. Any potential V such that $|V| \leq a|x|^{-\beta} + C$ belongs to $M^3(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ for all a, $C > 0$, $\beta \in (0, 1)$. If $|V| \leq a|x|^{-1}$, then (H) is satisfied if $a < 2/(\pi/2 + 2/\pi) \approx 0.9$. Moreover, any $V \in L^\infty(\mathbb{R}^3)$ satisfies (H) if $||V||_\infty < 1$.

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

$$\pm\Lambda^\pm(H_0 + \kappa V)\Lambda^\pm \geq \delta(\kappa)\Lambda^\pm \quad \textit{in } H^{1/2}(\mathbb{R}^3, \mathbb{C}^4)$$

Further min-max results: Talman's decomposition

$$\mathcal{H}_+^T = L^2(\mathbb{R}^3, \mathbb{C}^2) \otimes \left\{ \begin{pmatrix} 0 \\ 0 \end{pmatrix} \right\}, \quad \mathcal{H}_-^T = \left\{ \begin{pmatrix} 0 \\ 0 \end{pmatrix} \right\} \otimes L^2(\mathbb{R}^3, \mathbb{C}^2) ,$$

so that, for any $\psi = \binom{\varphi}{\chi} \in L^2(\mathbb{R}^3, \mathbb{C}^4)$,

$$\Lambda_+^T \psi = \begin{pmatrix} \varphi \\ 0 \end{pmatrix} , \quad \Lambda_-^T \psi = \begin{pmatrix} 0 \\ \chi \end{pmatrix} .$$

Assume also that the potential V satisfies

$$\lim_{|x| \to +\infty} V(x) = 0 , \quad -\frac{\nu}{|x|} - c_1 \leq V \leq c_2 = \sup(V) ,$$

with $\nu \in (0,1)$ and $c_1, c_2 \in \mathbb{R}$. Finally, define the 2-spinor space $W := C_0^\infty(\mathbb{R}^3, \mathbb{C}^2)$, and the 4-spinor subspaces of $L^2(\mathbb{R}^3, \mathbb{C}^4)$

$$W_+^T := W \otimes \left\{ \begin{pmatrix} 0 \\ 0 \end{pmatrix} \right\} , \quad W_-^T := \left\{ \begin{pmatrix} 0 \\ 0 \end{pmatrix} \right\} \otimes W$$

Theorem 2 *[J.D., Esteban, Séré] Under the previous assumptions, all eigenvalues of* H_0+V *in the interval* $(-1,1)$ *are given by the following (eventually finite) sequence of real numbers*

$$\inf_{\substack{F\subset W_+^T \\ F \text{ vector space} \\ \dim F=k}} \quad \sup_{\substack{\psi\in F\oplus W_-^T \\ \psi\neq 0}} \frac{((H_0+V)\,\psi,\psi)}{(\psi,\psi)}\,,$$

as long as they are contained in the interval $(-1,1)$*, assuming that the lowest of these min-max values is larger than* -1*.*

In particular, $$\lambda_1(V) = \inf_{\varphi\neq 0}\sup_{\chi}\frac{(\psi,(H_0+V)\psi)}{(\psi,\psi)} \text{ (Talman)}$$
where both φ and χ are in W and $\psi=\binom{\varphi}{\chi}$, as soon a the above inf-sup takes its values in $(-1,1)$. This theorem is a special case of an abstract result.

Abstract min-max approach

Let $\mathcal{H}$ be a Hilbert space and $A : D(A) \subset \mathcal{H} \to \mathcal{H}$ a self-adjoint operator. $\mathcal{F}(A)$ is the form-domain of A. Let $\mathcal{H}_+$, $\mathcal{H}_-$ be two orthogonal Hilbert subspaces of $\mathcal{H}$ such that $\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_-$. $\Lambda_\pm$ are the projectors on $\mathcal{H}_\pm$. We assume the existence of a core F such that :

(i) $F_+ = \Lambda_+ F$ and $F_- = \Lambda_- F$ are two subspaces of $\mathcal{F}(A)$.

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

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

(iii) $c_1 > a$, $b = \inf\ (\sigma_{\text{ess}}(A) \cap (a, +\infty)) \in [a, +\infty]$.

Definition: for $k \geq 1$, λ_k is the k^{th} eigenvalue of A in (a, b), counted with multiplicity, *if this eigenvalue exists*. If not, $\lambda_k = b$.

Theorem 3 *[J.D., Esteban, Séré] Assume (i)-(ii)-(iii).*

$$c_k = \lambda_k \ , \quad \forall k \geq 1$$

As a consequence, $b = \lim_{k\to\infty} c_k = \sup_k c_k > a$.

References on the min-max approach: Talman and Datta & Deviah for the computation of the first positive eigenvalue of Dirac operators with a potential. Other min-max approaches were proposed by Drake & Goldman and Kutzelnigg.

Esteban & Séré: Dirac operators with a Coulomb-like potential. Griesemer & Siedentop: first abstract theorem on the variational principle, *under conditions* (i), (ii), *and two additional hypotheses instead of* (iii)*:* $(Ax, x) > a\|x\|^2 \ \forall\, x \in F_+ \setminus \{0\}$, *the operator* $(|A| + 1)^{1/2} P_- \Lambda_+$ *is bounded. Here* Λ_+ *is the orthogonal projection of* $\mathcal{H}$ *on* $\mathcal{H}_+$ *and* P_- *is the spectral projection of* A *for the interval* $(-\infty, a]$, *i.e.* $P_- = \chi_{(-\infty,a]}(A)$.

[Griesemer, Lewis & Siedentop]: an alternative approach which extends the results of Griesemer & Siedentop and applies to Dirac operators with potentials having Coulomb singularities.

Additional comment: the difficult part to apply the previous theorem is condition (iii): *the first level of min-max has to be above the lower bound of the gap.* A possible method consists in deriving an abstract continuation method when the family of operators depends continuously on a parameter, for instance ν in case of $H_\nu := H_0 - \frac{\nu}{|x|}$. This allows us to take any $\nu \in (0,1)$ in the case of the Coulomb potential $V(x) = \frac{\nu}{|x|}$.

Proof: see the finite dimensional case (numerical approach).

A min-max approach of Hardy type inequalities
The case of Talman's min-max

As a subproduct of our method, we obtain Hardy type inequalities. In the case of the decomposition based on the projectors of the free Dirac operator, one gets a Hardy type inequality. A simpler form is obtained in case of Talman's decomposition.

For every $\varphi \in C_0^\infty(\mathbb{R}^3, \mathbb{C}^2)$ consider

$$\lambda(\varphi) = \sup_\chi \frac{(\psi, (H_0 + V)\,\psi)}{(\psi, \psi)} \quad \text{where} \quad \psi = \begin{pmatrix} \varphi \\ \chi \end{pmatrix}$$

This number is achieved by the function

$$\chi(\varphi) := \frac{-i\,(\sigma \cdot \nabla)\varphi}{1 - V + \lambda(\varphi)} = \frac{R\varphi}{1 - V + \lambda(\varphi)}$$

Moreover, $\lambda = \lambda(\varphi)$ is the unique solution to the equation

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

(uniqueness is an easy consequence of the monotonicity of both sides of the equation in terms of λ). Thus $\lambda_1(V)$ is the solution of the following minimization problem

$$\lambda_1(V) := \inf\{\lambda(\varphi) \; : \; \varphi \in C_0^\infty(\mathbb{R}^3, \mathbb{C}^2)\} \, .$$

This is by far simpler than working with Rayleigh quotients.

$\lambda_1(V)$ is the best constant in the inequality

$$\int_{\mathbb{R}^3} \frac{|(\sigma \cdot \nabla)\varphi|^2}{1 + \lambda_1(V) - V} \, dx + \int_{\mathbb{R}^3} (1 - \lambda_1(V) + V)|\varphi|^2 \, dx \; \geq \; 0$$

For any $\nu \in (0,1)$, the first eigenvalue of $H_\nu := H_0 - \frac{\nu}{|x|}$ is explicit:

$$\lambda_1\left(-\frac{\nu}{|x|}\right) = \sqrt{1-\nu^2}$$

$$\int_{\mathbb{R}^3} \frac{|(\sigma\cdot\nabla)\varphi|^2}{1+\sqrt{1-\nu^2}+\frac{\nu}{|x|}}\,dx + \left(1-\sqrt{1-\nu^2}\right)\int_{\mathbb{R}^3}|\varphi|^2\,dx \quad \geq \quad \nu\int_{\mathbb{R}^3}\frac{|\varphi|^2}{|x|}\,dx$$

Moreover this inequality is achieved. In the limit $\nu \to 1$, we get the optimal (but not achieved) inequality:

$$\int_{\mathbb{R}^3} \frac{|(\sigma\cdot\nabla)\varphi|^2}{1+\frac{1}{|x|}}\,dx + \int_{\mathbb{R}^3}|\varphi|^2\,dx \quad \geq \quad \int_{\mathbb{R}^3}\frac{|\varphi|^2}{|x|}\,dx$$

This inequality is not invariant under scaling.

The min-max associated with the projectors of the free Dirac operator: corresponding Hardy type inequality

Consider the splitting $\mathcal{H} = \mathcal{H}^f_+ \oplus \mathcal{H}^f_-$, with $\mathcal{H}^f_\pm = \Lambda^\pm \mathcal{H}$, where $\Lambda^+ = \chi_{(0,+\infty)}(H_0)$, $\Lambda^- = \chi_{(-\infty,0)}(H_0)$, *i.e.*

$$\Lambda^\pm = \frac{1}{2}\left(\mathbb{1} \pm \frac{H_0}{\sqrt{1-\Delta}}\right)$$

Theorem 4 *If* $\lim_{|x|\to+\infty} V(x) = 0$ *and* $-\frac{\nu}{|x|} - c_1 \le V \le c_2$ *with* $\nu \in (0,1)$, $c_1, c_2 \ge 0$, $c_1 + c_2 - 1 < \sqrt{1-\nu^2}$, *then*

$$c_k^f(V) = \lambda_k(V) \quad \forall\, k \ge 1\,.$$

Case $\nu < \frac{1}{2}$: [Esteban, Séré], case $\nu < \frac{2}{\frac{2}{\pi}+\frac{\pi}{2}}$: [J.D., Esteban, Séré]

$$\text{If } E \geq c_1^f(V)\,, \quad Q^f_{E,\nu}(\psi_+) \geq 0\,, \quad \forall\, \psi_+ \in \Lambda^+\left(C_0^\infty(\mathbb{R}^3, \mathbb{C}^4)\right)$$

$$Q^f_{E,\nu}(\psi_+) := ||\psi_+||^2_{H^{1/2}} - (\psi_+, (E-V)\psi_+) \\ + \left(\Lambda^-|V|\psi_+, \left(\Lambda^-(\sqrt{1-\Delta} + E + |V|)\Lambda^-\right)^{-1}\Lambda^-|V|\psi_+\right)$$

Proposition 2 *For all* $\nu \in [0,1]$, $\psi_+ \in \Lambda^+\left(C_0^\infty(\mathbb{R}^3, \mathbb{C}^4)\right)$,

$$\nu \int_{\mathbb{R}^3} \frac{|\psi_+|^2}{|x|}\,dx + \sqrt{1-\nu^2}\int_{\mathbb{R}^3}|\psi_+|^2\,dx \\ \leq \int_{\mathbb{R}^3}(\psi_+, \sqrt{1-\Delta}\,\psi_+)\,dx + \nu^2\int_{\mathbb{R}^3}\left(\Lambda^-\left(\frac{\psi_+}{|x|}\right), B^{-1}\Lambda^-\left(\frac{\psi_+}{|x|}\right)\right)dx$$

with $\quad B := \Lambda^-\left(\sqrt{1-\Delta} + \frac{\nu}{|x|} + \sqrt{1-\nu^2}\right)\Lambda^-$

Taking functions with support near the origin, we find, after rescaling and passing to the limit, a new homogeneous Hardy-type inequality. If

$$\Lambda^0_\pm := \frac{1}{2}\left(\mathbb{I} \pm \frac{\alpha \cdot \hat{p}}{|\hat{p}|}\right), \quad \hat{p} := -i\nabla$$

are the projectors associated with the zero-mass free Dirac operator, then for any $\psi_+ \in \Lambda^0_+\left(C_0^\infty(\mathbb{R}^3, \mathbb{C}^4)\right)$,

$$\int_{\mathbb{R}^3} \frac{|\psi_+|^2}{|x|}\,dx \le \int_{\mathbb{R}^3} (\psi_+, |\hat{p}|\psi_+)\,dx + \int_{\mathbb{R}^3} \left(\Lambda^0_-\left(\frac{\psi_+}{|x|}\right), (B^0)^{-1}\Lambda^0_-\left(\frac{\psi_+}{|x|}\right)\right)dx$$

$$\text{with } B^0 := \Lambda^0_-\left(|\hat{p}| + \tfrac{1}{|x|}\right)\Lambda^0_-$$

GENERALIZED HARDY INEQUALITY: AN ANALYTICAL PROOF

Notes from a discussion with M. Loss. Related works based on commutators of M.J. Esteban, L. Vega, Adimurthi containing improvements like logarithmic terms.

Proposition 3 *Let g be a bounded radial C^1 function such that* $\lim_{x\to 0} |x|\, g(x)$ *is finite. Then for any* $\varphi \in H^{1/2}(\mathbb{R}^3, \mathbb{C}^2)$*,*

$$\int_{\mathbb{R}^3} \frac{1}{g}\,|(\sigma\cdot\nabla)\varphi|^2\,dx + \int_{\mathbb{R}^3} g\,|\varphi|^2\,dx \;\geq\; 2\int_{\mathbb{R}^3} \frac{|\varphi|^2}{|x|}\,dx$$

Proof. Let $\phi \in H^{1/2}(\mathbb{R}^3, \mathbb{C}^2)$ and $\varepsilon = \pm 1$. In the case of the generalized Hardy inequality, take $g(x) = 1 + \frac{1}{|x|}$. From

$$\int_{\mathbf{R}^3} \left| \frac{1}{\sqrt{g}} (\sigma \cdot \nabla \phi) + \varepsilon \sqrt{g} \left(\sigma \cdot \frac{x}{|x|} \phi \right) \right|^2 dx \geq 0,$$ we get

$$\int_{\mathbf{R}^3} \frac{1}{g} |\sigma \cdot \nabla \phi|^2 \, dx + \int_{\mathbf{R}^3} g \, |\phi|^2 \, dx \geq \varepsilon \left(\phi, \left[\frac{1}{\sqrt{g}} (\sigma \cdot \nabla), \sqrt{g} \left(\sigma \cdot \frac{x}{|x|} \right) \right] \phi \right)_{L^2}$$

Let $L = ix \wedge \nabla$. A straightforward computation shows that

$$\left[(\sigma \cdot \nabla), \left(\sigma \cdot \frac{x}{|x|} \right) \right] = \frac{2}{|x|} (1 + \sigma \cdot L)$$

$$\left[\tfrac{1}{\sqrt{g}} (\sigma \cdot \nabla), \sqrt{g} \left(\sigma \cdot \tfrac{x}{|x|} \right) \right] = \tfrac{1}{2g} \left(\nabla g \cdot \tfrac{x}{|x|} \right) + \tfrac{2}{|x|} (1 + \sigma \cdot L) \, ,$$

$$\left[\tfrac{1}{\sqrt{g}} \sigma \cdot \left(\nabla - \tfrac{x}{|x|} \tfrac{\partial}{\partial r} \right), \sqrt{g} \left(\sigma \cdot \tfrac{x}{|x|} \right) \right] = \tfrac{2}{|x|} (1 + \sigma \cdot L) \, .$$

Lemma 4 *The spectrum of* $(1+\sigma\cdot L)$ *is* $\mathbb{Z}\setminus\{0\}$ *and* $L^2(\mathbb{R}^3,\mathbb{C}^2) = \mathcal{H}_-\oplus\mathcal{H}_+$ *with* $\mathcal{H}_\pm = P_\pm L^2(\mathbb{R}^3,\mathbb{C}^2)$, $P_\pm = \frac{1}{2}\left(1 \pm \frac{1+\sigma\cdot L}{|1+\sigma\cdot L|}\right)$. *As a consequence, for any nonnegative radial function* h,
if $\phi\in\mathcal{H}_\pm$, $\quad \pm\,(\phi, h\,(1+\sigma\cdot L)\,\phi)_{L^2} \geq \int_{\mathbf{R}^3} h\,|\phi|^2\,dx$

Let $\varphi\in H^{1/2}(\mathbb{R}^3,\mathbb{C}^2)$, $\varphi_\pm = P_\pm\varphi$. Apply Lemma 4 to φ_+ with $\varepsilon = +1$ (resp. to φ_- with $\varepsilon = -1$), $h = \frac{1}{|x|}$, $\nabla_\perp = \left(\nabla - \frac{x}{|x|}\frac{\partial}{\partial r}\right)$:

$$\int_{\mathbf{R}^3}\frac{1}{g}\,|\sigma\cdot\nabla_\perp\varphi_\pm|^2\;dx + \int_{\mathbf{R}^3} g\;|\phi_\pm|^2\;dx \geq \int_{\mathbf{R}^3}\frac{2}{|x|}\,|\varphi_\pm|^2\,dx$$

For any radial function h,

$$\int_{\mathbf{R}^3} h\,|\varphi|^2\,dx = \int_{\mathbf{R}^3} h\,|\varphi_-|^2\,dx + \int_{\mathbf{R}^3} h\,|\varphi_+|^2\,dx$$

$$\int_{\mathbf{R}^3} |\nabla\varphi|^2\,dx \geq \int_{\mathbf{R}^3} |\nabla_\perp\varphi_-|^2\,dx + \int_{\mathbf{R}^3} |\nabla_\perp\varphi_+|^2\,dx$$

A numerical algorithm for computing the eigenvalues of the Dirac operator

In principle one has to look for the minima of the Rayleigh quotient

$$\frac{((H_0 + V)\,\psi, \psi)}{(\psi, \psi)}$$

on "well chosen" subspaces of 4-spinors on which the above quotient is bounded from below. Direct approaches may face serious numerical difficulties. Our method is based on finding the best constant λ in the generalized Hardy inequality

$$\boxed{\int_{\mathbb{R}^3} \frac{|R\,\phi|^2}{\lambda + 1 - V}\,dx + \int_{\mathbb{R}^3} V|\phi|^2\ dx\ + (1-\lambda)\int_{\mathbb{R}^3} |\phi|^2\ dx \geq 0\ \forall\,\phi}$$

To do this, we minimize $\lambda = \lambda(\varphi)$, given by

$$\int_{\mathbb{R}^3} \left(\frac{|(\sigma \cdot \nabla)\varphi|^2}{1 - V + \lambda} + (1 + V)|\varphi|^2 \right) dx - \lambda \int_{\mathbb{R}^3} |\varphi|^2 \, dx = 0$$

w.r.t. φ. The discretized version of this equation on a finite dimensional space E_n of dimension n of 2-spinor functions is

$$A^n(\lambda)\, x_n \cdot x_n = 0 \,,$$

where $x_n \in E_n$ and $A^n(\lambda)$ is a λ-dependent $n \times n$ matrix. If E_n is generated by a basis set $\{\varphi_i, \ldots \varphi_n\}$, the entries of the matrix $A^n(\lambda)$ are the numbers

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

The matrix is monotone decreasing in λ. The ground state energy will then be approached from above by the unique λ for which the first eigenvalue of $A^n(\lambda)$ is zero.

The matrix $A^n(\lambda)$ is selfadjoint and has therefore n real eigenvalues:

$$\lambda_{1,n}(\lambda) < \lambda_{2,n}(\lambda) < ... \lambda_{1,n}(\lambda)$$

which are all monotone decreasing functions of λ.

The equation

$$A^n(\lambda)\, x_n \cdot x_n = 0 \ ,$$

means that x_n is an eigenvector associated to the eigenvalue $\lambda_{k,n}(\lambda) = 0$, for some k.

Minimizing λ is therefore equivalent to compute $\lambda_{1,n}$ as the solution of the equation

$$\lambda_{1,n}(\lambda) = 0$$

The uniqueness of such a λ comes from the monotonicity.

Moreover, if the approximating finite spaces $(E_n)_{n\in\mathbb{N}}$ is an increasing family which generates $H^1(\mathbb{R}^3;\mathbb{C}^2)$, since for a fixed λ

$$\lambda_{1,n}(\lambda) \searrow \lambda_1(\lambda) \quad \text{as} \quad n \to +\infty$$

we also have

$$\lambda_{1,n} \searrow \lambda_1 \quad \text{as} \quad n \to +\infty$$

This method has been tested on diatomic configurations (corresponding to a cylindrical symmetry) with B-splines basis sets. Approximations from above of the other eigenvalues of the Dirac operator, or excited levels, can also be computed by requiring successively that the second, third,... eigenvalues of $A^n(\lambda)$ are equal to zero.

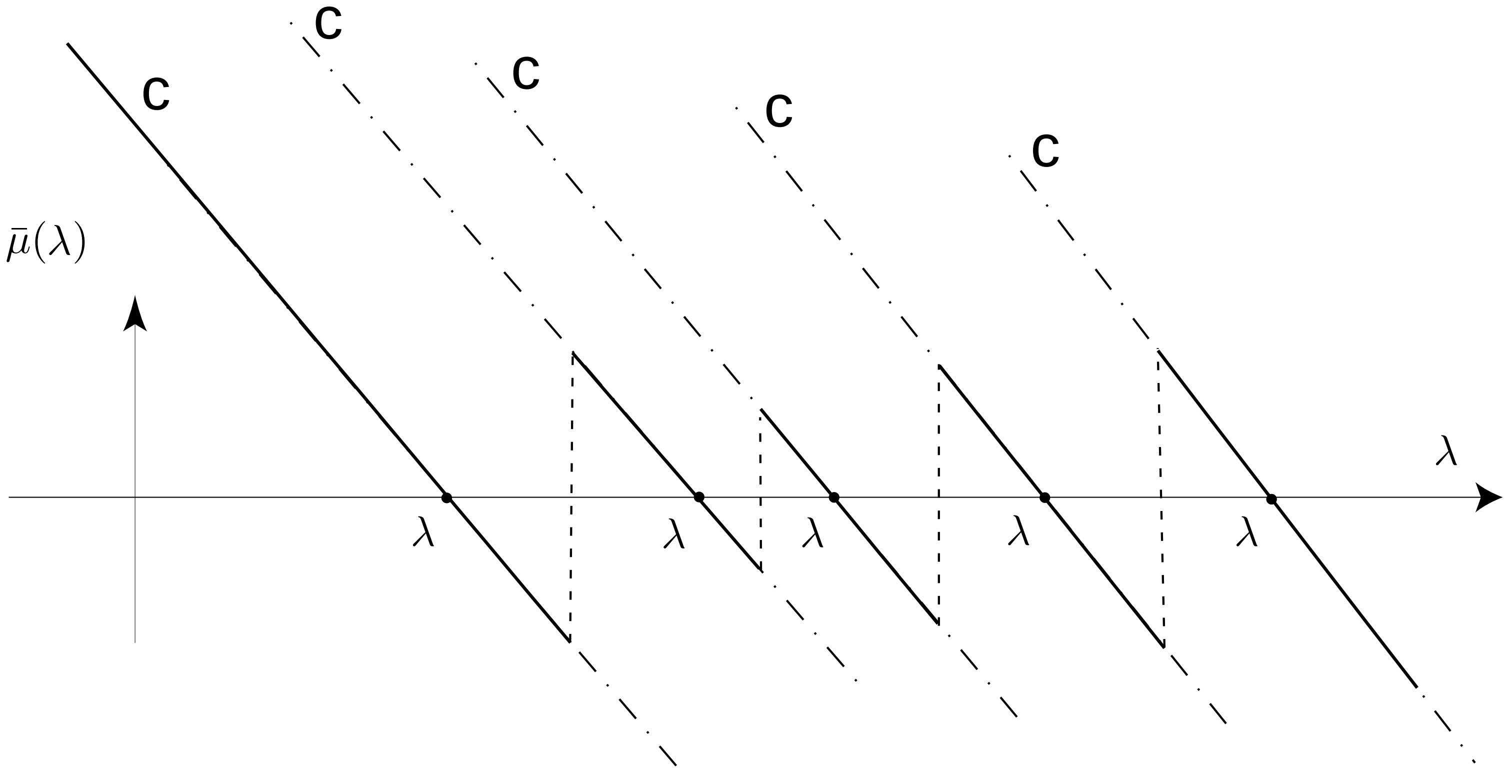

Figure 1: *Each eigenvalue $\mu_i(\lambda)$ of $A(\lambda)$, considered as a function of λ, is monotone decreasing. By looking for the zeros of the non continuous function $\lambda \quad \bar{\mu}(\lambda) = \inf_i \ \mu_i(\lambda)$, we obtain an efficient algorithm to compute all eigenvalues of the Dirac operator in the gap $(\quad 1, 1)$ and the corresponding eigenfunctions. The ground state of course corresponds to the smallest zero of $\bar{\mu}(\lambda)$ in $(\quad 1, 1)$. Moreover the method forbids variational collapse, no spurious states may appear and the only consequence of the approximation on a finite basis set is that eigenvalues are approximated from above.*

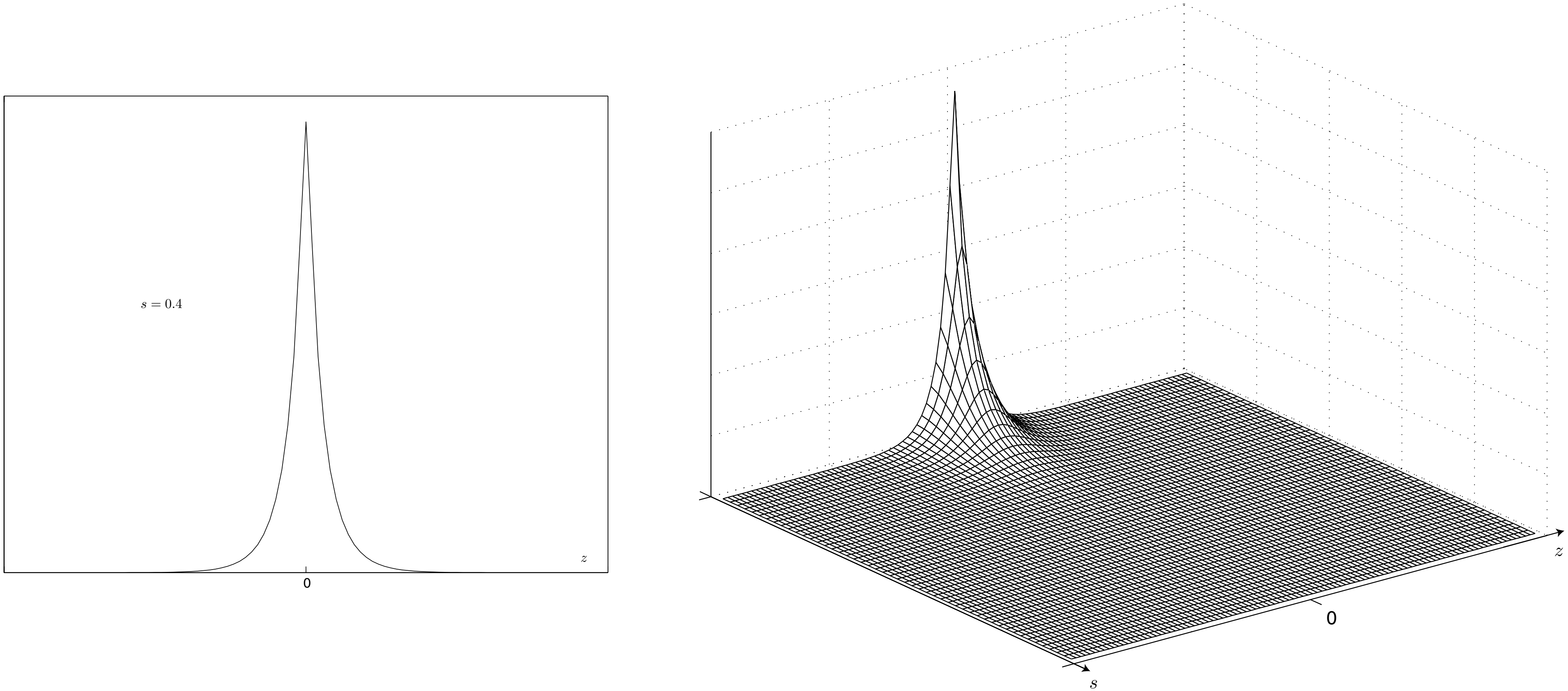

Figure 2: *Ground state of* Th^{89+} *corresponding to* $Z = 90$, *one atom, computed with* $s_{\max} = 10$, $z_{\max} = 10$, $h = 0.4$.

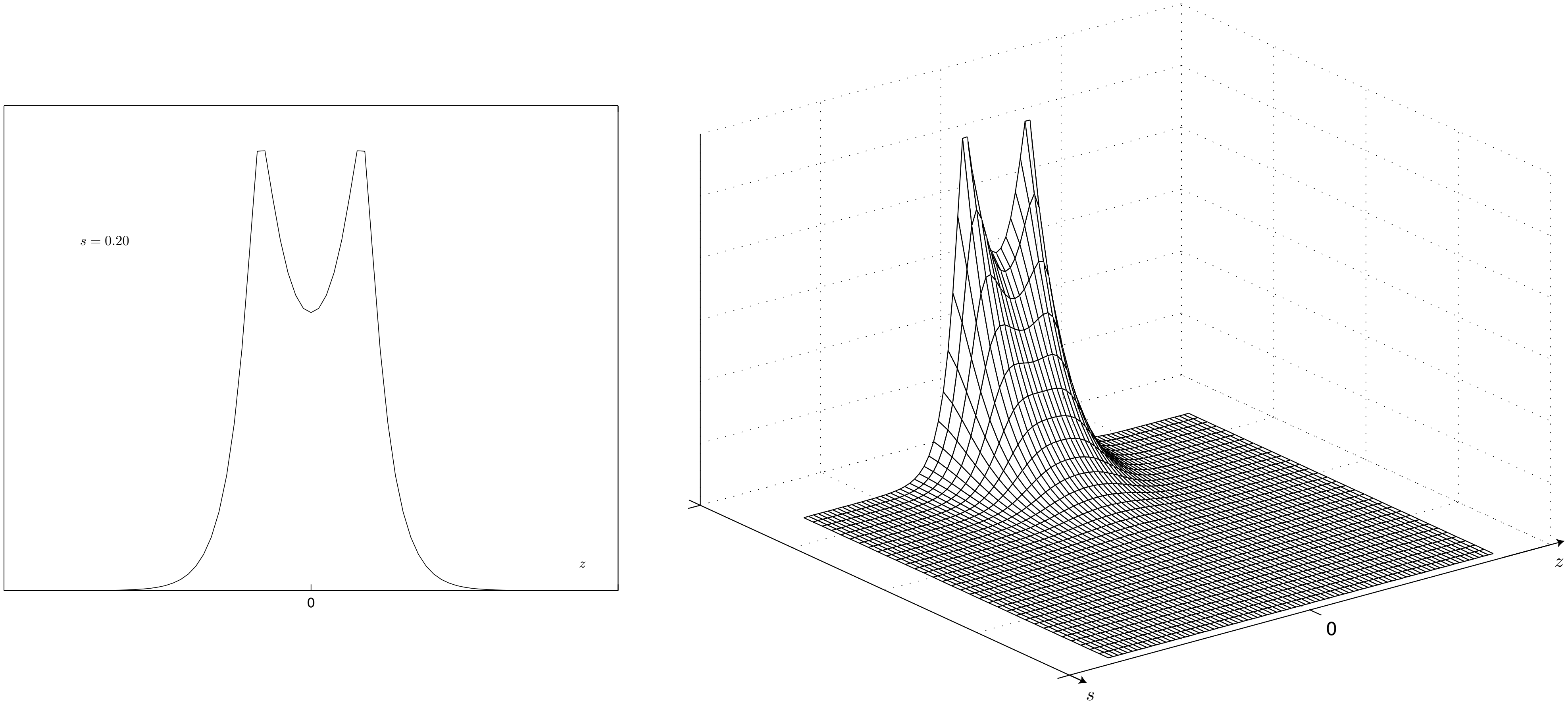

Figure 3: *Ground state of* H_2^+ *corresponding to* $Z = 1$*, two atoms, computed with* $s_{\max} = 700$*,* $z_{\max} = 820$*,* $h = 20$*.*

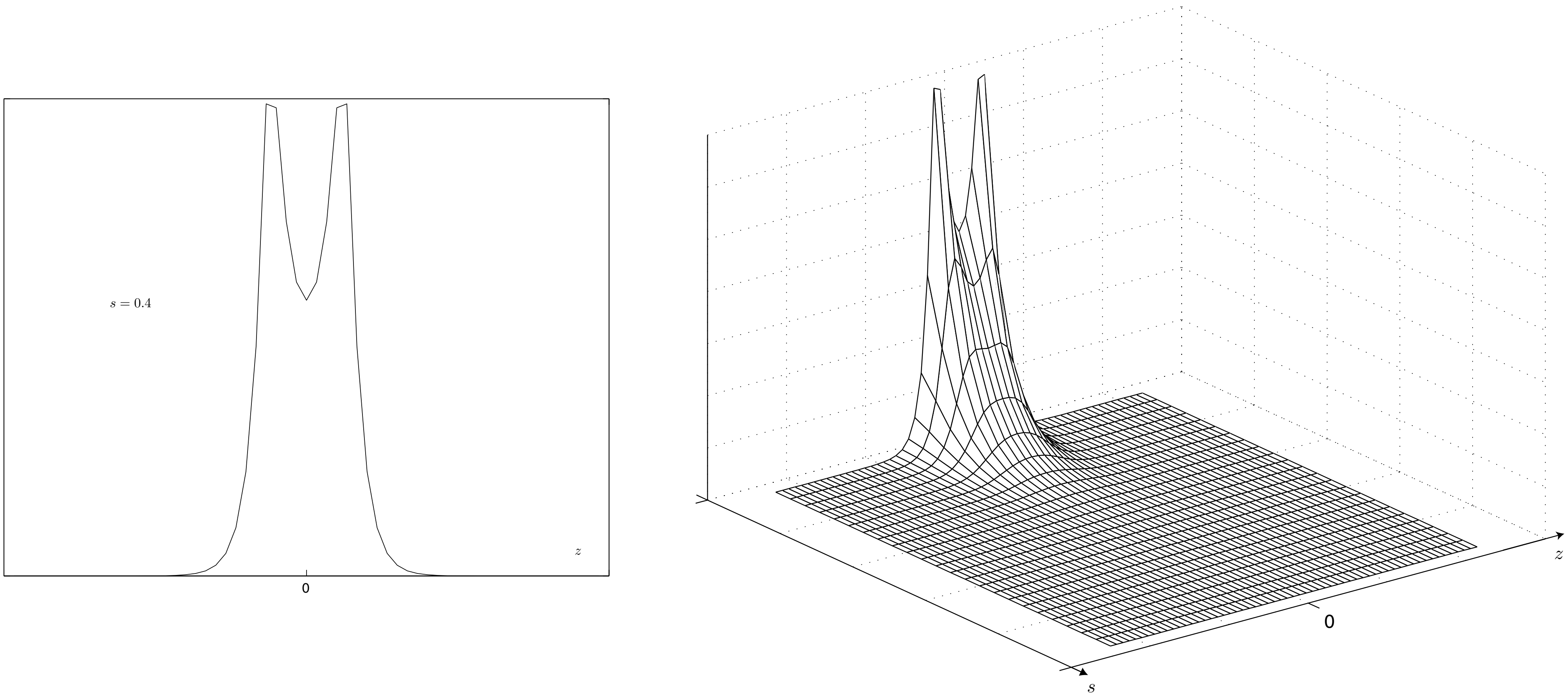

Figure 4: *Ground state of* Th_2^{179+} *corresponding to* $Z = 90$*, two atoms, computed with* $s_{\max} = 10$*,* $z_{\max} = 12$*,* $h = 0.4$*.*