

Stability and energy spectrum of the hydrogen atom in space with a compactified extra dimension and potential defined by Gauss' law

Martin Bureš

Institute of Theoretical Physics and Astrophysics Masaryk University Brno, Czech Republic Supervisor: Rikard von Unge

September 10, Corfu

- 3

S. P. Alliluev, Sov. Phys.-JETP 6, 156 (1958)

Extended Fock's method of stereographic projection to the case of d dimensions (d > 2).

- Michael Martin Nieto. "Hydrogen atom and relativistic pi-mesic atom in N-space dimensions". In: *Am. J. Phys.* (1979)
- Frank Burgbacher, Claus Lämmerzahl, and Alfredo Macias. "Is there a stable hydrogen atom in higher dimensions?" In: Journal of Mathematical Physics 40.2 (1999)
- Shi-Hai Dong. Wave Equations in Higher Dimensions. 2011



э

・ロット 御ママ キョマ キョン

A more physically relevant potential is the solution of Maxwell's equations for a point charge in the *d*-dimensional space:

$$V_d(|x|) \sim |x|^{2-d}, \qquad (d \neq 2)$$

• The corresponding Schrödinger equation reads

$$\left(-\frac{\hbar^2}{2m}\Delta_d - \frac{e_d^2}{|x|^{d-2}}\right)\psi = E\psi,$$

where e_d is the *d*-dimensional charge.



The model, questions raised, methods used

Underlying spaces

- extra dimensions of an infinite extent \mathbb{R}^d (especially d = 4)
- compactified extra dimensions: $\mathbb{R}^3 imes \mathcal{M}$ $(\mathcal{M} = \mathcal{T}^m, \ m = 1)$

Definition of operators

• Schrödinger operator of the hydrogen atom on the corresponding space (to be defined soon)

Questions raised, (main) methods used

- Stability/instability of the system, existence of bound states? (Functional analysis: Hardy's inequality, KLMN theorem, spectral theory)
- Energy spectrum due to extra dimensions? (Hamiltonian diagonalization)



Let $h(\cdot, \cdot)$ be a mapping from $Dom(h) \times Dom(h)$ to \mathbb{C} , with $Dom(h) \subset \mathcal{H}$ such that

$$\begin{array}{ll} h(\psi, a\phi + b\eta) &=& ah(\psi, \phi) + bh(\psi, \eta) \\ h(a\psi + b\phi, \eta) &=& \bar{a}h(\psi, \eta) + \bar{b}h(\phi, \eta) \end{array}$$

for all $\psi, \phi, \eta \in \text{Dom}(h)$ and all $a, b \in \mathbb{C}$. Then h is called the sesquilinear form and Dom(h) the domain of h.

Definition

The mapping $h[\cdot]$ from \mathcal{H} to \mathbb{C} defined by $h[\psi] = h(\psi, \psi)$ is called the quadratic form associated with the sesquilinear form h.



A D F A B F A B F A B F

A sesquilinear form h is said to be symmetric if $h(\psi, \phi) = \overline{h(\phi, \psi)}$ for all $\psi, \phi \in \text{Dom}(h)$. A symmetric form h is said to be bounded from below if there exists a real constant c such that $h[\psi] \ge c \|\psi\|^2$ for all $\psi \in \text{Dom}(h)$. If $c \ge 0$, the symmetric form is said to be non-negative.

Definition

Let h_0 be symmetric and bounded from below in \mathcal{H} . A symmetric form v (which need not be bounded from below) is said to be relatively bounded with respect to h_0 if

- $\operatorname{Dom}(v) \supset \operatorname{Dom}(h_0)$,
- $\forall \psi \in \text{Dom}(h_0), |v[\psi]| \le a|h_0[\psi]| + b||\psi||^2,$ where a, b are non-negative constants.



Let *h* be a symmetric sesquilinear form bounded from below. It is said to be closed if for any sequence $\{\psi_n\}_{n\in\mathbb{N}}\subseteq \text{Dom}(h)$ with $\psi_n \to \psi \in \text{Dom}(h)$ and $h[\psi_n - \psi_m] \to 0$ as $n, m \to \infty$, we have $h[\psi_n - \psi] = 0$ as $n \to \infty$. A symmetric sesquilinear form bounded from below is said to be closable if it can be extended to a closed form.



э

ヘロン 人間 とくほ とくほう

Theorem (KLMN)

Let h_0 : Dom $(h_0) \times$ Dom $(h_0) \rightarrow \mathbb{C}$ be a densely defined, symmetric, non-negative and closed sesquilinear form in \mathcal{H} . Let v be a symmetric sesquilinear form satisfying

- 1. $\operatorname{Dom}(h_0) \subset \operatorname{Dom}(v)$,
- 2. $\forall \psi \in \operatorname{Dom}(h_0), \quad |\mathbf{v}[\psi]| \le a h_0[\psi] + b \|\psi\|^2,$

where a, b are non-negative and a < 1. Then there exists a unique self-adjoint and bounded from below operator H, associated with the closed symmetric sesquilinear form

$$h := h_0 + v$$
, $\operatorname{Dom}(h) := \operatorname{Dom}(h_0)$.



Theorem (Kato-Rellich theorem)

 Let H₀ be self-adjoint and suppose V is a symmetric operator with Dom (V) ⊃ Dom (H₀) so that for some a < 1 and b,

 $\|V\phi\| \le a\|H_0\phi\| + b\|\phi\|$

for all $\phi \in \text{Dom}(H_0)$.

Then H₀ + V defined on Dom (H₀) ∩ Dom (V) ≡ Dom (H₀) is self-adjoint. If H₀ is bounded below, so is H = H₀ + V.

- The Kato-Rellich theorem is not always applicable: it requires the potential to belong to L² + L[∞]. This restricts the possible potentials −|x|^{-α} to singularities of the order 0 < α < 3/2.
- For stronger singularities, α < 2: KLMN theorem



Let H be a densely defined operator on a Hilbert space. H is called symmetric, or Hermitian, if and only if

$$\langle H\phi,\psi
angle = \langle \phi,H\psi
angle, \qquad orall \phi,\psi\in {
m Dom}\,(H).$$

A symmetric operator H is called self-adjoint if and only if

 $\operatorname{Dom}(H) = \operatorname{Dom}(H^*).$

References:

- Schrödinger operators and their spectra, David Krejčiřík
- 2 Methods of Modern Mathematical Physics, Reed M., Simon B.
- Hilbert Space Operators in Quantum Physics, Blank J., Exner P., Havlíček M.



3

・ 日 ・ ・ 一 ・ ・ ・ ・ ・ ・ ・ ・ ・ ・

Lemma (The classical Hardy inequality (for $d \ge 3$))

$$\forall \psi \in W^{1,2}(\mathbb{R}^d), \quad \int_{\mathbb{R}^d} |\nabla \psi(x)|^2 \mathrm{d}x \geq \frac{(d-2)^2}{4} \int_{\mathbb{R}^d} \frac{|\psi(x)|^2}{|x|^2} \mathrm{d}x.$$



(日) (個) (目) (目) (目) (目)

Extra dimension of an infinite extent





э

(日) (四) (日) (日) (日)

• Schrödinger's equation

$$\left(-\frac{\hbar^2}{2m}\Delta_4+V_4(x)\right)\psi(x)=E\psi(x),$$

with $V_4(x)=-e_4^2/|x|^2$, $x\in\mathbb{R}^4$

• We can rewrite it by using a dimensionless parameter $Z := 2me_4^2/\hbar^2$, where e_4^2 is the four dimensional charge:

$$\left(-\Delta_4-\frac{Z}{x^2}\right)\psi(x)=E'\psi(x).$$



3

・ロト ・雪 ト ・ ヨ ト ・ ヨ ト

Stability Z < 1: Application of Hardy's Inequality

• Free Hamiltonian $H_0 := -\Delta$, $Dom(H_0) := W^{2,2}(\mathbb{R}^4)$, is associated with the quadratic form

$$h_0[\psi] := \|\nabla \psi\|^2, \qquad \text{Dom}(h_0) := W^{1,2}(\mathbb{R}^4).$$

• $V(x) = |x|^{-2}$ with $x \in \mathbb{R}^4$ is associated with

- $\mathbf{v}[\psi] := \langle \psi, \mathbf{V}\psi \rangle, \qquad \operatorname{Dom}(\mathbf{v}) := \{\psi \in L^2(\mathbb{R}^4) : |\langle \psi, \mathbf{V}\psi \rangle| < \infty \}.$
- The classical Hardy inequality (for $d \ge 3$)

$$\forall \psi \in W^{1,2}(\mathbb{R}^d), \quad \int_{\mathbb{R}^d} |\nabla \psi(x)|^2 \mathrm{d} x \geq \frac{(d-2)^2}{4} \int_{\mathbb{R}^d} \frac{|\psi(x)|^2}{|x|^2} \mathrm{d} x.$$

• In d = 4 we get using the notation for quadratic forms that

$$\forall \psi \in \mathrm{Dom}\,(h_0), \qquad |\nu[\psi]| \leq h_0[\psi].$$



Stability Z < 1: Application of Hardy's Inequality

• Hardy inequality (for d = 4, notation for quadratic forms):

$$\forall \psi \in \mathrm{Dom}\,(h_0), \qquad |\mathbf{v}[\psi]| \leq h_0[\psi].$$

• By KLMN theorem, if Z < 1, the quadratic form

$$h[\psi] := h_0[\psi] - Zv[\psi], \qquad \operatorname{Dom}(h) := \operatorname{Dom}(h_0) = W^{1,2}(\mathbb{R}^4),$$

is symmetric, closed, and bounded from below, thus associated with a unique self-adjoint operator H that represents our Hamiltonian.

 \rightarrow H is stable, with non-negative spectrum $[0,\infty)$



э

A D > A D > A D > A D >

Instability Z > 1: Application of Hardy's Inequality

- Problem in the definition of our Hamiltonian:
 - $\rightarrow \infty$ number of s-a operators that act on functions from $C_0^{\infty}(\mathbb{R}^4 \setminus \{0\})$ as $\dot{H} := -\Delta ZV(x)$.
- There exists an optimizing sequence of functions $\{\psi_n\} \subset W^{1,2}(\mathbb{R}^4)$ for the Hardy inequality, for instance

$$\psi_n(x) := n^{-1/2} |x|^{(-1+1/n) \operatorname{sgn}(1-|x|)}.$$

• We analyse $\inf \langle \psi, H\psi \rangle$ by inserting φ_n :

$$\frac{\langle \varphi_n, H\varphi_n \rangle}{\|\varphi_n\|^2} = \frac{\|\nabla \varphi_n\|^2 - \langle \varphi_n, V\varphi_n \rangle - (Z-1)\langle \varphi_n, V\varphi_n \rangle}{\|\varphi_n\|^2} \to -\infty,$$

where we used that φ_n optimize the Hardy inequality.



In *d* dimensions, introducing the function $u(\rho) := \rho^{(d-1)/2} R(\rho)$, we obtain the operator

$$-\frac{\mathrm{d}^2}{\mathrm{d}\rho^2} + \left[\left(\frac{(d-1)(d-3)}{4} + l(l+d-2) \right) \frac{1}{\rho^2} - \frac{2me_d^2}{\hbar^2} \frac{1}{\rho^{d-2}} \right]$$

- For *d* = 4, the potential can be merged with the centrifugal term arising from radial reduction of the central potential.
- Because of the absence of a characteristic length, a procedure leading to dimensionless quantities, which works in the treatment of the radial equation for $d \neq 4$, cannot be used here!

$$ho' = lpha^{1/(4-d)}
ho$$
, with $lpha = m e_d^2/\hbar^2$



э

Instability for Z > 1: a more explicit argument

• Performing the transformation $R(\rho) = \rho^{-3/2} \tilde{R}(\rho)$, we get the radial operator acting in $L^2((0,\infty), d\rho)$:

$$\dot{H}_{\mathrm{rad}} := -\frac{\mathrm{d}^2}{\mathrm{d}\rho^2} - \frac{\gamma}{\rho^2},$$

where
$$\gamma = Z - 3/4 - I(I + 2)$$
.

"Boundary values for an eigenvalue problem with a singular potential"

Allan M Krall, J. Differ. Equations (1982).

• One of the results of is that spectrum of any H_{α} contains continuous branch $[0, +\infty)$ and negative eigenvalues having accumulation point at 0 and and $-\infty$.



Infinite extra dimension $(d = 4)^1$

- weak coupling $(0 \le Z \le 1)$: spectrum of H is the same as that of H_0 , i.e. consisting of a branch of the continuous one, without any negative eigenvalues \rightarrow Hamiltonian is stable without any bound states
- strong coupling (Z > 1): spectrum extends to $-\infty$ \rightarrow unstable hydrogen atom

Infinite extra dimensions, $d \ge 5$ Hydrogen atom is unstable: formally derived in earlier works:²

¹Martin Bureš and Petr Siegl. "Hydrogen atom in space with a compactified extra dimension and potential defined by Gauss' law". In: *Annals of Physics* 354 (Jan. 2015), pp. 316–327. arXiv: 1409.8530v1.

²L Gurevich and V Mostepanenko. "On the existence of atoms in n-dimensional space". In: *Physics Letters A* 35.3 (1971), pp. 201–202, Keith Andrew and James Supplee. "A hydrogenic atom in d-dimensions". In: *American Journal of Physics* 58 (1990), p. 1177.



Compactified extra dimension $(\mathbb{R}^3 \times S^1)$

• But, how about if one of the dimensions is compact? circular compactification: we idetify points $x_4 \rightarrow x_4 + 2\pi R$



• How does that change the story?



◆□▶ ◆圖▶ ◆臣▶ ◆臣▶ ─ 臣

Compactified extra dimension - method of images

• The basic idea - unroll the curled-up dimension to get an infinite space that repeats itself with a period of $2\pi R$





イロト イ押ト イヨト イヨト

To calculate the force between two particles, the method of images makes it easier





ж

イロト イポト イヨト イヨト

Definition of the system under consideration

 Main research goal: consequences of one additional compactified dimension for the stability of the non-relativistic hydrogen atom, defined through the potential

$$V(x) := -\sum_{n=-\infty}^{\infty} \frac{e_{4d}^2}{x_1^2 + x_2^2 + x_3^2 + (x_4 - c_n)^2}$$
$$= -\frac{e_{4d}^2}{2Rr} \frac{\sinh r/R}{\cosh r/R - \cos x_4/R},$$

where $r^2 := x_1^2 + x_2^2 + x_3^2$, $c_n := 2\pi Rn$, e_{4d} is the charge.





э

(日)、

For r ≪ R and x₄ ≪ R, the lowest-order term in the expansion of the potential is (ρ² := r² + x₄²):

$$V(r, x_4) = -e_{4d}^2/(r^2 + x_4^2) = -e_{4d}^2/\rho^2.$$

 \rightarrow the behaviour of the potential around the origin is the same as in the uncompactified case

• On the other hand, if $r \gg R$, we get

$$V(r, x_4) = -e_{4d}^2/2rR = -e_{3d}^2/r,$$

 \rightarrow the usual three-dimensional behaviour is restored

• relation between the 3-d and the 4-d charge:

$$e_{4d}^2 = 2Re_{3d}^2$$



・ロト ・聞 ト ・ 聞 ト ・ 聞 ト ・ 聞

Stability Z < 1: Application of Hardy's Inequality

• the Hardy inequality establishes the relative form-boundedness of ZV(x):

$$|v[\psi]| \le a|h_0[\psi]| + b||\psi||^2.$$

KLMN theorem

For any potential with the singularity $1/|x|^2$,

$$V(x)=-rac{1}{|x|^2}+W(x), \quad ext{with } W\in L^\infty(\mathbb{R}^3 imes\mathcal{S}^1),$$

the stability result remains the same as in \mathbb{R}^4 , *i.e.* the critical value Z = 1.



・ロト ・雪 ト ・ ヨ ト ・ ヨ ト

Critical Compactification Radius

• from the relation between charges $e_{4d}^2 = 2Re_{3d}^2$ we have:

$$Z := \frac{2me_{4d}^2}{\hbar^2} = \frac{4Rme_{3d}^2}{\hbar^2} = \frac{4R}{a_0}$$

• we infer the existence of a critical compactifion radius $R_{\rm c}$:

$$R_{\rm c} := Z_C \frac{a_0}{4} = \frac{a_0}{4} = \frac{\hbar^2}{4me_{3d}^2} \approx 1.32 \times 10^{-11} {\rm m}$$

- the atom is stable for $R < R_{
 m c}$ and not stable if $R > R_{
 m c}$
- current experimental bounds on the size of extra dimensions:³ $R^{-1} > 1.3 \text{TeV}$ at 95% C.L. $R \sim 10^{-18} \text{m}$

³E.g. Datta A., Patra A. and Raychaudhuri S.: Higgs Boson Decay Constraints on a Model with a Universal Extra Dimension, 2013, arXiv:1311.0926



Compatifiaction radius $R < a_0/4$

- System is stable!
- Essential spectrum remains $[0,\infty)$
- As a consequence of compactification, infinite number of negative energy eigenstates appear
- Bound states extend at least to the ground state of the hydrogen atom

Compatifiaction radius $R > a_0/4$

System is not stable (spectrum $(-\infty,\infty)$)

Martin Bureš and Petr Siegl. "Hydrogen atom in space with a compactified extra dimension and potential defined by Gauss' law". In: Annals of Physics 354 (Jan. 2015), pp. 316–327. arXiv: 1409.8530v1



We know that:⁴

- size of extra compactified dimension has to be smaller than $R = a_0/4$
- ground state energy for R = 0 equals the 3-dim hydrogen atom energy (no perturbation due to extra dimension)
- for $R = a_0/4$ the atom is unstable, so the energy should diverge $(E \to -\infty)$

Question: how does the spectrum change?

• Method used: Hamiltonian diagonalization⁵

⁴Martin Bureš and Petr Siegl. "Hydrogen atom in space with a compactified extra dimension and potential defined by Gauss' law". In: *Annals of Physics* 354 (Jan. 2015), pp. 316–327. arXiv: 1409.8530v1.

⁵Martin Bureš. "Energy spectrum of the hydrogen atom in a space with one compactified extra dimension, $\mathbb{R}^3 \times S^{1n}$. In: (2015). arXiv: 1505.08100 [quant-ph].



Basis constructed from the hydrogen atom eigenstates

$$\langle \vec{x} | n lmq
angle = R_{nl}(r) Y_{lm}(\Omega) rac{e^{iq\theta}}{\sqrt{2\pi}},$$

 $l \in \mathbb{N}, m \in \{-l, \dots, l\}, n \in \{l+1, l+2, \dots\}, q \in \mathbb{Z}.$

Matrix elements of the Hamiltonian:

$$\langle n'l'm'q'|\hat{H}|nlmq\rangle = \delta_{ll'}\delta_{mm'} \left\{ \delta_{nn'}\delta_{qq'} \left(-\frac{1}{n^2} + \frac{q^2}{R^2} \right) - \left(1 - \delta_{qq'} \right) M_{n,n';l}(1, |q-q'|/R) \right\},$$

where

$$\begin{split} M_{n,n';l}(g,\mu) &= \frac{g}{2} \left(\frac{4}{nn'}\right)^{l+2} \sqrt{\frac{(n-l-1)!(n'-l-1)!}{(n+l)!(n'+l)!}} \frac{(2l+1)!}{\sigma^{2l+2}} \sum_{k=0}^{\min(n-l-1,n'-l-1)} \binom{n+l}{n-l-1-k} \\ &\times \binom{n'+l}{n'-l-1-k} \binom{k+2l+1}{k} \left(\frac{2}{n\sigma}\right)^k \left(\frac{2}{n'\sigma}\right)^k \left(1-\frac{2}{n\sigma}\right)^{n-l-1-k} \left(1-\frac{2}{n'\sigma}\right)^{n'-l-1-k}, \end{split}$$

with $\sigma(|q - q'|/R) = 1/n + 1/n' + |q - q'|/R$.



э

(日)、

Basis constructed from exponential functions

$$\langle \vec{x} | iq \rangle = 2\alpha_i^{3/2} e^{-\alpha_i r} \frac{e^{iq\theta}}{\sqrt{2\pi}}, \quad i \in \{1, 2, \dots, I\}, \ q \in \{-Q, \dots, Q\}$$

Matrix elements of the Hamiltonian:

$$\langle jp|\hat{H}|iq\rangle = \left[\langle jp|iq
angle\left(lpha_ilpha_j + rac{q^2}{R^2}
ight) - rac{(2\sqrt{lpha_ilpha_j})^3}{(lpha_i + lpha_j + |q-p|/R)^2}
ight],$$

where

$$\langle jp|iq\rangle = 4(\alpha_m \alpha_n)^{3/2} \int_0^\infty \mathrm{d}r r^2 e^{-(\alpha_i + \alpha_j)r} \frac{1}{2\pi} \int_0^{2\pi} e^{\mathrm{i}(q-p)\theta} = \left(\frac{2\sqrt{\alpha_i \alpha_j}}{\alpha_i + \alpha_j}\right)^3 \delta_{p,q}$$

are the overlap integrals.



(日)、

Energy shifts due to a compactified extra dimension



Energy shifts due to a compactified extra dimension



(a) Ground state energy dependence on basis size (hydrogen atom basis, N = 7, $Q = 1, \ldots, 50$) (b) Ground state energy dependence on basis size (exponential basis, N = 7, $Q = 1, \dots, 50$)

Figure : Energy eigenvalues (in units $e^2/2a$) as a function of the compactification radius R (in units of the Bohr radius a). Hydrogen atom basis (left-hand side), exponential basis (right-hand side). The computational step in R was adjusted according to the second derivative of the curves between $\Delta R = 0.005$ and $\Delta R = 0.03$.



Lifting of degeneracy



Figure : The lifting of degeneracy of energy levels (hydrogen atom basis, N = 7, Q = 30): $n = \{2, 3\}$: l = 0 (solid line) l = 1 (dashed line), m = 0. The almost vertical curve represents the first Kaluza-Klein state n = 1, q = 1.

æ

Electron probability density in the (r, θ) plane



(a) Hydrogen atom basis (N = 10, Q = 30)



(b) Exponential basis (N = 10, Q = 30)



æ



Σας ευχαριστώ πολύ για την προσοχή σας!





<ロ> (四) (四) (日) (日) (日)

If we are given a symmetric and bounded from below operator H, then the sesquilinear form, defined as

 $h(\phi,\psi) := \langle \phi, H\psi \rangle$ for all $\phi, \psi \in \text{Dom}(h)$,

with Dom(h) := Dom(H), is also symmetric and bounded from below. Such form is closable and by the first representation theorem, the operator associated with its closure is self-adjoint and bounded from below, with the same lower bound of the spectrum as the original symmetric operator H.



Theorem (The first representation theorem)

Let $h : Dom(h) \times Dom(h) \to \mathbb{C}$ be a densely defined, symmetric, bounded from below and closed sesquilinear form in \mathcal{H} . Then there exists a self-adjoint operator H such that

- i) $\operatorname{Dom}(H) \subset \operatorname{Dom}(h)$ and $h(\phi, \psi) = \langle \phi, H\psi \rangle$ for every $\phi \in \operatorname{Dom}(h)$ and $\psi \in \operatorname{Dom}(H)$;
- ii) Dom(H) is a core of h;

iii) if ψ ∈ Dom (h), η ∈ H, and h(φ, ψ) = ⟨φ, η⟩ holds for every φ belonging to a core of h, then ψ ∈ Dom (H) and Hψ = η. The self-adjoint operator H is uniquely determined by the condition i).



Theorem

Let H be a self-adjoint operator on \mathcal{H} . A point λ belongs to $\sigma(H)$ if, and only if, there exists a sequence $\{\psi_n\}_{n\in\mathbb{N}}\subset \text{Dom}(H)$ such that $\|\psi_n\| = 1$ for all $n \in \mathbb{N}$ and $\lim_{n\to\infty} \|(H-\lambda)\psi_n\| \to 0$. Moreover, λ belongs to $\sigma_{\text{ess}}(H)$ if, and only if, in addition to the above properties the $\{\psi_n\}$ converges weakly to zero in \mathcal{H} .



ヘロン 人間 とくほ とくほう