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Atomic potential and stability due to compactified extra dimensions

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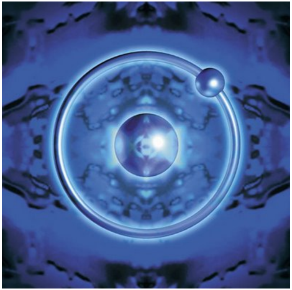
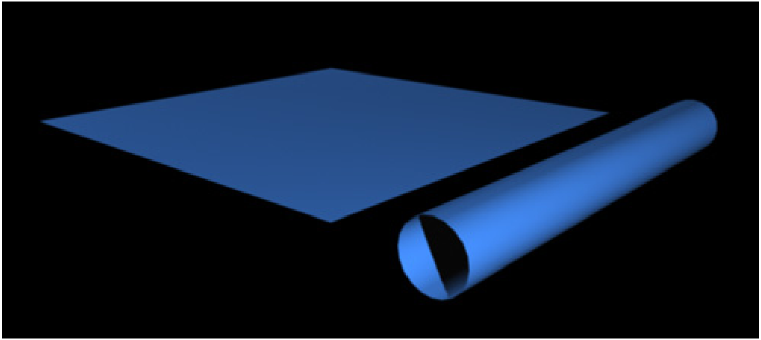
Hydrogen atom in higher dimensions

To understand hydrogen is to understand all of physics!"
...Much of what we know about the universe has come from looking at hydrogen and it cannot be denied that the universe itself is made almost entirely of hydrogen." [1]



[1] "The Yin and Yang of Hydrogen", D. Kleppner, Phys. Today, April 1999

Consequences of compactification for atomic physics



d-dimensional hydrogen atom with $1/r$ potential

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

d-dim hydrogen atom with potential from Gauss' law

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: $\mathbb{R}^3 \times \mathcal{M}$ ($\mathcal{M} = T^m$, $m = 1$)

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 thm, spectral theory)
- Energy spectrum due to extra dimensions?
  (diagonalization of the Hamiltonian)

Hamiltonians defined as quadratic forms

Definition

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

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

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

Symmetry and relative boundedness of forms

Definition

A sesquilinear form h is said to be symmetric if $h(\psi, \phi) = \overline{h(\phi, \psi)}$ for all $\psi, \phi \in \mathrm{Dom}\,(h)$.

A symmetric form h is said to be bounded from below if there exists a real constant c such that $h[\psi] \geq c\|\psi\|^2$ for all $\psi \in \mathrm{Dom}\,(h)$. If $c \geq 0$, 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

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

Closedness of a sesquilinear form

Definition

Let h be a symmetric sesquilinear form bounded from below. It is said to be closed if for any sequence $\{\psi_n\}_{n\in\mathbb{N}} \subseteq \mathrm{Dom}\,(h)$ with $\psi_n \to \psi \in \mathrm{Dom}\,(h)$ 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.

KLMN (Kato-Lions-Lax-Milgram-Nelson) theorem

Theorem (KLMN)

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

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

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*

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

Kato-Rellich theorem

Theorem (Kato-Rellich theorem)

- *Let H_0 be self-adjoint and suppose V is a symmetric operator with $\mathrm{Dom}\,(V) \supset \mathrm{Dom}\,(H_0)$ so that for some $a < 1$ and b,*

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

  for all $\phi \in \mathrm{Dom}\,(H_0)$.
- *Then $H_0 + V$ defined on $\mathrm{Dom}\,(H_0) \cap \mathrm{Dom}\,(V) \equiv \mathrm{Dom}\,(H_0)$ is self-adjoint. If H_0 is bounded below, so is $H = H_0 + V$.*

- The Kato-Rellich theorem is not always applicable: it requires the potential to belong to $L^2 + L^\infty$. This restricts the possible potentials $-|x|^{-\alpha}$ to singularities of the order $0 < \alpha < 3/2$.
- For stronger singularities, $\alpha > 3/2$, up to the border case $\alpha = 2$ of "meaningful" quantum mechanical potentials: KLMN theorem

Self-adjoint vs. symmetric operators

Definition

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

$$\langle H\phi, \psi \rangle = \langle \phi, H\psi \rangle\,, \qquad \forall \phi, \psi \in \mathrm{Dom}\,(H).$$

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

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

References:

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

Hardy's inequality

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

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

Summary : Hardy's inequality + KLMN theorem $\rightarrow$ stability

Extra dimension of an infinite extent

Definition of the system under consideration

- Schrdinger'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:

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

Stability $Z < 1$: Application of Hardy's Inequality

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

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

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

$$v[\psi] := \langle\psi, V\psi\rangle, \qquad \mathrm{Dom}\,(v) := \{\psi \in L^2(\mathbb{R}^4) : |\langle\psi, V\psi\rangle| < \infty\}.$$

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- In $d = 4$ we get

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

Stability $Z < 1$: Application of Hardy's Inequality

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

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

- By KLMN theorem, if $Z < 1$, the quadratic form

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

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 $[0, \infty)$

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

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

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

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

  where we used that φ_n optimize the Hardy inequality.

Infinite extra dimension - Schrdinger's equation

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!
  $\rho' = \alpha^{1/(4-d)} \rho$, with $\alpha = me_d^2/\hbar^2$

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 $L^2((0,\infty), \mathrm{d}\rho)$:

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

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

"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 dimensions - summary

Infinite extra dimension,[2] space $\mathbb{R}^4$

- weak coupling ($0 \leq Z \leq 1$): spectrum of H is the same as that of H_0 (free particle), i.e. $(0, +\infty)$
  $\rightarrow$ Hamiltonian is stable without any bound states
- strong coupling ($Z > 1$): spectrum extends to $-\infty$
  $\rightarrow$ unstable hydrogen atom

Infinite extra dimensions, space $\mathbb{R}^d$, $d \geq 5$

Hydrogen atom is unstable: formally derived in earlier works:[3]

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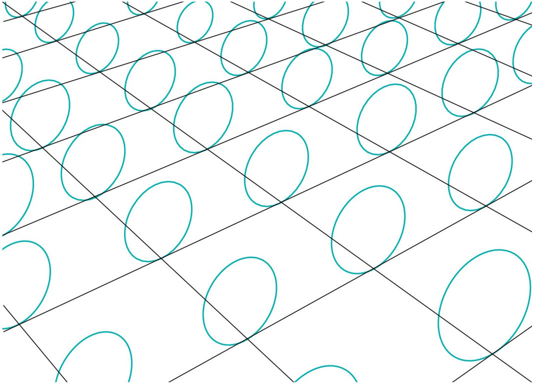
[2] Martin Bureš and Petr Siegl (2015). "Hydrogen atom in space with a compactified extra dimension and potential defined by Gauss' law". In: *Annals of Physics* 354, pp. 316–327. arXiv: 1409.8530v1.

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

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

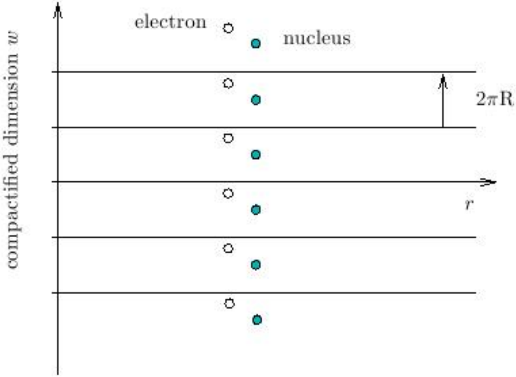
- But, how about if one of the dimensions is compact?
  circular compactification: we idetify points $x_4 \to x_4 + 2\pi R$



- How does that change the story?

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 $2\pi R$



Compactified extra dimension - method of images

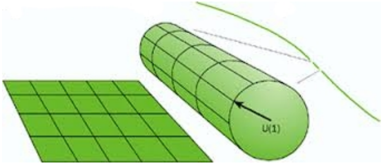
To calculate the force between two particles, the method of images makes it easier

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



Behaviour of the potential

- For $r \ll R$ and $x_4 \ll R$, the lowest-order term in the expansion of the potential is ($\rho^2 := r^2 + x_4^2$):

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

$\rightarrow$ 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:

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

Stability $Z < 1$: Application of Hardy's Inequality

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

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

- KLMN theorem

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

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

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

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 $R_{\rm c}$:

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

- the atom is stable for $R < R_{\rm c}$ and not stable if $R > R_{\rm c}$
- current experimental bounds on the size of extra dimensions:[4]
  $R^{-1} > 1.3\mathrm{TeV}$ at 95% C.L. $R \sim 10^{-18}$m

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

Summary of results for $\mathbb{R}^3 \times \mathcal{S}^1$ (compactified case)

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

Relativistic case

- The critical dimension for the hydrogen atom is three, instead of four (unlike the non-relativistic case).
- Thus, already in three spatial dimensions there exists a critical value of the coupling constant, above which the atom becomes unstable.
- Proof, *cf.* Lieb and Seiringer 2010, Lemma 10.3, also Lieb and Seiringer 2010, Chap. 8. The ground state energy is

$$E_0 = \inf_{\psi \in \mathcal{H}_0^+, \|\psi\|_2 = 1} [(\psi, D_0 \psi) - Z\alpha(\psi, |x|^{-1}\psi)]$$

Lemma (Stability of Hydrogen)

There is a critical $(Z\alpha)_c$*, with* $2/\pi \leq (Z\alpha)_c \leq 4/\pi$*, such that* E_0 *satisfies* $E_0 > \infty$ *for* $Z\alpha < (Z\alpha)_c$ *and* $E_0 = -\infty$ *for* $Z\alpha > (Z\alpha)_c$*.*

(Since $|p|$ and $1/|x|$ both scale like an inverse length, there is a critical coupling constant above which even stability of the first kind fails. Lieb and Seiringer 2010, Remark 8.5)

Relativistic case

- The relativistic Hardy inequality reads [Lieb and Seiringer 2010, Remark 8.5] function in $H^{1/2}(\mathbb{R}^d)$. Then there is the strict inequality

$$(\psi(x), |p|\psi(x)) > 2\left(\frac{\Gamma\left(\frac{d+1}{4}\right)}{\Gamma\left(\frac{d-1}{4}\right)}\right)^2 \int_{\mathbb{R}^d} \frac{|\psi(x)|^2}{|x|}\mathrm{d}x$$

- Moreover, the constant is sharp, i.e., for any bigger constant the inequality fails for some function in $H^{1/2}(\mathbb{R}^d)$. For $d = 3$ the constant in the relativistic Hardy inequality is $2(\Gamma(1)/\Gamma(1/2))^2 = 2/\pi$.
- The spectral properties of the operator $(p^2 + m^2)^{1/2} - Ze^2/r$ were examined in [Herbst 1977].
- Lieb, Yau, "The stability and instability of relativistic matter" [Lieb and Yau 1988].

Relativistic case - Klein-Gordon equation

- Analysis of stability for the following operator [Herbst 1977]

$$H = \sqrt{-\Delta + m^2} - m + ZV_(x)$$

The square root of the Klein-Gordon equation can be interpreted as a pseudodifferential operator [Laemmerzahl 1993]. The difficulty of its treatment is given by its non-locality.

- For simplicity, we set $m = 0$. The simple inequality $\sqrt{p^2 + m^2} - m \geq |p| - m$ shows that stability also holds in the case of non-zero mass whenever it holds with zero mass [Lieb and Seiringer 2010, Remark 8.5].
- Stability of relativistic matter implies stability of non-relativistic matter [Lieb and Seiringer 2010, Remark 8.6], hence the conclusions of [Bureš and Siegl 2015] are a special case of the above results.

Space Dimension Dynamics and Modified Coulomb Potential of Quarks - Dubna Potential

- Quarkonium spectroscopy indicates that between valence quarks inside hadrons, the potential on small scales has $D = 3$ Coulomb form and at hadronic scales has $D = 1$ Coulomb one.
- We may form an effective potential in which at small scales dominates $D = 3$ component and at hadronic scale - $D = 1$, the Coulomb-plus-linear potential (the "Cornell potential"):

$$V(r) = -\frac{k}{r} + \frac{r}{a^2} = \mu(x - \frac{k}{x}),\ \mu = 1/a = 0.427 GeV,\ x = \mu r,$$

where $k = \frac{4}{3}\alpha_s = 0.52 = x_0^2,\ x_0 = 0.72$ and $a = 2.34 GeV^{-1}$ were chosen to fit the quarkonium spectra [Eichten et al 1978].

Space Dimension Dynamics and Modified Coulomb Potential of Quarks - Dubna Potential

- We consider the dimension $D(r)$ of space of hadronic matter dynamically changing with r and corresponding Coulomb potential

$$V_D(r) \sim r^{2-D(r)},$$

  where effective dimension of space $D(r)$ changes from 3 at small r to 1 at hadronic scales ~ 1fm.
- Cornell potential contains QCD dynamics. We may compare it with Coulomb potential with dynamical dimension. We define dimension of space from the equality of $V(r) = \mu(x - \frac{k}{x})$ and $V(D, r) = -\alpha(D)r^{2-D}$:
- In[5] we constructed such a potential and effective dimension as a functions of r.

[5] Martin Bureš and Nugzar Makhaldiani (2019). “Space Dimension Dynamics and Modified Coulomb Potential of Quarks - Dubna Potentials”. In: *Physics of Elementary Particles and Atomic Nuclei, Letters* 16 (6).

Space Dimension Dynamics and Modified Coulomb Potential of Quarks - Dubna Potential

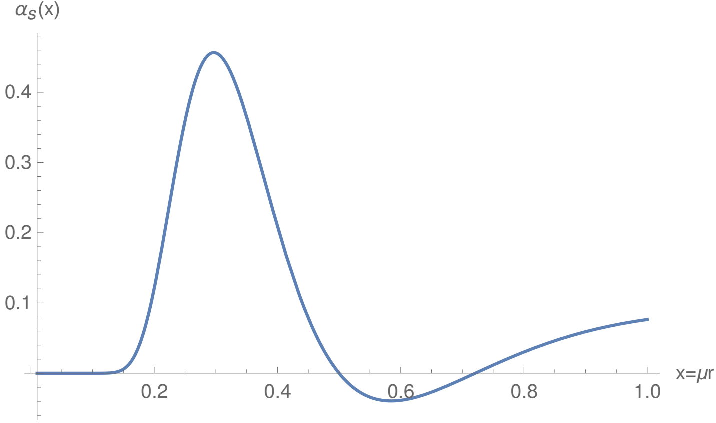


Figure: α_s as a function of $x = \mu r \in (0.01, 1.0)$

Space Dimension Dynamics and Modified Coulomb Potential of Quarks - Dubna Potential

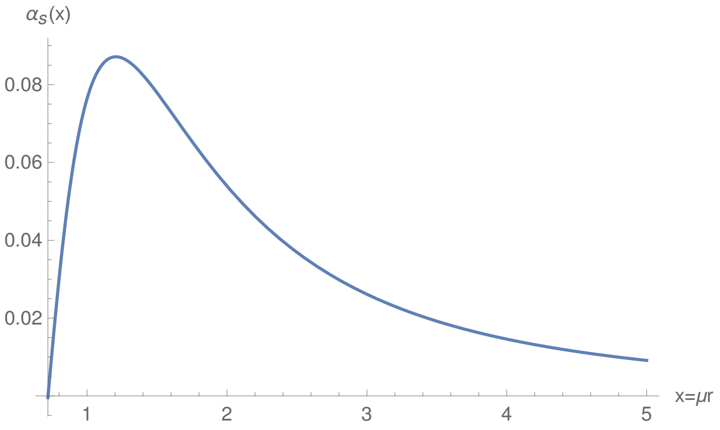


Figure: α_s as a function of $x = \mu r \in (0.72, 5)$

Energy shifts due to a compactified extra dimension

We know that:[6]

- 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: diagonalization of the Hamiltonian[7]

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

[7] Martin Bureš (2015). "Energy spectrum of the hydrogen atom in a space with one compactified extra dimension, $R^3 \times S^1$". In: *Annals of Physics* 363, pp. 354–363. arXiv: 1505.08100 [quant-ph].

Energy shifts due to a compactified extra dimension

Basis constructed from the hydrogen atom eigenstates

$$\langle \vec{x} | nlmq \rangle = R_{nl}(r) Y_{lm}(\Omega) \frac{e^{iq\theta}}{\sqrt{2\pi}},$$
$$l \in \mathbb{N},\ m \in \{-l, \ldots, l\},\ n \in \{l+1, l+2, \ldots\},\ q \in \mathbb{Z}.$$

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

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

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

Energy shifts due to a compactified extra dimension

Basis constructed from exponential functions

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

Matrix elements of the Hamiltonian:

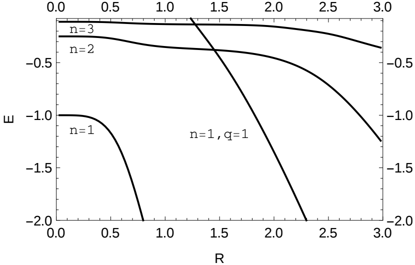
$$\langle jp | \hat{H} | iq \rangle = \left[\langle jp | iq \rangle \left(\alpha_i \alpha_j + \frac{q^2}{R^2} \right) - \frac{(2\sqrt{\alpha_i \alpha_j})^3}{(\alpha_i + \alpha_j + |q - p|/R)^2} \right],$$

where

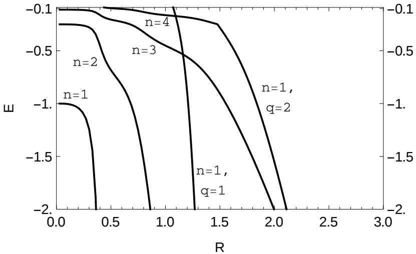
$$\langle jp | iq \rangle = 4(\alpha_m \alpha_n)^{3/2} \int_0^\infty \mathrm{d}r r^2 e^{-(\alpha_i + \alpha_j)r} \frac{1}{2\pi} \int_0^{2\pi} e^{\mathrm{i}(q-p)\theta} = \left(\frac{2\sqrt{\alpha_i \alpha_j}}{\alpha_i + \alpha_j} \right)^3 \delta_{p,q}$$

are the overlap integrals.

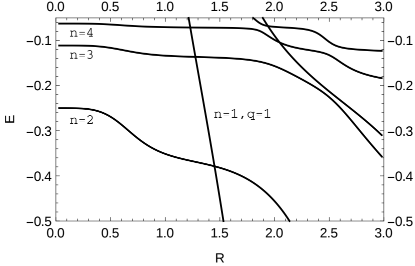
Energy shifts due to a compactified extra dimension

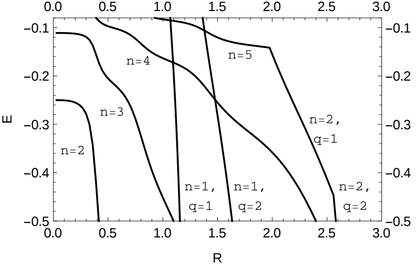


(a) Energy levels: hydrogen basis ($l = m = 0$, size $N = 10$, $Q = 30$)

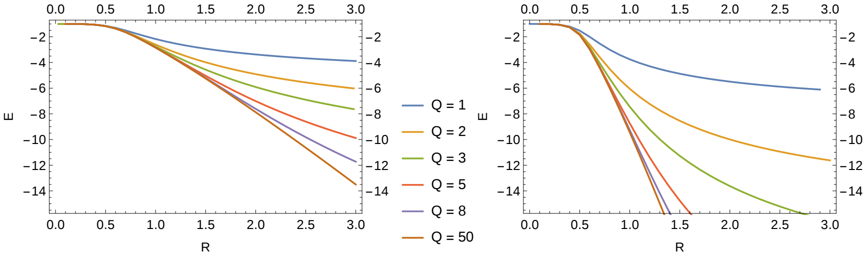


(b) Energy levels: exponential basis ($l = m = 0$, size $N = 10$, $Q = 30$)





Energy shifts due to a compactified extra dimension



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

(g) Ground state energy dependence on basis size (exponential basis, $N = 7,\ Q = 1, \ldots, 50$)

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

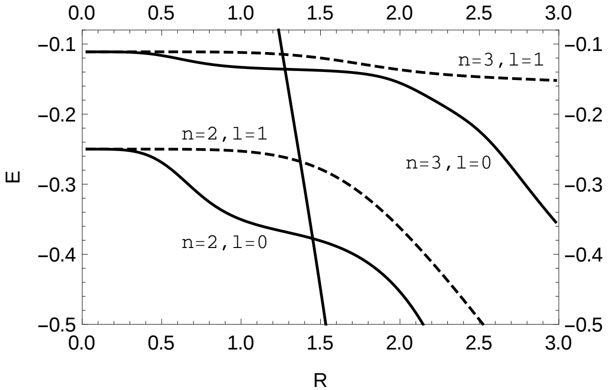
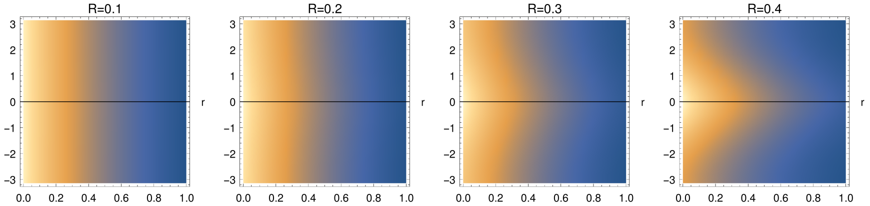
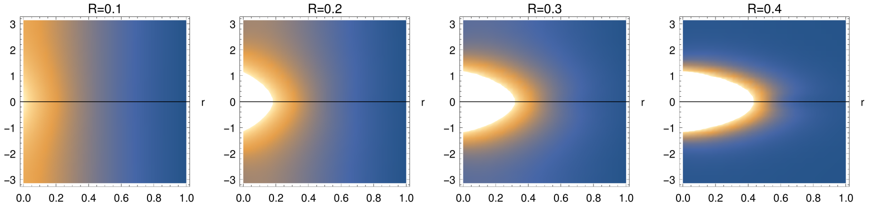


Figure: The lifting of degeneracy of energy levels (hydrogen atom basis, $N = 7$, $Q = 30$): $n = \{2, 3\}$: $l = 0$ (solid line) $l = 1$ (dashed line), $m = 0$. The almost vertical curve represents the first Kaluza-Klein state $n = 1, q = 1$.

Electron probability density in the (r, θ) plane



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



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

Thank you!

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The Friedrichs extension

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

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

with $\mathrm{Dom}\,(h) := \mathrm{Dom}\,(H)$, 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.

The first representation theorem

Theorem (The first representation theorem)

Let $h : \mathrm{Dom}\,(h) \times \mathrm{Dom}\,(h) \to \mathbb{C}$ *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) $\mathrm{Dom}\,(H) \subset \mathrm{Dom}\,(h)$ *and* $h(\phi, \psi) = \langle \phi, H\psi \rangle$ *for every* $\phi \in \mathrm{Dom}\,(h)$ *and* $\psi \in \mathrm{Dom}\,(H)$;

ii) $\mathrm{Dom}\,(H)$ *is a core of* h;

iii) *if* $\psi \in \mathrm{Dom}\,(h)$, $\eta \in \mathcal{H}$, *and* $h(\phi, \psi) = \langle \phi, \eta \rangle$ *holds for every* ϕ *belonging to a core of* h, *then* $\psi \in \mathrm{Dom}\,(H)$ *and* $H\psi = \eta$. *The self-adjoint operator* H *is uniquely determined by the condition* i).

Weyl's criterion

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 $\{\psi_n\}_{n\in\mathbb{N}} \subset \mathrm{Dom}\,(H)$ 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 $\sigma_{\mathrm{ess}}(H)$ if, and only if, in addition to the above properties the $\{\psi_n\}$ converges weakly to zero in $\mathcal{H}$.