A numerical study of the 1d hydrogen atom

Héctor Mejía-Díaz, Luis Fabian Garcia-Mendoza, Wolfgang Bietenholz

Instituto de Ciencias Nucleares, UNAM

The 3d Hydrogen Atom

- Two particles: proton and electron, spinless
- Non-relativstic quantum mechanics
- Electron subjected to Coulomb potential

$$V_{3d}(r) = -\frac{e^2}{4\pi\epsilon_0 r}$$

- Energy spectrum

$$E_n = -\left[\frac{\mu}{2\hbar^2}\left(\frac{e^2}{4\pi\epsilon_0}\right)^2\right]\frac{1}{n^2}$$

The one-dimensional hydrogen atom

We define the 1d Coulomb potential as

$$V(x) = -\frac{e^2}{4\pi\epsilon_0}\frac{1}{|x|}.$$

Why is it more delicate than in 3d?

- Its expectation value,

$$\langle V \rangle = -\frac{e^2}{4\pi\epsilon_0}\int \frac{|\psi(x)|^2}{|x|}\,dx$$

  contains a divergent integrand
- The solutions of Schrödinger's equation must be in $\mathbb{R} - \{0\}$
- It's not clear how to connect the $x > 0$ and $x < 0$ solutions

Energy spectrum of 1d hydrogen atom

- Loudon (1959):
  - Potential barrier at $x = 0$
  - Infinitely-negative binding energy
  - All excited states doubly degenerated
- Andrews (1976):
  - No degeneracy of excited states
  - Solutions for $x > 0$ or $x < 0$ only
- Criticism due to no-degeneracy theorem
- Moshinsky (1992):
  - There's no potential barrier
  - Ground state energy might be minus infinite

Energy spectrum of 1d hydrogen atom

- Nouri, Palma and Raff (2002)
  - For $n = 1, 2, 3 \ldots$

$$E_n^{1d} = -\frac{\mu e^4}{2(4\pi\epsilon_0)^2\hbar^2}\frac{1}{n^2}$$

    as in the 3d case

- Abramovici and Avishai (2009)
  - The potential is a perfect reflector
  - Two types of solutions

$$E_n^{1d} \propto \frac{1}{n^2}$$

$$\tilde{E}_n^{1d} \propto \frac{1}{(n+\frac{1}{2})^2}$$

Energy spectrum of 1d hydrogen atom

- Numerical studies: diagonalize $\hat{H}$
  - Dziubak and Matulewski (2013): no state with infinite energy
  - Gebremedhin and Weatherford (2014): $1/\sqrt{x^2+\beta^2}$, $\beta \to 0$
    - Excited states $\propto 1/(2n^2)$
    - Ground state with $E \to -\infty$

Main controversies

- $x = 0$ acts as an impenetrable barrier ?
- Only consider $x > 0$ or $x < 0$?
- Ground state energy finite or divergent ?

- We give clear evidence of the behavior of the ground state and the first excited state of the 1d hydrogen atom

Virial Theorem

For a Hamiltonian of the form

$$\hat{H} = \hat{T}(\hat{p}) + \hat{V}(\hat{x}),$$

the Virial Theorem identifies

$$\langle \hat{T} \rangle = \frac{1}{2} \left\langle x \frac{dV(x)}{dx} \right\rangle$$

Instead of Coulomb potential ($e^2/(4\pi\epsilon_0) = 1$, $\hbar = 1$, $\mu = 1$)

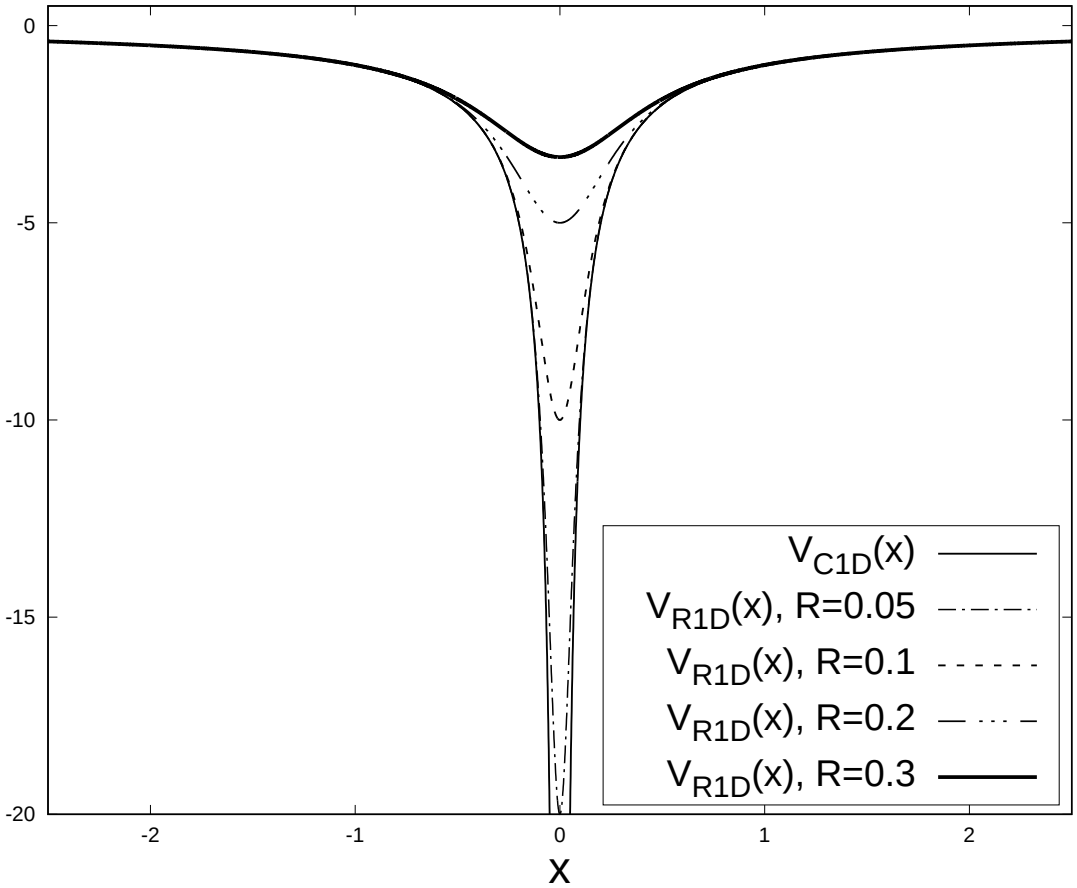
$$V_C(x) = -\frac{1}{|x|},$$

we consider the regularized potential

$$V_R(x) = \left(-\frac{1}{|x|} \right) \frac{\exp(2|x|/R) - 1}{\exp(2|x|/R) + 1} \overbrace{\longrightarrow}^{R \to 0} V_C(x)$$

Regularized potential

- $V_R(x) \to V_C(x)$ if $|x| \gg R$, $\quad R(0) = \frac{1}{R}$
- $0.006 \leq R \leq 0.3$



Path integral formulation

Expectation value of observable A

$$\langle A \rangle = \frac{\int \mathcal{D}x \, \exp(-S[x(\tau)])A[x(\tau)]}{\int \mathcal{D}x \, \exp(-S[x(\tau)])}$$

where $[x(\tau)]$ represents any possible path

Ground state energy of regularized 1d hydrogen atom

$$E_1(R) \simeq -\left\langle \frac{1}{N} \sum_{i=1}^{N} \left[\frac{\exp(2|x_{\tau_i}|/R) - 1}{2|x_{\tau_i}|(\exp(2|x_{\tau_i}|/R) + 1)} + \frac{2\exp(2|x_{\tau_i}|/R)}{R(\exp(2|x_{\tau_i}|/R) + 1)^2} \right] \right\rangle$$

Monte Carlo simulations

- Numerical approximation for expectation value:

$$\langle A \rangle = \frac{1}{M} \sum_{\text{paths}}^{M} \frac{1}{N} \sum_{i=1}^{N} A[x^k(\tau_i)]$$

- Paths $[x^k]$ with probability $p[x^k] \propto \exp(-S([x^k]))$
- Markov chain $\longrightarrow$ detailed balance

$$\frac{P(x^k(\tau) \to x^j(\tau))}{P(x^j(\tau) \to x^k(\tau))} = \frac{p[x^j]}{p[x^k]}$$

for transition probability $P(x^k \to x^j)$

- Ergodicity: all paths are attainable in a finite number of steps

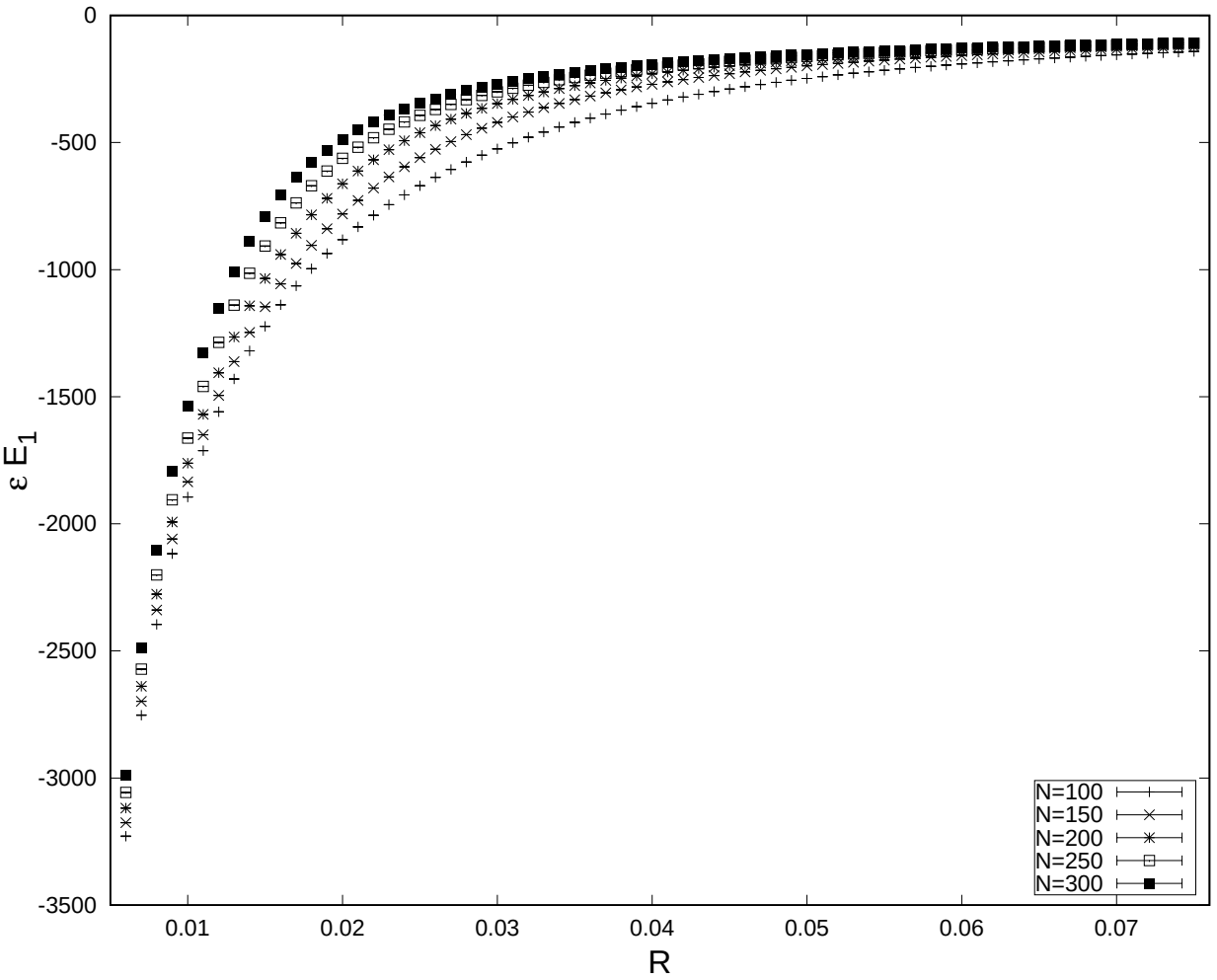
Simulation overview

- Initial path $\{x^{initial}\}$: $100 \leq N \leq 300$ random $x(\tau_k)$-values in $[-2, 2]$
- Fix parameter R
- Fix temporal interval of size $20 \gg$ correlation length, $\epsilon := \frac{20}{N}$
- Suggest update step $x_{\tau_k} \to x_{\tau_k} + (2r - 1)R$ for $r \in [0, 1]$
- Metropolis acceptance probability:

$$P = \begin{cases} 1 & \text{if} \quad \Delta S \leq 0 \\ e^{-\Delta S} & \text{otherwise} \end{cases}$$

- Thermalization: skip $10\,000N$ steps $=10\,000$ sweeps
- Decorrelation: measure observable in independent paths separated by 100 sweeps

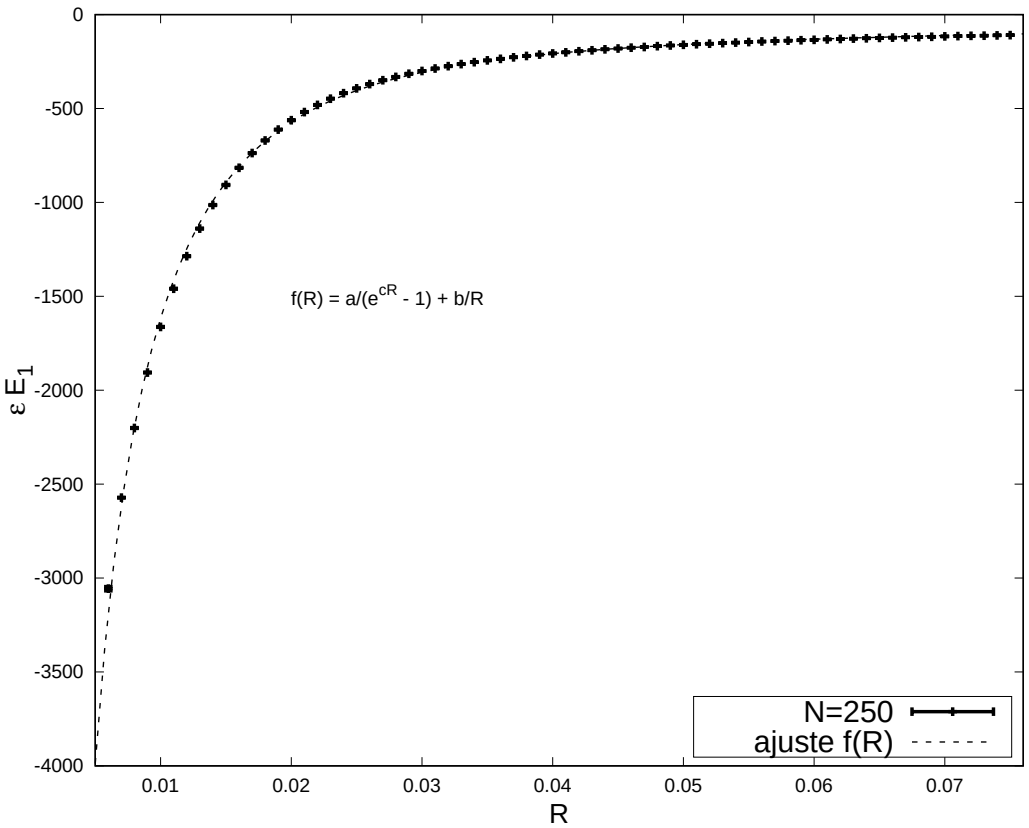
Numerical results: Ground state energy



Numerical results: Ground state energy

Fit the data to

$$f(R) = \frac{a}{\exp(cR) - 1} + \frac{b}{R},$$



Numerical results: Ground state energy

$$f(R) = \frac{a}{\exp(cR) - 1} + \frac{b}{R},$$

- Fitting parameters

N	a	b	c	$\frac{a}{c} + b$
150	-757(35)	-6.8(5)	51(4)	-21(1)
200	1416(56)	7.9(1)	92 (3)	-23.2(8)
250	-2186(70)	-7.80(7)	128(3)	-24.8(7)
280	-2717(87)	-7.65 (5)	150(3)	-25.7(7)
300	-3180(93)	-7.56(4)	166(3)	-26.7(7)

Numerical results: Ground state energy

From Laurent series

$$f(R) = \frac{\frac{a}{c} + b}{R} - \frac{a}{2} + \frac{Rac}{12} + \mathcal{O}(R^3)$$

If

$$g(a, b, c; N) = \frac{a}{c} + b \neq 0,$$

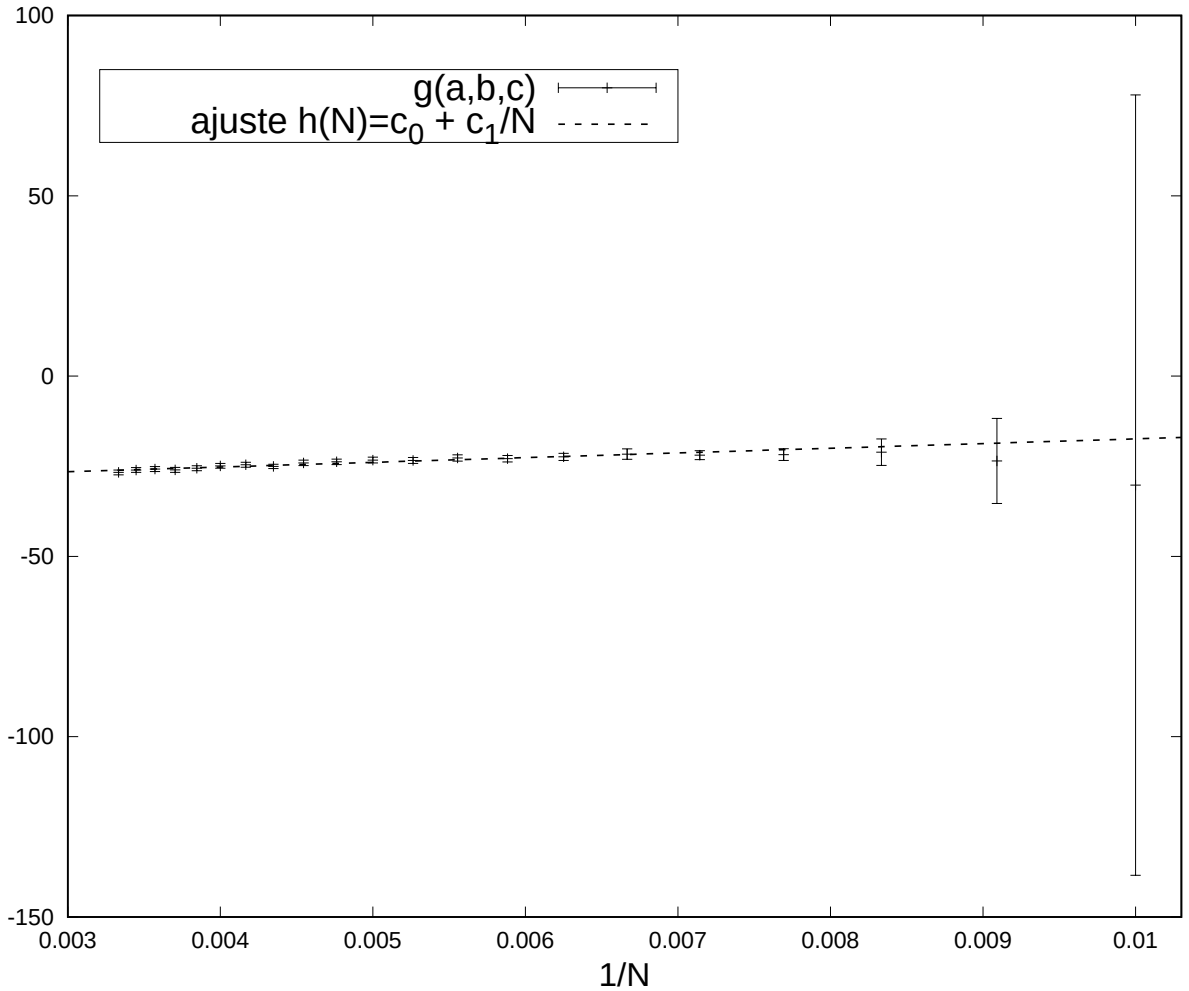
the ground state energy diverges in the limit $R \to 0$.

Continuum extrapolation: we fit $g(a, b, c; N)$ to

$$h(N) = c_0 + \frac{c_1}{N}$$

Numerical results: Ground state energy

$c_0 = -30.4(4)$



Correlation function

The first energy gap can be measured through the two-point correlation function.
Using translation invariance and periodicity one obtains

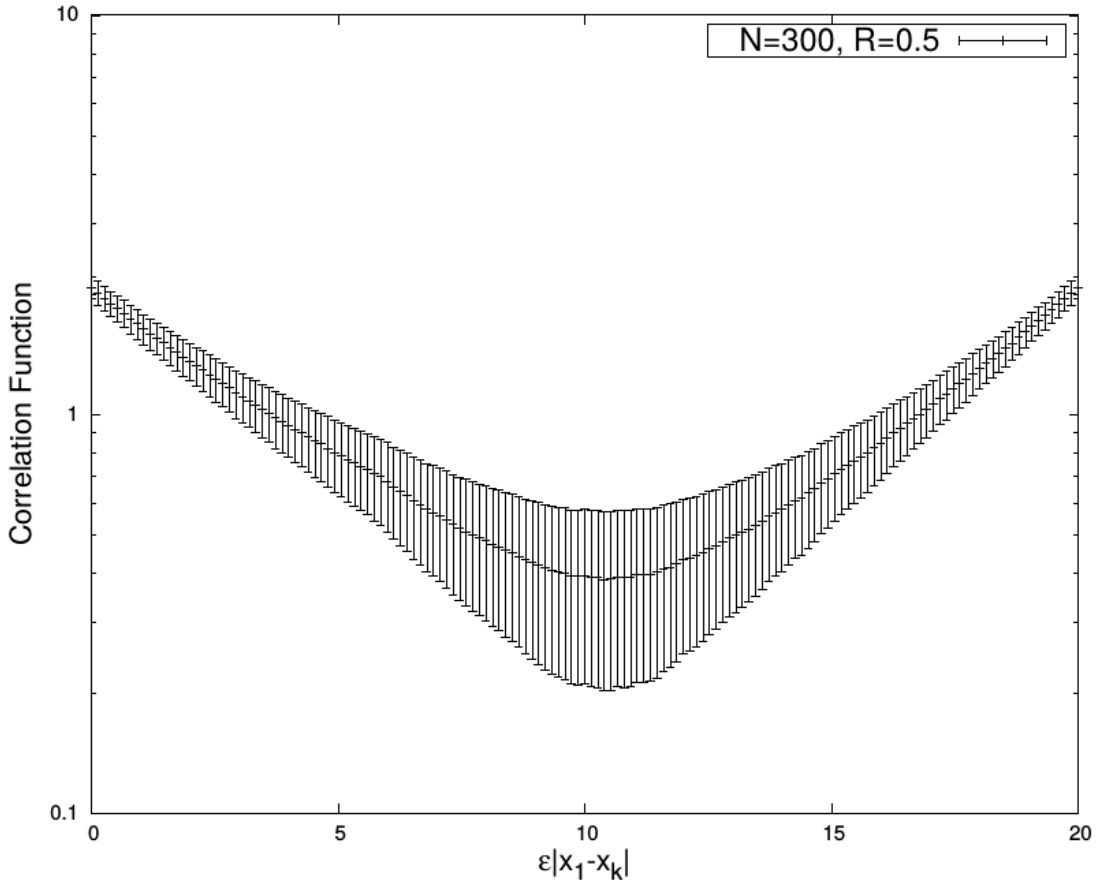
$$\langle x_{\tau_i} x_{\tau_j} \rangle \propto \cdot \cosh \left(\frac{|x_{\tau_i} - x_{\tau_j}| - \frac{N}{2}}{\xi} \right)$$

where ξ is the correlation length

$$\xi = \frac{1}{E_2 - E_1}$$

Numerical results: first energy gap

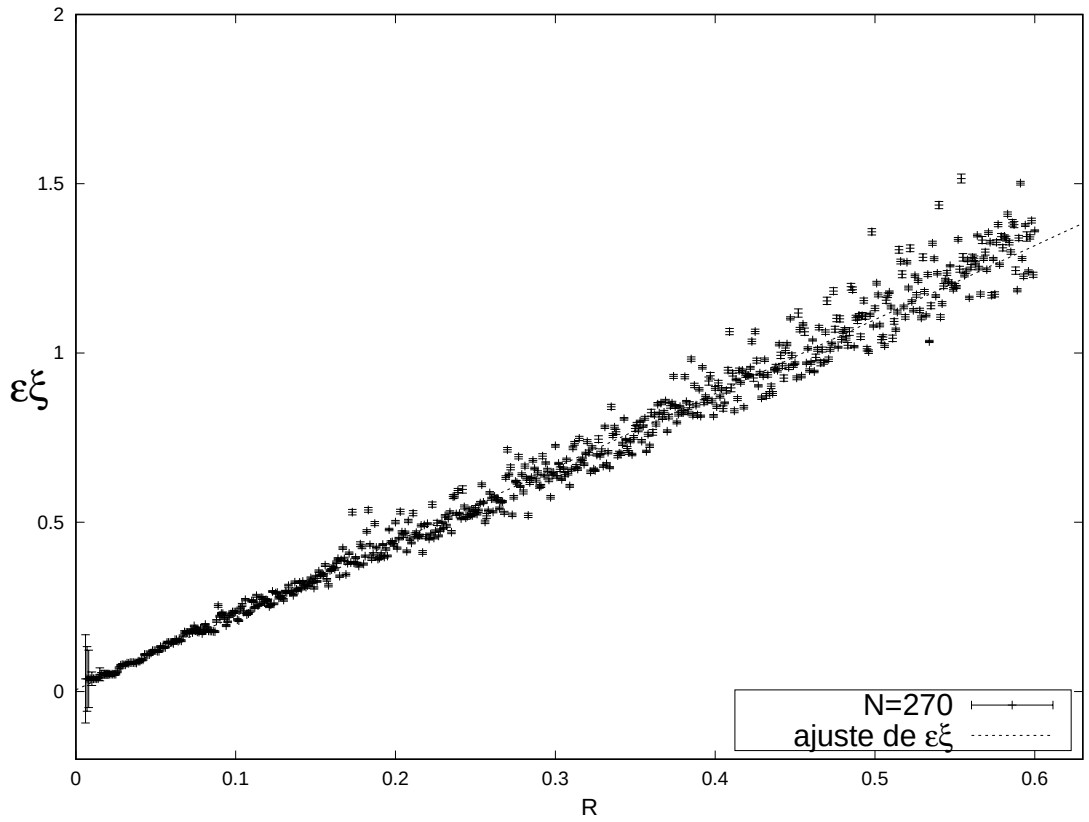
$$\langle x_{\tau_1} x_{\tau_k} \rangle = \lim_{M\to\infty} \frac{1}{M} \sum_{i=1}^{M} x_R^i(\tau_1) x_R^i(\tau_k)$$



Numerical results: first energy gap

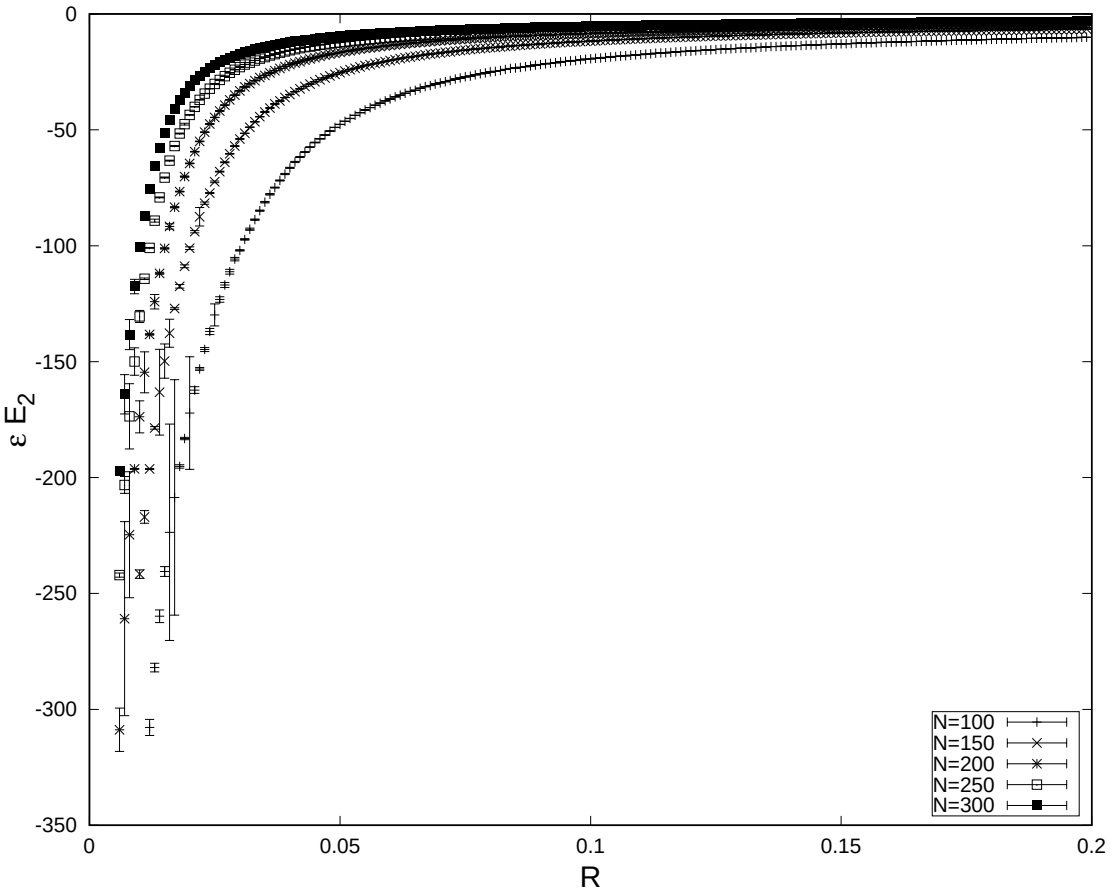
Correlation length

$$\xi = \frac{1}{E_2 - E_1}$$



Numerical results: first energy gap

$$E_2 = \left(\frac{1}{\xi} + E_1 \right)$$



Numerical results: first energy gap

Treatment of E_2 analogous to E_1

$$f(R) \approx \frac{\frac{a}{c} + b}{R} - \frac{a}{2} + \frac{Rac}{12}$$

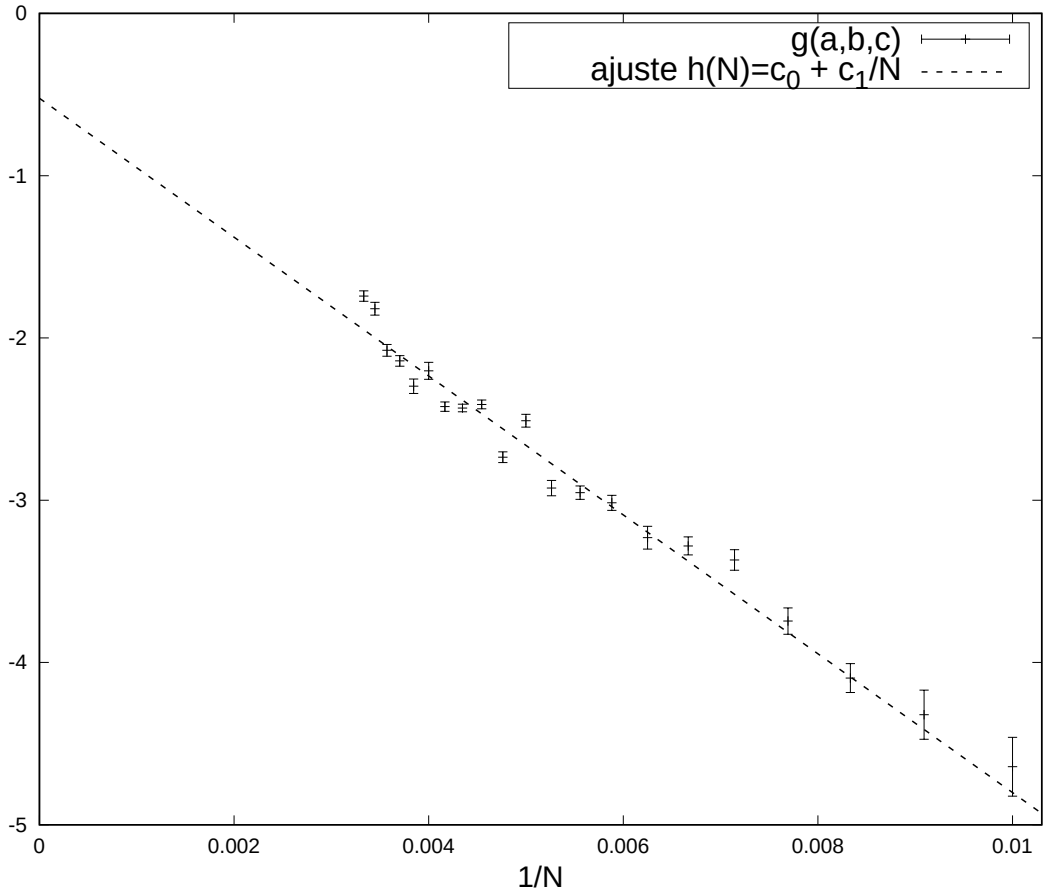
leads to a divergence if

$$g(a, b, c) = \frac{a}{c} + b \neq 0$$

Numerical results: first energy gap

Since $h < 0$, $E_2 \to -\infty$

$c_0 = -0.5(1)$



Summary

1. We treated the Coulomb problem in one dimension introducing a smoothly regularized potential, in the range of the parameter R. This enables the application of the Virial Theorem
2. After considering the ground state energy for various values of N, our fitting function reveals its divergence, as $N \to \infty$ $R \to 0$: $E_1 \to -\infty$
3. The study of the two point correlation function also shows that the first energy gap is divergent, $(E_2 - E_1) \to \infty$
4. Still, the first excited energy eigenvalue is $E_2 \to -\infty$
5. **The one-dimensional hydrogen atom does not represent a sensible quantum mechanical model**