

La ambigüedad en el tratamiento de la ecuación de Schrödinger con el potencial de paredes infinitas disipada 90 años más tarde

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Real Academia de Ciencias

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1. Introducción

Esta no es (¡¡ no debe ser !!) una conferencia para investigadores en el campo:
Reunión Anual conjunta entre Académicos Numerarios y Correspondientes Nacionales de la Sección de Exactas (RAC, 1/06/2016).

Conferencias ya impartidas sobre G. Gamow, el efecto túnel, el potencial de paredes infinitas, “soluciones planas” del problema lineal de Schroedinger y mi artículo de 2015:

J. I. Díaz, On the ambiguous treatment of the Schrödinger equation for the infinite potential well and an alternative via flat solutions: the one-dimensional case. *Interfaces and Free Boundaries*, **17** (2015), 333–351.

Tours (2012), Valencia (2013), Cambridge (2014), Nápoles (2015), Tenerife (2016), ...



Plan de la conferencia

2. Gamow, Schroedinger, Cabrera, Rey Pastor y Dou.
3. Confinamiento para la onda de Schroedinger: el efecto túnel de Gamow.
4. Ambigüedad en el potencial de paredes infinitas: resultados rigurosos.
5. Demostraciones y observaciones adicionales.

2. Gamow, Schroedinger, Cabrera, Rey Pastor y Dou.

In his 1928 pioneering article Gamow proved, for the first time, the *tunneling effect* which, among many other applications lead to the construction of the electronic microscope and the correct study of the alpha radioactivity. Most of his study was concerning with *bound states* $\psi(x, t) = e^{-iEt}u(x)$ of the Schrödinger equation in \mathbb{R}^N , $N \geq 1$, [1925]

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \Delta \psi + V(x)\psi, \text{ in } (0, \infty) \times \mathbb{R}^N,$$

associated to the potential $V(x)$, for a single elementary particle of mass m and energy E which we shall denote also by λ). Here $i = \sqrt{-1}$ and \hbar is the renormalized Plank constant.
Gamow was specially interested in the Coulomb potential

$$V(x) = \frac{k}{|x|}, \quad x \in \mathbb{R}^N,$$

Personal historical researches (Galindo, Sánchez-del Río, Sánchez Ron,...)

Zur Quantentheorie des Atomkernes.

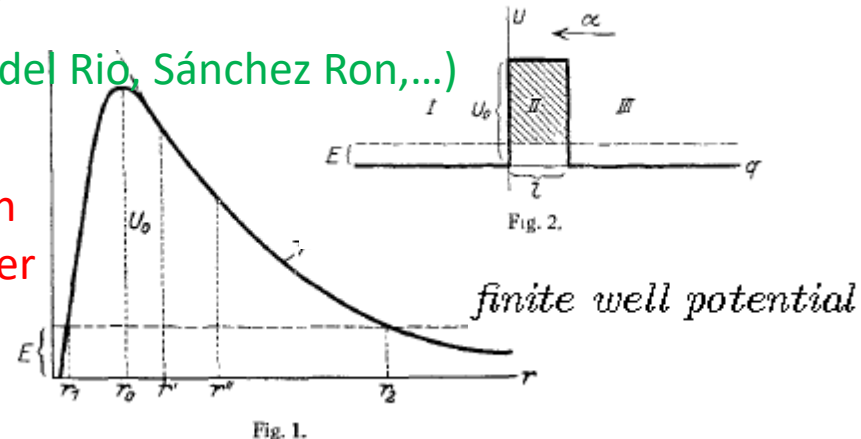
Von G. Gamow, z. Zt. in Göttingen.

Mit 5 Abbildungen. (Eingegangen am 2. August 1928.)

Traducción
Uwe Brauer

Göttingen, Institut für theoretische Physics

Mention to a 1927 paper by E. Rutherford





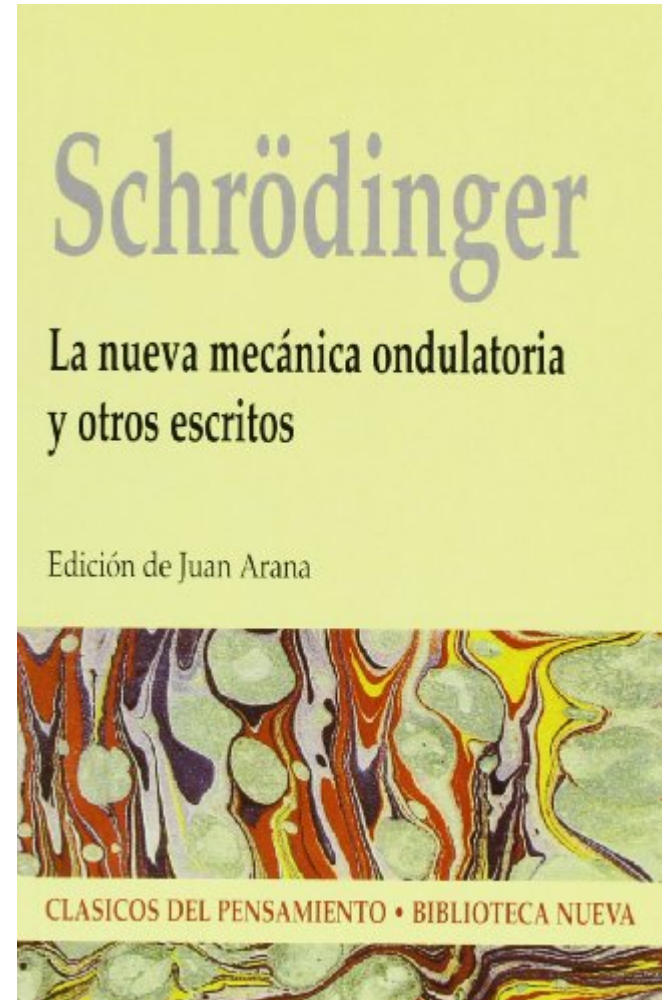
George Gamow
(Odessa, Ukrania 1904-Boulder (Colorado, USA), 1958)



[Erwin Schrödinger \(Viena, 1887-1961\)](#)

Curso de Verano en la U. I. de Verano (Santander) 1934

Las bases de la nueva ciencia físico-matemática fue el nombre elegido para una serie de cursos en los que Maurice Fréchet y Esteban Terradas hablaron sobre probabilidad, y Blas Cabrera, que había sucedido a Ramón Menéndez Pidal como rector de la Universidad Internacional de Verano, presentó las bases de la relatividad y de la estructura atómica. Pero la estrella indiscutible del curso fue Schrödinger, ese hombre entusiasta y de aspecto algo extravagante que había recibido el premio Nobel de Física, junto con Paul Dirac y Werner Heisenberg, el año anterior.



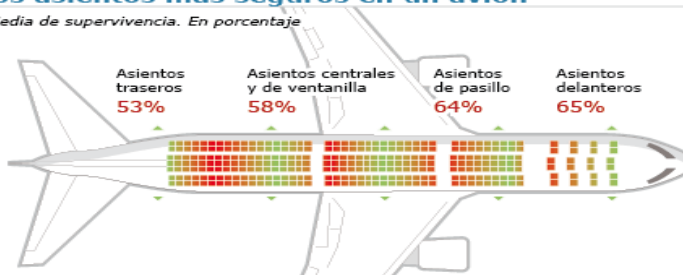


Blas Cabrera (1878-1945)

1934. Presidente de la Academia de Ciencias de Madrid, cargo que ocupa hasta el año 1937 en que se exilia. Rector de la Universidad Internacional de Verano de Santander, de la que había sido uno de los fundadores en el año 1933

Los asientos más seguros en un avión

Media de supervivencia. En porcentaje



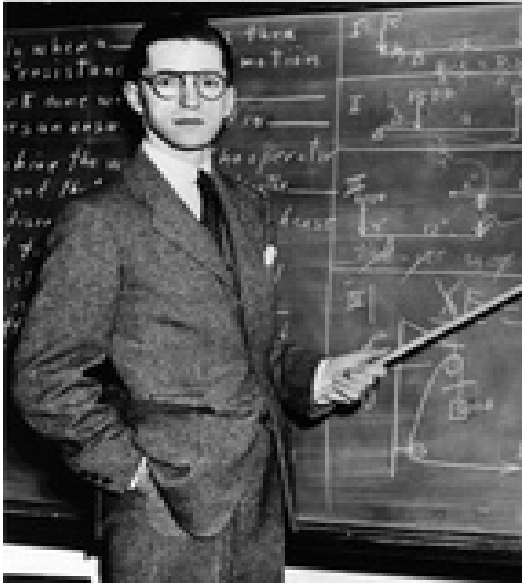
Distancia de la salida de emergencia

Según el estudio de la universidad de Greenwich, sobre 105 accidentes con aterrizajes forzados y fuegos a bordo, los asientos más peligrosos son los que se encuentran a seis o más filas de la salida de emergencia.



Piloto de la física española anterior a la Guerra Civil (1936)

Biografía de la física



At the University, Gamow made friends with three other students of theoretical physics, Lev Landau, Dmitri Ivanenko, and Matvey Bronshtein (who was later arrested in 1937 and executed in 1938 by the Soviet regime). The four formed a group known as the **Three Musketeers** which met to discuss and analyze the ground-breaking papers on quantum mechanics published during those years. He later used the same phrase to describe the Alpher, Bethe (fictitious), and Gamow "group." (**alfa-beta-gamma**)

On graduation, he worked on quantum theory in Göttingen (Max Born), where his research into the atomic nucleus provided the basis for his doctorate. He then worked at the Theoretical Physics Institute of the University of Copenhagen (Niels Bohr), from 1928 to 1931, with a break to work with Ernest Rutherford at the Cavendish Laboratory, Cambridge.

George Gamow was the father (1946) of the hot **"big bang" theory** of the expanding universe.

After the discovery of the structure of **DNA** in 1953 by Francis Crick, James D. Watson, Maurice Wilkins and Rosalind Franklin, Gamow attempted to solve the problem of how the order of the four different kinds of bases (adenine, cytosine, thymine and guanine) in DNA chains could control the synthesis of proteins from amino acids. Crick has said that Gamow's suggestions helped him in his own thinking about the problem. As related by Crick,[33] **Gamow suggested that the twenty combinations of four DNA bases taken three at a time corresponded to the twenty amino acids that form proteins.** This led Crick and Watson to enumerate the twenty amino acids common to proteins. Gamow's contribution to solving the problem of genetic coding gave rise to important models of biological degeneracy.

In 1956, he was awarded the Kalinga Prize by UNESCO for his work in popularizing science with his **Mr. Tompkins...** series of books (1939–1967), his book One, Two, Three...Infinity, and other works.

Göttingen, Institut für theoretische Physics

47 Nobel Prize



Carl Friedrich Gauss, mathematician



Bernhard Riemann, mathematician



David Hilbert, mathematician



Felix Klein, mathematician



Constantin Carathéodory, mathematician



Peter Gustav Lejeune Dirichlet, mathematician



Max Born, physicist



J. Robert Oppenheimer, physicist



Max Planck, physicist



Walther Nernst, chemist



Friedrich Wöhler, chemist



Heinrich Heine, poet



Brothers Grimm, writers



Arthur Schopenhauer, philosopher



Rudolf von Jhering, jurist



Otto von Bismarck, "Iron Chancellor" of the second German Empire



Richard von Weizsäcker, former President of Germany



Gerhard Schröder, former Chancellor of Germany



Max Weber, sociologist



Jürgen Habermas, sociologist



John von Neumann, mathematician



Gottlieb Burckhardt, psychiatrist



Werner Heisenberg, Physicist



Enrico Fermi, Physicist



Wolfgang Pauli, Physicist



Irving Langmuir, Chemist/Physicist



Max Von Laue, Physicist



Rudolph Sohm, lawyer and Church historian



William Graham Sumner, Sociologist



Göttingen also had a focus on natural science, especially mathematics. Carl Friedrich Gauss taught here in the 19th century. Bernhard Riemann, Peter Gustav Lejeune Dirichlet and a number of significant mathematicians made their contributions to mathematics here. By 1900, David Hilbert and Felix Klein had attracted mathematicians from around the world to Göttingen, which made Göttingen a world mecca of mathematics at the beginning of the 20th century.



Alberto Dou (1915-2009)

Actos de celebración de su centenario Real Academia de Ciencias,
24 de febrero de 2016

J. I. Díaz, Alberto Dou: su obra matemática y su papel en el progreso de la matemática española, La Gaceta de la RSME, Vol. 12 (2009), 227-243

J.I. Díaz, Alberto Dou y sus valores científicos Rev. R. Acad. Cienc. Exact. Fis. Nat., Vol. 103, Nº 2 (2009).



Courant Institut (F. John)
Univ. Paris VI (J.L. Lions)

Piloto de la matemática española anterior a la Guerra Civil (1936)



Julio Rey Pastor

(Logroño, 1888 –Buenos Aires, 1962).

Pensionado en 1913 en Berlin y Gottingen (transformaciones conformes: Koebe y Bieberbach)

3. Confinamiento para la onda de Schroedinger: el efecto túnel de Gamow.

We recall that in Quantum Mechanics,

$\psi : [0, \infty) \times \mathbb{R}^N \rightarrow \mathbb{C}$ the matter wave function (L. de Broglie 1924: wave-particle duality)

$\hbar > 0$ renormalized Plank constant, m mass of the elementary particle,

$V(x) \in \mathbb{R}$ the external potential

Crucial fact: $|\psi(x, t)|^2$ represents the probability density (Max Born 1926) to find the particle at point x and time t :

$$\frac{\partial}{\partial t} |\psi|^2 + \operatorname{div} \mathbf{J} = 0$$

$$\mathbf{J} := \frac{i\hbar}{2m} (\psi \nabla \psi^* - \psi^* \nabla \psi) = \frac{\hbar}{2m} \operatorname{Re} \left(\frac{1}{i} \psi^* \nabla \psi \right)$$

(ψ^* =the complex conjugate of ψ).

Question: how to "confine" (or "localize") the particle (and how to measure its linear momentum \mathbf{p}) ??

Simplifications for the linear Schrödinger equation (attributed by him, in 1935, to George Gamow (1904-1968) and repeated in any text book in Quantum Mechanics):

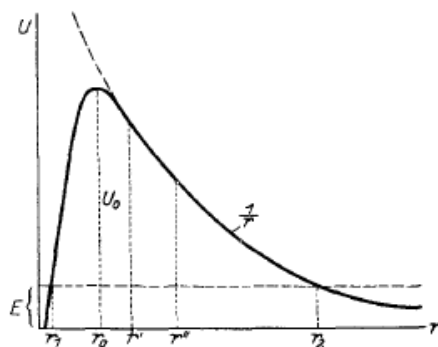


Fig. 1.

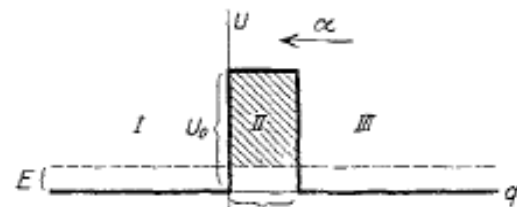


Fig. 2.

$$\psi(x, t) = e^{-iEt}u(x)$$

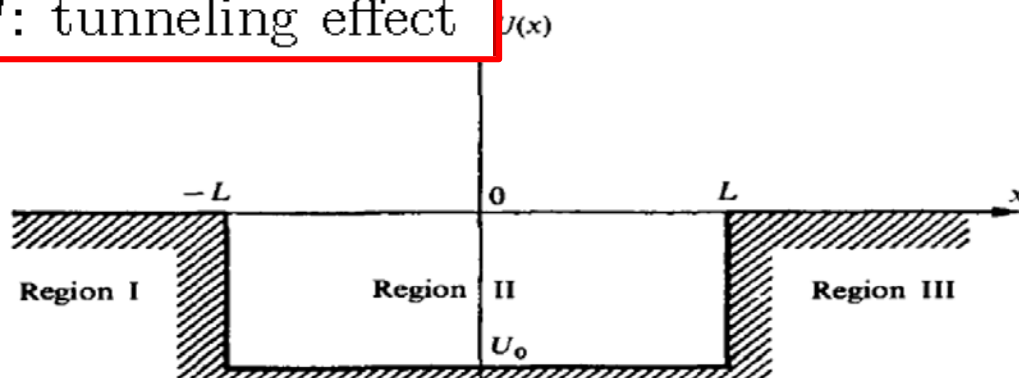
$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \Delta \psi + V(x)\psi, \text{ in } (0, \infty) \times \mathbb{R}^N,$$

For simplicity $m = 1$, $\hbar = 1$ and $E = \lambda$

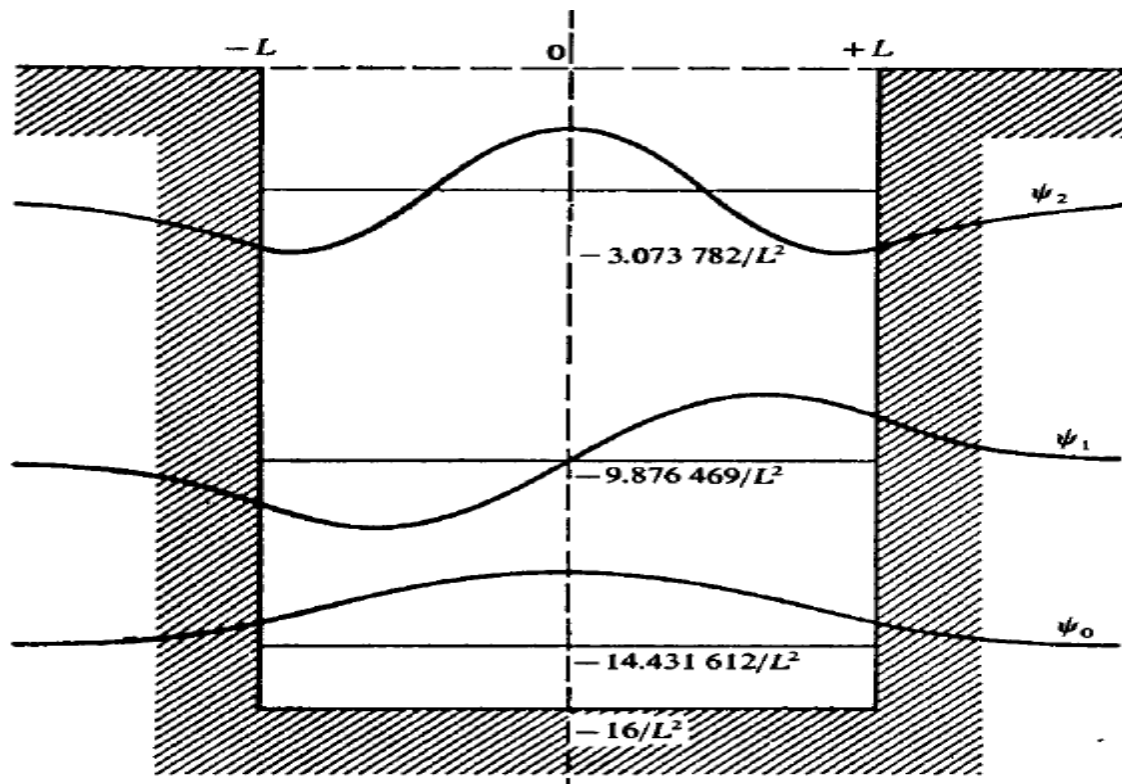
$$-\Delta u + V(x)u = \lambda u \quad \text{in } \mathbb{R}^N,$$

"the square well potential": tunneling effect

$$V_q(x; R, V_0) = \begin{cases} V_0 & \text{if } x \in (-R, R), \\ q & \text{if } x \notin (-R, R). \end{cases}$$



In his 1928 article, Gamow consider the *finite well potential* by solving the problem in a weak sense: the solution was not C^2 but merely C^1 . The notion of "solution" used by him was not explicitly mentioned in the paper but it is coherent with the notion of weak solution introduced several years later by J. Leray, L. Sobolev and L. Schwartz.



Wave functions and potential for a square potential well with $L|U_0|^{1/2} = 4$

Microscopios de Efecto Túnel (en inglés *Scanning tunneling microscope* o **STM**)

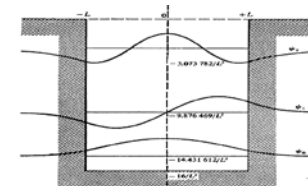
Binnig y H. Rohrer (de IBM Zürich),
1981: Premio Nobel de Física de 1986

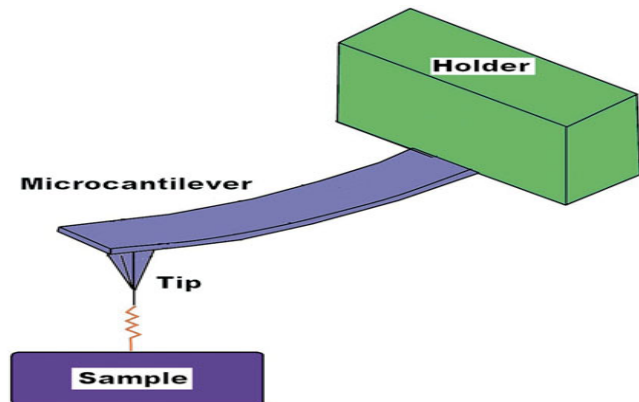
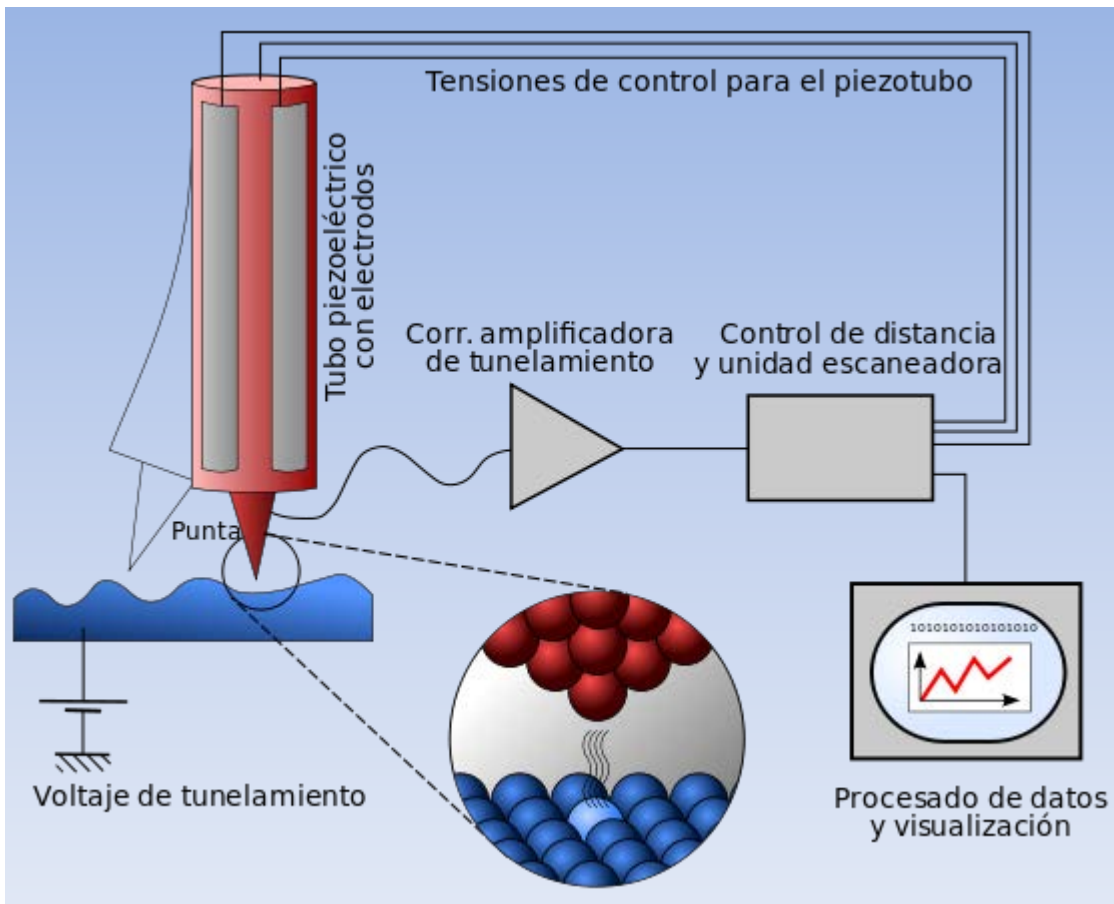
- imágenes de superficies a nivel atómico.
- resolución de 0.1 nm

Efecto túnel:

En su pionero artículo de 1928
George Gamow probó, por
primera vez, el efecto túnel
que conduce a la construcción
del microscopio electrónico y
el estudio adecuado de la
radiactividad alfa.

$$-\Delta u + V(x)u = \lambda u$$





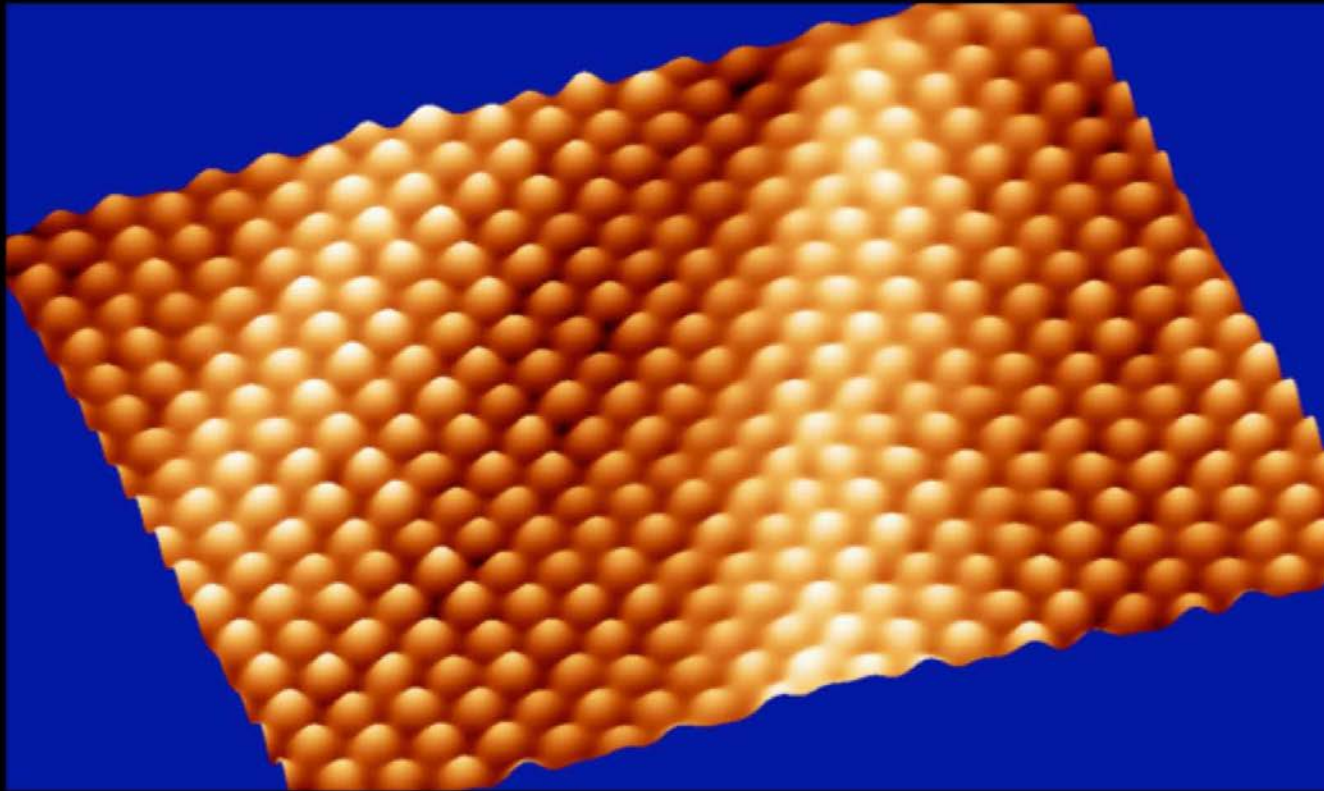


Como David y Goliat.

En la fotografía puede verse claramente la diferencia de tamaños entre un microscopio electrónico de transmisión, conocido como TEM (al fondo) y un microscopio de efecto túnel (en la mano del investigador).

Abajo, a la derecha, se presenta una fotografía del microscopio de efecto túnel, STM.

Ambos microscopios pueden llegar a ver átomos, pero resulta sorprendente cómo utilizando las ideas de la física cuántica se puede construir un microscopio tan pequeño y tan potente.

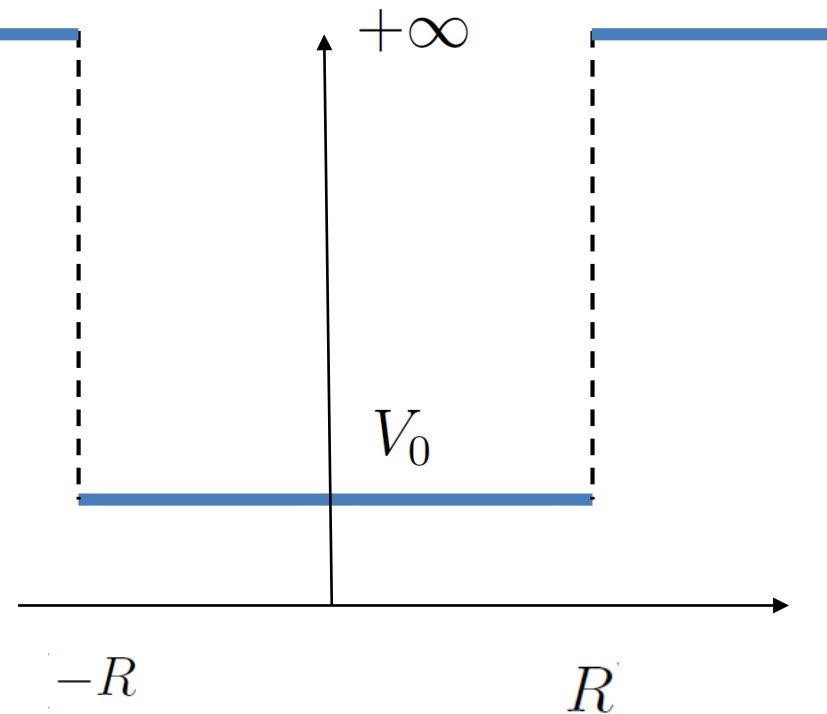


Paisajes del nanomundo. Cada una de estas “bolas” es un átomo en una superficie de oro. Esta imagen fue obtenida con un microscopio de efecto túnel (STM) operando en ultra alto vacío. Veinticinco siglos después de que Demócrito propusiese la existencia de los átomos, se han construido microscopios que nos permiten verlos, manipularlos y construir tecnología con ellos. La distancia que separa cada uno de los átomos es más de diez mil veces más pequeña que el grosor de un cabello humano.

4. The ambiguity in the infinite well potential and my results.

"the infinite well potential"

$$V_\infty(x : R, V_0) = \begin{cases} V_0 & \text{if } x \in (-R, R), \\ +\infty & \text{if } x \notin (-R, R), \end{cases}$$



Lemma Given $q > 0$ and $V_q(x : R, V_0)$ problem (1), with $N = 1$, has a nonnumerable sequence of eigenvalues $\lambda_n(q)$ and eigenfunctions $u_{q,n}(x)$ (renormalized such that $\|u_{q,n}\|_{L^2(\mathbb{R})} = 1$). Moreover, as $q \rightarrow +\infty$,

$$\lambda_n(q) \rightarrow \left(\frac{\pi}{2R}\right)^2 n^2, \quad \text{with } n \in \mathbb{N},$$

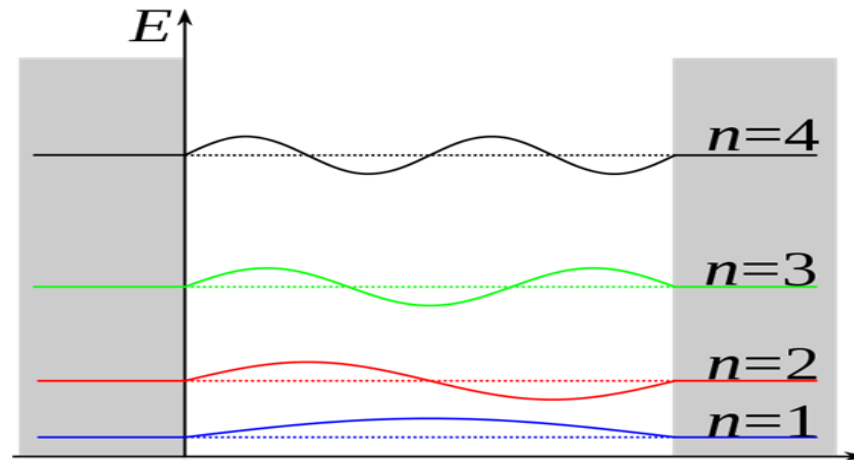
and $u_{q,n} \rightarrow u_n$ weakly in $H^1(\mathbb{R})$, with u_n given by

$$\begin{cases} u_n(x) = \begin{cases} C \sin \frac{n\pi}{2R}(x + R) & \text{if } x \in (-R, R), \\ 0 & \text{if } x \notin (-R, R), \end{cases} \\ \lambda_n - V_0 = \left(\frac{\pi}{2R}\right)^2 n^2, \quad n = 1, 2, \dots \end{cases}$$

In terms of the original value of the parameters m and \hbar and denoting again the energy by E we get the discrete set of energies

$$E_n := \frac{\hbar^2}{2m} \lambda_n$$

Finally, $(u_n)_{xx}$ generate two family of Dirac deltas (depending on $n \in \mathbb{N}$): one at $x = R$ and the other at $x = -R$.



The ambiguity in this mathematical treatment arises because the derivatives of such u_n are discontinuous at the points $x = \pm R$, and thus such u_n are not solutions of the equation in the whole domain \mathbb{R} in the sense of distributions

$$-\frac{\hbar^2}{2m} \frac{d^2 u_n}{dx^2} + V(x)u_n = E_n u_n, \quad \text{in } \mathbb{R},$$

but they satisfy a different equation

$$-\frac{\hbar^2}{2m} \frac{d^2 u_n}{dx^2} + V(x)u_n = E_n u_n + k_n(R)\delta_{\{R\}} - k_n(-R)\delta_{\{-R\}}, \quad \text{in } \mathbb{R}, \quad (1)$$

since the second derivative develops two Dirac deltas (see Lemma above). Here

$$k_n(-R) = \frac{\hbar^2}{2m} \frac{\sqrt{2}}{R^{3/2}} n\pi \quad \text{and} \quad k_n(R) = \frac{\hbar^2}{2m} \frac{\sqrt{2}}{R^{3/2}} n\pi (-1)^n.$$

The presence of such discontinuities was noticed previously in the literature (see, e.g. the book by Galindo and Pascual (1990)) but, as far as we know, it seems that a careful analysis of this ambiguity, and the study of some alternative potential $V(x)$ preventing it, was not considered before.

My purpose was to give an answer to the following *inverse free boundary problem*: can we find a potential $V(x)$ and some values of the energy λ such that the solution of $-\frac{d^2 u}{dx^2} + V(x)u = \lambda u$ in \mathbb{R} , gives rise to a free boundary given by $\partial\Omega$ in the sense that $u \equiv 0$ on $\mathbb{R} \setminus \Omega$ and $\frac{du}{dx}(\pm R) = 0$?

After submitting my paper I became aware of the survey:

M. Belloni and R.W. Robinett, The infinite well and Dirac delta function potentials as pedagogical, mathematical and physical models in quantum mechanics, *Physics Reports* 540 (2014) 25–122 [with 248 references].

[120] L. Yinji, H. Xianhuai, A particle ground state in the infinite square well, *Amer. J. Phys.* 54 (1986) 738.

[121] R. Seki, On boundary conditions for an infinite square well potential in quantum mechanics, *Amer. J. Phys.* 39 (1971) 929–931.

[122] E.F. Cummings, The particle in a box is not simple, *Amer. J. Phys.* 45 (1977) 158–159.

[123] D. Branson, Continuity conditions on the Schrödinger wave function at discontinuities of the potential, *Amer. J. Phys.* 47 (1979) 1000–1003.

[124] M. Andrews, Matching conditions on wave functions at discontinuities of the potential, *Amer. J. Phys.* 49 (1981) 281–282.

[125] D. Home, S. Sengupta, Discontinuity in the first derivative of the Schrödinger wave function, *Amer. J. Phys.* 50 (1982) 552–554.

Fortunately, my results were not anticipated by anyone !!!

Curiously, in this important survey the first work dealing with the infinite square well is not attributed to Gamow but to the book:

N.F. Mott, *An Outline of Wave Mechanics*, Cambridge University Press, 1930.

As it is said in an excellent text book

D.J. Griffiths, Introduction to Quantum Mechanics, Prentice Hall, 1995,

“This potential is awfully artificial, but I urge you to treat it with respect. Despite its simplicity – or rather, precisely because of its simplicity – it serves as a wonderfully accessible test case for all the fancy stuff that comes later”.

This problem appears simple and accessible because it has a simple classical analog (a particle in a box) and its energy eigenfunctions are analogous to the classical normal modes of a string. In fact, the infinite square well problem has become a staple of textbooks (from quantum mechanics through introductory physics) since it provides a convenient starting point for the discussion of bound-state problems.

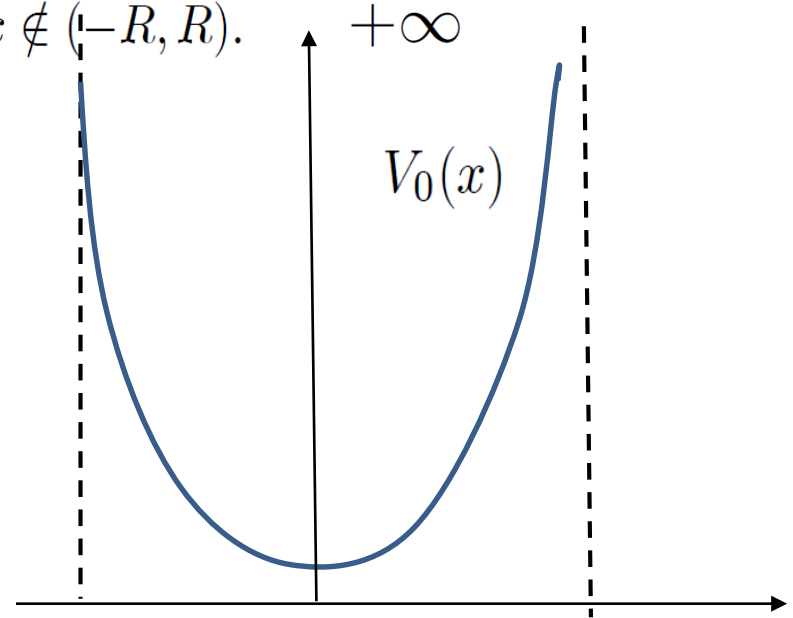
In addition, many computational methods used to solve quantum-mechanical systems (such as the shooting method) rely on putting the problem in a box to force proper Dirichlet boundary conditions: see, e.g.

H. Gould, J. Tobochnik, W. Christian, Introduction to Computer Simulation Methods, Addison Wesley, 2006.

M. Belloni, W. Christian, Time development in quantum mechanics using a reduced Hilbert space approach, Amer. J. Phys. 76 (2008) 385–392.

As a matter of fact, after the work by Gamow, several authors considered many generalizations of the *infinite well potential* corresponding to the case in which the constant value V_0 is replaced by a general function $V_0(x)$ leading to the potential

$$V_\infty(x : R, V_0(\cdot)) = \begin{cases} V_0(x) & \text{if } x \in (-R, R), \\ +\infty & \text{if } x \notin (-R, R). \end{cases}$$



The quantum bouncer, the "half quantum oscillator", etc. (see, e.g. references in the survey Belloni and Robinett (2014)). The general case $V_0 \in L^1(-R, R)$ was already considered in the 1968 monograph by M.A. Naimark. The more singular case $V_0(x) = \delta_0(x)$, the Dirac delta applied to $x = 0$, related with the so called *Quantum Dot*, was also considered in the literature (see, e.g., Joglekar (2009) and the mentioned survey).

In contrast with the case of the tunneling effect (corresponding to the treatment of the finite well potential, the usual study of the *infinite well potential*, such as it is presented in most of the textbooks, contains an ambiguity which, curiously enough, it seems unseen before: it is said in many textbooks that to solve the equation in \mathbb{R}^N outside Ω ($\Omega = (-R, R)$ before) it is necessary to impose that the solution $u(x)$ of the equation in \mathbb{R}^N let $u(x) \equiv 0$ if $x \notin \Omega$. Thus the study of the problem in \mathbb{R}^N leads to solve the associated Dirichlet problem on Ω

$$DP(V, \lambda, \Omega) \begin{cases} -\Delta u + V(x)u = \lambda u & \text{in } \Omega, \\ u = 0 & \text{on } \partial\Omega. \end{cases}$$

The main goal of my 2015 paper was to present a set of results offering some kind of alternative.

In particular, here we shall deal merely with nonnegative solutions $u \geq 0$ of $DP(V, \lambda, \Omega)$, and in fact in the one-dimensional case, $\Omega = (-R, R)$.

My purpose was to give an answer to the following *inverse free boundary problem*: can we find a potential $V(x)$ and some values of the energy λ such that the solution of $-\frac{d^2u}{dx^2} + V(x)u = \lambda u$ in \mathbb{R} , gives rise to a free boundary given by $\partial\Omega$ in the sense that $u \equiv 0$ on $\mathbb{R} \setminus \Omega$ and $\frac{du}{dx}(\pm R) = 0$?

The case of higher dimensions is the object of a separated work by this author.

It is useful to introduce the following notation (already used in the literature):

We say that a function $u \in H_0^1(\Omega)$ is a (positive) “*flat solution*” of problem $DP(V, \lambda, \Omega)$ if u satisfies $DP(V, \lambda, \Omega)$, $u > 0$ and $\frac{du}{dx}(\pm R) = 0$.

Theorem 1 *Let $\Omega = (-R, R)$ and let $V \in L_{loc}^1(\Omega)$ be such that*

$$\frac{\underline{C}}{d(x, \partial\Omega)^\alpha} \leq V(x) \leq \frac{\overline{C}}{d(x, \partial\Omega)^\alpha} \quad \text{a.e. } x \in \Omega = (-R, R), \quad (2)$$

for some $\alpha \in [0, 2]$ and some $\overline{C} > \underline{C} > 0$. Then:

1. If $\alpha \in [0, 2)$ then no positive solution of $DP(V, \lambda, \Omega)$ may be a flat solution for any $\lambda \geq 0$.
2. If $\alpha = 2$, for any value of \overline{C} and \underline{C} , there exists $\lambda^\# = \lambda^\#(R) \geq \left(\frac{\pi}{2R}\right)^2$ such that problem $DP(V, \lambda^\#, \Omega)$ has a nonnegative solution $u^\#$.

3. If $\alpha = 2$, there exists two positive constants $C_* < C^*$ such that if

$$C_* \leq \underline{C} \leq \overline{C} < C^* \quad (3)$$

then problem $DP(V, \lambda^\#, \Omega)$ has a positive flat solution $u^\#$. Moreover there exists $m \in [0, 1)$ such that $u \in \mathcal{C}^{2/(1-\overline{m})}(\overline{\Omega})$ and

$$\underline{K}d(x, \partial\Omega)^{2/(1-m)} \leq u^\#(x) \leq \overline{K}d(x, \partial\Omega)^{2/(1-m)} \quad \text{for any } x \in \overline{\Omega}, \quad (4)$$

for some constants $\overline{K} > \underline{K} > 0$.

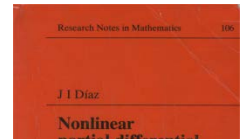
We recall that if $\Omega = (-R, R)$ then $\lambda_1 = \left(\frac{\pi}{2R}\right)^2$ is the first eigenvalue of the linear problem

$$\begin{cases} -u_{xx} = \lambda u & \text{in } \Omega \\ u = 0 & \text{on } \partial\Omega. \end{cases}$$

Corollary 2 Let $\Omega = (-R, R)$ and $V_\infty(x : R, V_0(\cdot))$ with $V_0(\cdot)$ satisfying (2) and (3) with $\alpha = 2$. Then there exists $\lambda^\# > 0$ such that the Schrödinger equation admits a solution $u \in \mathcal{C}^{2/(1-\overline{m})}(\mathbb{R})$ satisfying (4), for suitable $m \in (0, 1)$, $\overline{K} > \underline{K} > 0$, and such that $u \equiv 0$ on $\mathbb{R} \setminus \Omega$.

As far as we know, the above theorem is the first result in the literature showing the existence of a flat solution **for a linear elliptic problem**. We recall that the first result in the literature on solutions with compact support for elliptic problems was raised in the works Brezis and Stampacchia (1973) related

to an obstacle problem formulated for the study of subsonic flows. Later the existence of solutions with compact support was extended to other semilinear (sublinear) problems in Brezis (1974) and Benilan, Brezis and Crandall (1975). Many other results for nonlinear problems can be found, for instance, in my book Díaz (1985). Of course the existence of the flat solution is only possible when the strong maximum principle cannot be applied (see e.g. Protter-Weimberger (1984), Vázquez (1984) and the book by Pucci and Serrin (2007).



When $C = \underline{C}$ potentials $V(x)$ satisfying (2), with $\alpha = 2$, are called "Hardy type potentials" on the distance to the boundary variable. There is a long literature dealing with problems involving such potentials. We emphasize that here we are considering the so called "absorption case" and that, in contrast with other authors considering the formation of a free boundary (see, *e.g.*, Bandle-Pozio (2015), **the main problem under consideration in this paper is linear.**

□

After the above comments on the literature on solutions with compact support for nonlinear problems perhaps it is not too strange to say that we use here some auxiliary nonlinear problem giving rise to flat solutions in order to prove the theorem. To be more precise, we shall start considering the nonlinear eigenvalue type problem

$$P(R, m, V_0, \lambda) \equiv \begin{cases} -\frac{d^2v}{dx^2} + V_0v^m = \lambda v, & v \geq 0 \text{ in } (-R, R), \\ v(\pm R) = 0, \end{cases}$$

for a given $V_0 > 0$ and $m \in (0, 1)$. We shall prove:

Proposition 3 *For any $\lambda \geq \left(\frac{\pi}{2R}\right)^2$ there exists a unique nonnegative solution v_m of $P(R, m, V_0, \lambda)$. Moreover, there exists a $\lambda^*(m) > \left(\frac{\pi}{2R}\right)^2$ such that: a) If $\lambda \geq \lambda^*(m)$ then*

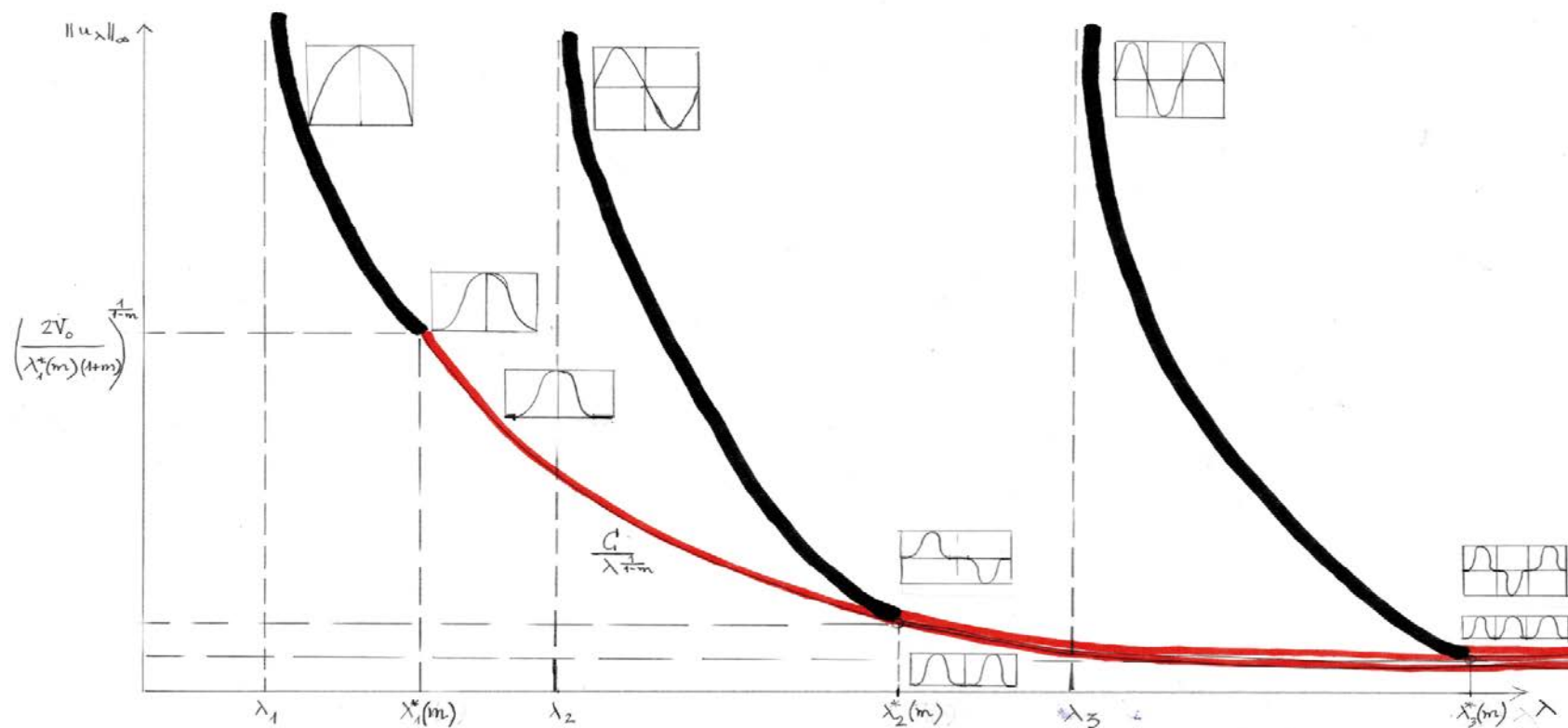
$$v_m(x) \leq \overline{K}d(x, \partial\Omega)^{2/(1-m)} \quad \text{for any } x \in \overline{\Omega} = [-R, R], \quad (5)$$

for some constant \overline{K} . In particular $\frac{dv_m}{dx}(\pm R) = 0$. b) If $\lambda \leq \lambda^(m)$ then*

$$\underline{K}d(x, \partial\Omega)^{2/(1-m)} \leq v_m(x) \quad \text{for any } x \in \overline{\Omega} = [-R, R], \quad (6)$$

for some constant \underline{K} . In particular $v_m > 0$ in Ω . c) If $\lambda = \lambda^(m)$ inequalities (5) and (6) hold for some $\overline{K} > \underline{K} > 0$.*

Concerning the case of nodal solutions of the semilinear problem $P(R, m, V_0, \lambda)$ constructed in Díaz- Hernández (2015) we have:



Corollary 4 *Estimates (5) and (6) also apply to the nodal solutions of the semilinear problem $P(R, m, V_0, \lambda)$ corresponding to suitable values $\lambda_n^*(m)$ of the parameter λ in branches bifurcating at the infinity from the simple eigenvalues λ_n for any $n \in \mathbb{N}$.*

As a particular consequence of the above Corollaries and it is possible to offer a correct alternative to the "localizing" process suggested by Gamow in his 1928 paper.

Corollary 5 *For any $R > 0$, $n \in \mathbb{N}$ and $m \in (0, 1)$ there exists a countable set of values of the parameter $\lambda = \lambda_n^*(m)$ (in branches bifurcating at the infinity from the simple eigenvalues λ_n , of the linear Schroedinger equation, and there exists a countable set of infinite well type potentials $V_{n,m}(x) = V_\infty(x : R, V_{0,n,m}(\cdot))$ such that the associated Schrödinger equation*

$$-\Delta u + V_{n,m}(x)u = \lambda_n^*(m)u \quad \text{in } \mathbb{R},$$

admits a solution $u_{n,m} \in C^{\frac{2}{1-m}}(\mathbb{R})$, changing sign n -times, such that $u_{n,m}(x) = 0$ for any $x \notin (-R, R)$ (and in particular $u'_{n,m}(\pm R) = 0$). Moreover $V_\infty(x : R, V_{0,n,m}(x))u_{n,m}(x) = 0$ for any $x \notin (-R, R)$ (i.e. no Dirac delta is generated on the boundaries $x = \pm R$).

2d. Proofs and additional remarks

As mentioned, the key point in the proof of the main Theorem is the set of estimates stated in the auxiliary Proposition for the **semilinear** problem $P(R, m, V_0, \lambda)$.

The existence of a branch of positive solutions for the semilinear problem for $\lambda \in (\lambda_1, \lambda^*(m))$ was proven in Díaz-Hernández (2015).

The critical eigenvalue $\lambda^*(m)$ of the main theorem depends crucially on the main assumption $m \in (0, 1)$:

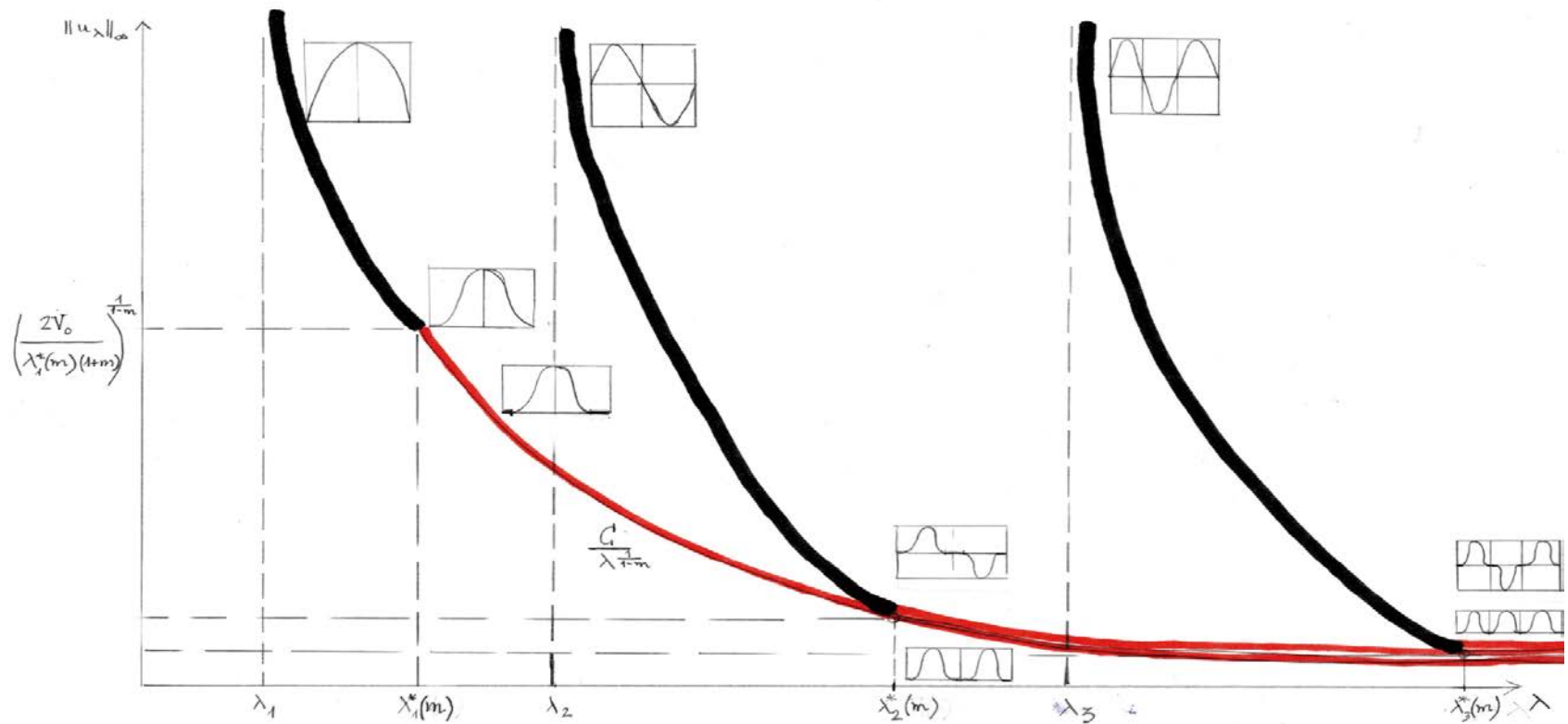
$$\lambda^*(m) = \frac{1}{2R^2} \left(\int_0^{(2/(1+m))^{1/(1-m)}} \frac{dr}{(F(\mu) - F(r))^{1/2}} \right)^2 \quad (10)$$

with

$$F(r) = \frac{r^2}{2} - \frac{r^{m+1}}{m+1}, \quad \mu = \|u\|_\infty \quad (11)$$

It is shown in Díaz-Hernández (2015) that the (unique) positive solution for $\lambda = \lambda^*(m)$ has a peculiar behaviour near the boundary: it is a "flat positive solution" in the sense that $u > 0$ in Ω and

$$\frac{\partial u}{\partial n}(x) = 0 \text{ on } \partial\Omega.$$



The associated solution $u_{\lambda^*(m), V_0}$ (when extended by zero to the whole real line \mathbb{R}) gives rise to a continuum of nonnegative solutions u_{λ, V_0} for any $\lambda > \lambda^*(m)$ through a double rescaling (in amplitude and in the argument of application). This type of solutions have compact support in the sense that

$$\text{support}(u_{\lambda, V_0}) \subsetneq \Omega.$$

The main novelties of the Proposition are the estimates (5) and (6). In order to prove them we need to reconstruct some of the arguments of the proof of Theorem 1 of Díaz-Hernández (2015). We make the change of variables

$$v_{\lambda, V_0}(x) = \left(\frac{V_0}{\lambda} \right)^{\frac{1}{1-m}} v(\sqrt{\lambda}x) \quad (12)$$

where v is now the solution of the renormalized problem

$$P(L) \begin{cases} -v'' = f(v) & \text{in } (-L, L), \\ v(\pm L) = 0, \end{cases} \quad (13)$$

with $f(v) = v - v^m$ and $L = \sqrt{\lambda}R$. We introduce

$$F(r) = \int_0^r f(s)ds = \frac{r^2}{2} - \frac{r^{m+1}}{m+1}$$

and note that $f(s) < 0$ if $0 < s < 1 := r_f$ and $f(s) > 0$ if $1 < s$. On the other hand $F(s) < 0$ if $0 < s < r_F = (2/(1+m))^{1/(1-m)}$ and $F(s) > 0$ for $s > r_F$.

Proof of the Proposition. For $\mu \in [r_F, +\infty)$ we define

$$\gamma(\mu) := \frac{1}{\sqrt{2}} \int_0^\mu \frac{dr}{(F(\mu) - F(r))^{1/2}}. \quad (14)$$

It is shown in Díaz-Hernández (2015) that the mapping $\gamma : [r_F, +\infty) \rightarrow \mathbb{R}$ has the following properties: (i) $\gamma \in C[r_F, \infty) \cap C^1(r_F, \infty)$; (ii) $\gamma'(\mu) \rightarrow -\infty$ as $\mu \downarrow r_F$; (iii) For any $\mu > r_F$ $\gamma'(\mu) < 0$, (iv) $\lim_{\mu \rightarrow +\infty} \gamma(\mu) = \frac{\pi}{2}$. Moreover, it was also shown there that if we call

$$\lambda^*(m) = \frac{1}{2R^2} \left(\int_0^{r_F} \frac{dr}{(-F(r))^{1/2}} \right)^2 \quad (15)$$

For $\mu > r_F$ we define the mapping $\gamma : [r_F, +\infty) \rightarrow \mathbb{R}$ given by (14). Now we use the following fact: a function v is a positive solution of problem $P(L)$ if and only if

$$\frac{1}{\sqrt{2}} \int_{v(x)}^{\mu} \frac{dr}{(F(\mu) - F(r))^{1/2}} = |x|, \text{ for } |x| \leq L,$$

where $\mu := \|v\|_{L^\infty}$ (such that $\mu \in (r_F, \infty)$) and $L > 0$ are related by the equation $\gamma(\mu) = L$. In particular, if $\mu > r_F$ we get that

$$v'(\pm L) = \mp A^{-1}(F(\mu)) \text{ where } A(r) := \frac{r^2}{2}. \quad (17)$$

which proves part ii) of the Proposition for the case of $\lambda < \lambda^*(m)$ since we know that it corresponds to the case in which the transformed function v by the change of variables has a maximum μ such that $\mu > r_F$. In the case of $\lambda = \lambda^*(m)$ the associated function v is such that $\mu = r_F$ and in consequence $v'(\pm L) = 0$. Moreover, since

$$\frac{1}{1+m} r^{1+m} \geq \frac{1}{1+m} r^{1+m} - \frac{1}{2} r^2 \geq \frac{(1-m)}{2(1+m)} r^{1+m} \quad \text{for } r \in (0, 1),$$

we get that there exist two positive constants $\underline{M} < \overline{M}$ such that

$$\underline{M} \tau^{\frac{1-m}{2}} \leq \frac{1}{\sqrt{2}} \int_0^\tau \frac{dr}{\sqrt{-F(r)}} \leq \overline{M} \tau^{\frac{1-m}{2}} \quad (10)$$

for any $\tau \in (0, 1)$ which leads to conclusion iii) of the Proposition and obviously also ii) for $\lambda = \lambda^*(m)$). Finally, since we know that for $\lambda > \lambda^*(m)$ the nonnegative solutions are generated extending by zero the function $v_{\lambda^*(m), V_0}$ outside $(-R, R)$ we get part i) of the Proposition thanks to the estimate (10).

Now we are in conditions to prove the main result of this paper:

Proof of the Theorem. Part 1 holds since if $\alpha < 2$ then $\frac{dv}{dx}(-R) > 0$ and $\frac{dv}{dx}(R) < 0$. The proof is an easy adaptation of the Hopf strong maximum principle: see, *e.g.* Protter-Weimberger (1984) or Bertsch- Rostamian (1985). In order to prove Part 2, for any $h \in L^2(\Omega)$ ($\Omega = (-R, R)$) we define the operator $Th = z \in H_0^1(\Omega)$ solution of the linear problem

$$\begin{cases} -\Delta z + V(x)z = h & \text{in } \Omega, \\ z = 0 & \text{on } \partial\Omega. \end{cases} \quad (11)$$

This operator is well defined since problem (11) has a unique (weak) solution $z \in H_0^1(\Omega)$. This follows from applying the Lax-Milgram Lemma to the associated bilinear form in $H_0^1(\Omega)$

$$a(u, v) = \int_{\Omega} \nabla u \cdot \nabla v dx + \int_{\Omega} V(x)uv dx$$

which is well-defined, continuous and coercive. Indeed, taking into account that

$$V(x) \leq \frac{\overline{C}}{d(x, \partial\Omega)^\alpha} \quad \text{a.e. } x \in \Omega,$$

(thanks to assumption (2)) Hardy's inequality implies that

$$\frac{1}{\overline{C}} \int_{\Omega} V(x) u^2 dx \leq \int_{\Omega} \frac{u^2}{d(x)^2} dx \leq k \int_{\Omega} |\nabla u|^2 dx$$

for some suitable constant $k = k(\Omega)$ and then

$$a(u, u) \leq C \|u\|_{H_0^1(\Omega)}^2$$

for some $C > 0$, which implies that a is continuous (the coerciveness of a is a routine matter). Thus, for any $h \in L^2(\Omega)$, there exists a unique $Th \in H_0^1(\Omega)$ solution of the above equation and it is easy to see that the composition with the (compact) embedding $H_0^1(\Omega) \subset L^2(\Omega)$ is a selfadjoint compact linear operator $\tilde{T} = i \circ T : L^2(\Omega) \rightarrow L^2(\Omega)$ for which we obtain in the usual way a sequence of eigenvalues $\nu_n \rightarrow +\infty$. If we call $\lambda^\# = \nu_1$ then, by well-known results we know that $\lambda^\# > 0$. In fact, since $V(x) \geq 0$, we know that $\lambda^\# > \lambda_1(R) = \left(\frac{\pi}{2R}\right)^2$.

The proof of Part 3 (i.e. the associated eigenfunctions have zero normal derivatives on the boundary) will result of the application of the iterative method of super and subsolutions (since the comparison principle does not apply directly to solutions of the problem (DP)). We start by proving that if $\lambda^\#$ is the eigenvalue mentioned in Part 2 then we can chose $m^\# \in [0, 1)$ such that

$$\lambda^\# = \lambda^*(m^\#) \quad (12)$$

with $\lambda^*(m)$ the critical eigenvalue of the nonlinear problem $P(R, m, V_0, \lambda)$ given in Proposition 1.5. Indeed, for any $m \in [0, 1)$ we have

$$\lambda^*(m) = \frac{\varphi(m)}{2R^2}$$

where $\varphi(m) := \int_0^{\mu(m)} \frac{dr}{\sqrt{\frac{r^{m+1}}{m+1} - \frac{r^2}{2}}}$, with $\mu(m) := \left(\frac{2}{1+m}\right)^{\frac{1}{(1-m)}}$. Obviously function $\varphi(m)$ is continuous, $\varphi(m) > 0$ for any $m \in [0, 1)$ and

$$\lim_{m \nearrow 1} \varphi(m) = +\infty.$$

Moreover, it is not difficult to check that

$$\int_a^b \frac{dr}{\sqrt{r - \frac{r^2}{2}}} = \sqrt{2}(\arcsin(1 - a) - \arcsin(1 - b)),$$

and thus

$$\varphi(0) = \int_0^2 \frac{dr}{\sqrt{r - \frac{r^2}{2}}} = \sqrt{2}\pi.$$

Then property (12) holds since we know that

$$\lambda^\# \geq \left(\frac{\pi}{2R}\right)^2 > \frac{\sqrt{2}\pi}{2R^2} = \lambda^*(0).$$

On the other hand the comparison principle holds, for solutions of the problem

$$DP(V, f) \begin{cases} -\frac{d^2u}{dx^2} + V(x)u = f(x) & \text{in } \Omega, \\ u = 0 & \text{on } \partial\Omega, \end{cases}$$

in the sense that, since $\frac{C}{d(x, \partial\Omega)^2} \leq V(x)$, if $\underline{f}, \bar{f} \in H^{-1}(\Omega)$ and $\underline{f} \leq \bar{f}$ in $H^{-1}(\Omega)$ then there exist $\underline{u}, \bar{u} \in H_0^1(\Omega)$ solutions of $DP(V, \underline{f})$ and $DP(V, \bar{f})$, respectively, such that $\underline{u}(x) \leq \bar{u}(x)$ a.e. $x \in \Omega$. The proof of this follows by applying again the Hardy inequality. Then we can apply the iterative method of super and subsolutions: we start by building the supersolution of $DP(V, \lambda^\#, \Omega)$ of the form $\bar{u}(x) = v_{\lambda^*(m^\#)}(x : \bar{V}_0)$ with $v_{\lambda^*(m^\#)}(x : \bar{V}_0)$ the flat solution of $P(R, m^\#, \bar{V}_0, \lambda^*(m^\#))$. Thanks to estimates (5) and (6) and assumption (2) for any $x \in \bar{\Omega}$ we have

$$\frac{\bar{V}_0}{|v_{\lambda^*(m^\#)}(x)|^{1-m^\#}} \leq \frac{\bar{V}_0}{(\underline{K}^\#)^{1-m^\#}} \frac{1}{d(x, \partial\Omega)^2} \leq V(x)$$

if the condition

$$\frac{\bar{V}_0}{(\underline{K}^\#)^{1-m^\#}} \leq \underline{C}, \quad (13)$$

holds. As a matter of fact, from the Proof of Proposition 1.5 we can see that (13) is equivalent to

$$\frac{1}{\underline{K}^{1-m^\#}} \leq \underline{C} \quad (14)$$

where \underline{K} is the bound associated to the "direct case" $\bar{V}_0 = 1$ and $\lambda = 1$. Then, if we assume (14)

$$\begin{aligned} \lambda^*(m^\#) v_{\lambda^*(m^\#)} &= -\frac{d^2 v_{\lambda^*(m^\#)}}{dx^2} + \bar{V}_0 v_{\lambda^*(m^\#)}^{m^\#} = -\frac{d^2 v}{dx^2} + \frac{\bar{V}_0}{|v_{\lambda^*(m^\#)}(x)|^{1-m^\#}} v_{\lambda^*(m^\#)} \\ &\leq -\frac{d^2 v_{\lambda^*(m^\#)}}{dx^2} + \frac{\bar{V}_0}{(\underline{K}^\#)^{1-m^\#}} \frac{v_{\lambda^*(m^\#)}}{d(x, \partial\Omega)^2} \leq -\frac{d^2 v_{\lambda^*(m^\#)}}{dx^2} + V(x) v_{\lambda^*(m^\#)}, \end{aligned}$$

which proves that $v_{\lambda^*(m^\#)}(x : \bar{V}_0)$ is a supersolution (notice that for the moment \bar{V}_0 is arbitrary).

The construction of a subsolution is more delicate. In fact we shall built a continuum of subsolutions. Given $\widehat{V}_0 > 0$ (to be chosen later) we shall take a suitable $\lambda > \lambda^*(m^\#)$ and $\underline{u}(x) = v_\lambda(x : \widehat{V}_0)$ solution of $P(R, m^\#, \widehat{V}_0, \lambda)$. By properties d) mentioned in the proof of the Proposition, if $\lambda = \lambda^*(m^\# : \widehat{V}_0)\omega$ with $\omega > 1$ we have a family $S_1(\lambda)$ of compact support nonnegative solutions with connected support defined by

$$v_{\lambda, \widehat{V}_0}(x) = \frac{1}{\omega^{\frac{1}{1-m^\#}}} v_{\lambda^*(m^\#), \widehat{V}_0}(\sqrt{\omega}x - z) \quad (15)$$

where the shifting argument z is arbitrary among the points $z \in (-R, R)$ such that support $v_{\lambda, \widehat{V}_0}(\cdot) \subset (-R, R)$. Then, arguing as in the case of the supersolution, we have

$$-\frac{d^2 \underline{u}}{dx^2} + V(x)\underline{u} \leq -\frac{d^2 \underline{u}}{dx^2} + \widehat{V}_0 \underline{u}^{m^\#} - (\lambda - \lambda^*(m^\#))\underline{u} = \lambda^*(m^\#)\underline{u}$$

assumed

$$\overline{C} \leq \frac{\omega}{(\overline{K}^\#)^{1-m^\#}} - (\lambda - \lambda^*(m^\#))R^2, \quad (16)$$

since we have

$$\left(\frac{\omega}{(\overline{K}^\#)^{1-m^\#}} - \lambda^*(m^\#)(\omega - 1)R^2 \right) \frac{1}{d(x, \partial\Omega)^2} \leq \widehat{V}_0 \underline{u}^{m^\#-1} - (\lambda - \lambda^*(m^\#)),$$

with \overline{K} is the upper bound associated to the "direct case" $\widehat{V}_0 = 1$ and $\lambda = 1$. If we define $\varepsilon := \lambda - \lambda^*(m^\#)$ then

$$\omega = \frac{\lambda}{\lambda^*(m^\#)} = \frac{\lambda^*(m^\#) + \varepsilon}{\lambda^*(m^\#)}$$

and condition (16) can be written as

$$\overline{C} \leq \frac{\frac{\lambda^*(m^\#) + \varepsilon}{\lambda^*(m^\#)} - \varepsilon R^2 (\overline{K})^{1-m^\#}}{(\overline{K})^{1-m^\#}} = \frac{1 + \varepsilon \left(\frac{1}{\lambda^*(m^\#)} - R^2 (\overline{K})^{1-m^\#} \right)}{(\overline{K})^{1-m^\#}}.$$

and this implies that \underline{u} is a subsolution.

Finally, to apply the super and subsolution method we must check

$$\underline{u}(x) \leq \overline{u}(x) \text{ for any } x \in \Omega. \quad (17)$$

From the definitions of $\underline{u}(x)$ and $\overline{u}(x)$ we have that (17) holds if

$$\frac{\widehat{V}_0}{\lambda} \leq \frac{\overline{V}_0}{\lambda^*(m^\#)}, \quad (18)$$

or equivalently

$$\frac{\lambda^*(m^\#) + \varepsilon}{\lambda^*(m^\#)} \geq \frac{\widehat{V}_0}{\overline{V}_0}. \quad (19)$$

Thus we can proceed as follows; we assume

$$\overline{C} < \frac{1}{(\overline{K})^{1-m^\#}}. \quad (20)$$

Then, if $\frac{1}{\lambda^*(m^\#)} - R^2(\overline{K})^{1-m^\#} \geq 0$ then we can take $\varepsilon > 0$ arbitrary and then \overline{V}_0 and \widehat{V}_0 such that (19) holds. If by the contrary $\frac{1}{\lambda^*(m^\#)} - R^2(\overline{K})^{1-m^\#} < 0$ then we take

$$\varepsilon < \frac{1 - \overline{C}(\overline{K})^{1-m^\#}}{(R^2(\overline{K})^{1-m^\#} - \frac{1}{\lambda^*(m^\#)})}$$

and again \overline{V}_0 and \widehat{V}_0 such that (19) holds.

Then, by the super and subsolution method, we get the existence of a minimal $\underline{u}^*(x)$ and maximal $\overline{u}^*(x)$ solution of (DP) such that

$$\underline{u}(x) \leq \underline{u}^*(x) \leq \overline{u}^*(x) \leq \overline{u}(x) \text{ for any } x \in \Omega.$$

Since there is a continuum of subsolutions we can shift them in order to get that $\overline{u}^*(x) > 0$ for any $x \in \Omega$. Moreover from the spectral theory necessarily $\underline{\Lambda} \underline{u}^*(x) = u^\# = \overline{\Lambda} \overline{u}^*(x)$ for some $\underline{\Lambda}, \overline{\Lambda} > 0$ and the estimates (4) hold for the solutions of the linear problem holds thanks to the Proposition. \square

Proof of Corollary 4. As it is shown in Díaz-Hernández (2015), the nodal solutions $v_{\lambda_n^*(m)}$ of the semilinear problem $P(R, m, V_0, \lambda)$ corresponding to suitable values $\lambda_n^*(m)$ of the parameter λ bifurcating at the infinity from the simple eigenvalues λ_n , $n \in \mathbb{N}$, are obtained by rescaling, gluing and translating the unique positive flat solution corresponding to $\lambda^*(m)$. Thus the conclusion is an obvious consequence of the Proposition. \square

Remark. It is possible to get many variants of the above mentioned results. For instance the spatial interval $\Omega = (-R, R)$ can be replaced by any other bounded interval not necessarily symmetric or even by an unbounded interval of the form $\Omega = (0, +\infty)$. In this last case the assumptions on the potential $V(x)$ are

$$\frac{C}{x^2} \leq V(x) \leq \frac{\overline{C}}{x^2} \text{ for any } x \in (0, x_0) \text{ for some } x_0 > 0, \quad (21)$$

and

$$\underline{C} \leq \liminf_{x \rightarrow +\infty} V(x)x^2 \leq \limsup_{x \rightarrow +\infty} V(x)x^2 \leq \overline{C}. \quad (22)$$

Notice that under the above condition the spectrum is still countable (see, e.g. Galindo-Pascual (1990)). The study of flat solutions at $x = 0$ under condition (21) when assumption (22) fails (as for instance for the "effective potential" associated to the Yukawa potential: also called "screened Coulomb potential")

$$W(r) = \frac{L_0}{\mu r^2} + \frac{k}{r} e^{-\frac{r}{a}}$$

with L_0 the angular momentum, μ the reduced mass and $k \in \mathbb{R}, a > 0$ some parameters, can be considered by means of the local techniques.

Notice that, again,

$$V_0 v^m \geq \frac{V_0 K^{(m-1)}}{d(x, \partial\Omega)^2} v$$

(and analogously for the reverse estimate).

Remark 6. The estimate $v(x) \leq Kd(x, \partial\Omega)^{-2/(m-1)}$ a.e. $x \in \Omega$ was also proved for the large solution of the higher order semilinear equations

$$LSSP(m, V_0) \begin{cases} (-\Delta)^\alpha v + V_0 v^m = f_0 & \text{in } \Omega, \\ v = +\infty & \text{on } \partial\Omega, \end{cases}$$

for a given $\alpha \in \mathbb{N}$, when Ω is a ball and $f_0 \geq 0$:

J. I. Díaz, M. Lazzo, P.G. Schmidt, Asymptotic Behavior of Large Radial Solutions of a Polyharmonic Equation with Superlinear Growth. Journal Differential Equations (August 2014).

The extension to the associate **linear** problem is in progress.

Remark 7. Many new results concerning this type of potentials can be obtained: existence of large solutions ($u(x) \uparrow +\infty$ on $\partial\Omega$), localization properties for the original evolution equation

$$\begin{cases} i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \Delta \psi + V(x)\psi & \text{in } (0, \infty) \times \mathbb{R}, \\ \psi(0, x) = \psi_0(x) & \text{on } \mathbb{R}, \end{cases} ,$$

$\text{supp}\psi_0 \subset \bar{\Omega}$ implies that $\text{supp}\psi(t, \cdot) \subset \bar{\Omega}$ for any $t > 0$; *symmetric rearrangement* comparison results, etc.

**Thanks for
your attention**