# On physical analysis of numerical methods in the 1D Coulomb problem

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Diverse numerical studies of the 1D Coulomb problem have suggested the existence of an infinite binding-energy ground-state and definite parity eigenstates in this system. We exhibit that such conclusions about the 1D Coulomb problem are wrong. The origin of the mistakes are to be found not in the numerical techniques employed but in the careless extrapolation of their results. Any numerical technique used for solving the 1D Coulomb problem must be supplemented by a detailed analysis of the effect of the impenetrable barrier produced by the $-|x|^{-1}$ singularity in order to obtain valid conclusions.

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## I. INTRODUCTION.

The 1D Coulomb problem, also known as the 1D hydrogen atom, described by the Schödinger equation (in atomic units $\hbar = m = e = 1$)

$$H_C\psi(x) = -\frac{1}{2}\frac{d^2\psi(x)}{dx^2} - \frac{Z}{|x|}\psi(x) = E\psi(x), \quad Z \quad \text{the atomic number,} \tag{1}$$

where $H_C$ is the Coulomb Hamiltonian operator with potential energy $V_C = -Z/|x|$, $\psi(x)$ stands for the system's eigenfuctions, and $E$ for its energy eigenvalues, has produced an extensive literature which includes its uses in many fields of physics [1–39, 41, 42]. We should mention that some of the previous theoretical studies of the system (e.g. [5, 20, 30, 36, 44]) made erroneus claims that have been disproved based on rigorous physical and mathematical analyses [7, 14, 32, 42, 43, 45, 46]. Let us first remark that the Hamiltonian $H_C$ is not self-adjoint an important fact which we discuss later on [7, 23]. As examples of its uses, the Hamiltonian (1) has been used for calculating the optical absorption spectra for direct interband transitions in a 1D electron-hole system within the effective-mass approximation were special care was taken to avoid the assumed —but inexistent, as we show here— divergence in the spectrum of the 1D hydrogen atom [17]. Moreover, very recently it was employed as a model in the effective-mass approximation, to study electron states in a nanotube placed in the electric field of a charged ring, such field may create a potential-well describable by a 1D Coulomb-like potential [38]. A related phenomena, also approximately described by $H_C$ (1), has been observed in the spontaneous formation of quasi one-dimensional hydrogen gas hydrates within single-wall nanotubes [39], [40].

Several numerical approaches have tried to provide insight on the physical proterties of the 1D Coulomb problem. In order to deal with the singularity of the potential in (1) different approximations have been used to make the problem numerically solvable. Such approximations go from introducing a parameter to ameliorate the singularity, for example, the following two,

$$V_\alpha^1 = -\frac{Z}{|x| + \alpha}, \quad \alpha > 0, \quad \text{and} \quad V_\alpha^2 = -\frac{Z}{\sqrt{x^2 + \alpha^2}}, \quad \alpha \neq 0; \tag{2}$$

at the end they need $\alpha$ to vanish in order to recover the singular Hamiltonian (1) and be able to obtain conclusions, but these cannot be obtained from any numerical calculation. We can just obtain hints on some features on the systems behavior that should be checked in non-numerical

 

fashion. Another used approach is simulating the interaction of the regularized 1D hydrogen atom with an harmonic electromagnetic field —*e.g.* a laser pulse— to observe features of the numerical solutions which may help understand the behavior of the singular system (1) [34–37].

A common conclusion of such studies is the degeneracy of the energy eigenvalues of the 1D hydrogen atom and, in some cases, the existence of an infinite binding-energy non-degenerate ground-state, described by a Dirac-$\delta$ wave function — though this kind of state is sometimes regarded as an improper or unphysical solution [36, 37]. Such conclusions may occur because those analyses were not really based on solid physical or mathematical grounds but only on numerical interpretations. Some of the previous results may have suggested that the wave function should vanish at the origin—this would make $H_C$ self-adjoint. This is known as the Dirichlet condition, which is **not** the only boundary condition making $H_C$ self-adjoint [23, 41], the use of this condition does indeed provoke the breakdown of parity in the system [32, 42].

Such considerations exhibit that generalizing from purely numerical results to general properties of singular quantum systems is prone to fail if the appropiate considerations (such as a careful assesment of the conditions needed in order to invoke adequate convergence results for the sequences of operators used in the studies) are not taken into account [33, 47]. Any numerical procedure needs to be supplemented by detailed physical and mathematical analyses of the singular problem for the conclusions drawn from them to be meaningful. The paper is organized as follows: In section II we show that the ground state of infinite binding energy for the 1D Coulomb problem does not exist. In section III we show that no eigenstates can be defined in the whole real line, such feature can be understood as the manifestation of a superselection rule acting in the problem [10, 13, 32, 42]. In section IV we discuss the conclusions obtained from the numerical results of [34–37]. In section V we sum up our conclusions. Appendix A explains the notion of *spectral pollution*, a concept that is used in section II.

## II. NON-EXISTENCE OF THE INFINITE ENERGY GROUND STATE.

Back in 1980, Gesztezy established that the energy of the ground state of the 1D Coulomb problem is $E_{gs} = -1/2$ [7], a result that has been corroborated in more recent analyses [11, 32, 46]. Some numerical analyses used an approximation to the singular 1D Coulomb potential $V_C$ by means of regularized potentials, $V_\alpha^i$ in (2), parametrized by the real number $\alpha$, or use cut-off approximations to investigate the $E_0$ energy eigentstate of (1). Their results apparently corroborate that such eigenvalue is indeed unbounded by below when $\alpha \to 0$ [3, 34, 36, 37]. But, as we said

 

before, we can ascertain that there is not an infinite binding-energy eigenstate in this system. Thus, some of the numerical approaches seems to be flawed, and this is so because it is known that numerical evidence gathered from regularizing perturbations of a singular Hamiltonian are inconclusive when used to investigate the nature of its spectrum.

The heart of the problem lies in a mathematical intricacy: the spectra of a series of operators $H_n$ that converge to a singular operator $H$ are not related in any natural way to the spectrum of $H$, unless very restrictive conditions are satisfied [47]. As an example of such an anomaly we can mention the phenomenon known as spectral pollution, in which a sequence of eigenvalues of $H_n$ converges to a value that *is not* in the spectrum of $H$ [48]. Related to this issue is the fact that there exist several different notions of convergence of operators, but only the strongest types of convergence ensure that spectral pollution will not occur [49]. As an example that illustrates the implications related to different types of convergence, we discuss in some detail the work of Gesztezy [7]. In order to calculate the spectrum of the singular 1D Columb Hamiltonian (1), Gesztezy used the Friedrichs extension [55] $H_D$ of the kinetic operator $p^2/2$ in (1) to construct the family of operators

$$S_\alpha = H_D + V_\alpha^i, \tag{3}$$

and showed that $H_C$ is the limit, in the sense of strong norm convergence, [56] of the family $S_\alpha$ as $\alpha \to 0$. Gestezy further showed that $S_\alpha \geq -1/2$ for all $\alpha > 0$ considering $V_\alpha^1$ (1) and, as a consequence, the spectrum of $H_C$ is bounded from below by $-1/2$ regardless of the approach to $V_C$ ($V_\alpha^2$ with $\alpha \neq 0$, the cut-off approximation, or others). As an immediate consequence the inexistence of a ground state with unbounded negative energy is established. Let us note that the sequence of operators

$$T_\alpha = -\frac{p^2}{2} + V_\alpha^i, \tag{4}$$

thus not considering the Friedrichs extension, also converges to $H_C$ as $\alpha \to 0$, but only in the strong graph limit sense, [57] and therefore no useful information about the spectrum can be inferred (see Appendix A). In this case, the spectra of $T_\alpha$ are unbounded from below, a fact that misled several authors to believe that the energy of the fundamental state of $H_C$ was also unbounded (*i.e.* $E_{gs} = -\infty$) [3, 6, 34–37].

We should also notice that admitting the ground state eigenfunction as a Dirac-$\delta$ function is completely untenable since the corresponding probability density, which would be the square of a distribution, would generate all kind of interpretation problems on its own. Besides, let us assume

 

the Dirac-$\delta$ as an eigenfunction for the 1D hydrogen atom, by taking its Fourier transform we can see that its equivalent eigenfunction in the momentum representation would be

$$\Phi_0(p) = \frac{1}{\sqrt{2\pi\hbar}}. \tag{5}$$

But the eigenfunction with quantum number $n = 0$ in momentum representation is known to be $\Phi_0(p) = 0$, which contradicts our initial assumption [32]. Our above discussion shows that the observed numerical fact that the base-state energy is consistently getting larger in absolute value as $\alpha$ (14), or as the cut-off approach shrinks, is of no consequence for establishing conclusions about the value of the ground energy of the 1D Coulomb problem [10].

## III. ON THE NON-EXISTENCE OF PARITY EIGENFUNCTIONS.

Another source of controversy related to the spectrum of the 1D hydrogen atom is wether the wave functions of the system possess a certain kind of definite parity. Numerical studies have tried to address this property of the system by means of both the regularized potentials and the atom-laser interaction [34–37]. In a system with a regularized Coulomb potential states with definite parity do exist, however the singularity of the potential $V_C$ induce an spontaneous breaking of parity —which was not taken into account in the limit of the numerical approximations. The strongest effects of such symmetry breakdown may be interpreted as the existence of a superselection rule operating on the system [13, 42].

Such issue may be set straight by proving that the 1D Coulomb problem does not admit eigenfunctions defined over the whole $x$-axis. Although not explicitly stated, all the aforementioned solutions for the 1D Coulomb problem assume that the wavefunctions vanish at the origin, $\psi(0) = 0$. This Dirichlet boundary condition guarantees that the Hamiltonian $H_C$ is self-adjoint [23, 31, 33].

In [32] we found that the eigenfunctions, $\psi_n^{\pm}(x)$, and corresponding energy eigenvalues, $E_n$, of the 1D Coulomb problem are

$$\begin{aligned} \psi_n^{\pm}(x) &= \Theta(\pm x) 2 n^{-3/2} (-1)^{n-1} x L_{n-1}^1(2x/n) \exp(-z/n), \\ E_n &= -\frac{1}{2n^2}, \qquad n = 1, 2, 3, \ldots, \end{aligned} \tag{6}$$

where $\Theta(x)$ is the unit step function and $L_{n-1}^1$ are the generalized Laguerre polynomials [32, 50]. Notice that, as proved above, the $n = 0$ value is not allowed. Nevertheless, it would be easy to use the above eigenfunctions to build apparently valid normalized doubly-degenerate even and odd

 

states as follows

$$\psi^{even} = \frac{1}{\sqrt{2}}(\psi^{+} + \psi^{-}), \qquad \psi^{odd} = \frac{1}{\sqrt{2}}(\psi^{+} - \psi^{-}), \tag{7}$$

which are defined for $-\infty < x < \infty$. However, the definition of $\psi^{even}$ and $\psi^{odd}$ is not valid because the functions $\psi^{+}$ and $\psi^{-}$ cannot be joined to produce eigenfunctions valid for all real $x$. For, when a potential $V(x)$ is singular at $x = 0$ but not a Dirac-$\delta$ potential —as happens for the 1D Coulomb problem— we can obtain upon integrating the Schrödinger equation

$$\lim_{\epsilon \to 0} \int_{0-\epsilon}^{0+\epsilon} V(x)\psi^{even}(x)dx = \frac{1}{2}\left(\psi(0^{+}) - \psi(0^{-})\right) = 0; \tag{8}$$

whereas, by using (6) directly we obtain

$$\psi_n^{even}(0^{+}) - \psi_n^{even}(0^{-}) = (-1)^{n-1}\sqrt{8/n} \tag{9}$$

as in [42]. Therefore, the even states cannot be part of the spectrum of the system, which means that no even-parity eigenfunctions exist [11, 32]. On the other hand, if we accept the existence of odd eigenfunctions, $\psi^{odd}$, the matrix elements of both the position, $\hat{q} = x$, and the momentum, $\hat{p} = -id/dx$, operators between any two eigenfunctions of the system, would necessarily vanish

$$< \psi_1|\hat{q}|\psi_2 >= \int_{-\infty}^{\infty} x\psi_1^{*}\psi_2 dx = 0 \quad \text{and} \quad < \psi_1|\hat{p}|\psi_2 >= -i\int_{-\infty}^{\infty} \psi_1^{*}\frac{d\psi_2}{dx}dx = 0. \tag{10}$$

We thus get the contradictory result that any operator which may be expressed in terms of $\hat{q}$ and $\hat{p}$ should vanish. Our conclusion is then that no eigenfunction can be defined on the whole configuration space $(-\infty, \infty)$. The eigenstates then necessarily describe states confined wholly to the left or wholly to the rigth of the singularity and so the origin, $x = 0$, is completely forbidden for the quantum particle [22] as it is clearly exhibited by the vanishing of the quantum flux

$$j = i\left(\psi^{*}\frac{\partial\psi}{\partial x} - \psi\frac{\partial\psi^{*}}{\partial x}\right)\Big|_{x=0} = 0. \tag{11}$$

Even at positive energies there cannot be particle flow from the right to the left of the singularity or vice versa, in complete agreement with the matching condition $\psi(0) = 0$. It is known that in each of the regions $x > 0$ and $x < 0$, equation (1) has two linearly independent solutions, one of these, and also the only one with physical meaning for this problem, is the so-called regular Whittaker function

$$M_{\kappa\mu}(x) = \exp(-x/2)x^{\mu+1/2}M(\mu - \kappa + 1/2, 1 + 2\mu; x), \tag{12}$$

which is analytic in the vicinity of $x = 0$; and the other is not. one

$$W_{\kappa\mu}(x) = \exp(-x/2)x^{\mu+1/2}U(\mu - \kappa + 1/2, 1 + 2\mu; x), \tag{13}$$

 

with a logarihtmic singularity such that its derivative at $x = 0$ is infinite, and where the symbols $M(a, b; c)$ and $U(a, b; c)$ stand for Kummer functions [51]. The fact that only one solution is acceptable on each half-line implies that at positive energies there can be no transmission to the other side, because the only acceptable solution that contains no incoming wave, as required for transmission, is the trivial one. Thus, in the 1D Coulomb problem the boundary condition $\psi(0) = 0$ acts as an impenetrable potential barrier [4, 22, 23, 32, 42].

## IV. PHYSICAL ANALYSIS OF NUMERICAL RESULTS.

We have explained why the numerical evidence offered by [34–37] and others do not imply the existence of wave functions with any kind of definite parity nor the existence of an infinite binding-enegy ground state with Dirac-$\delta$ eigenfunction. We emphasize that no numerical approach is enough to settle controversies on non-perturbative properties of quantum systems. Despite the symmetry of the system, the superselection rule provoke a breaking of parity. The physical consequences of the ensuing superselection rule [12, 32, 33, 42] cannot be explicitly appreciated in numerical results. Every numerical approach should take into account that if an arbitrary sequence of Hamiltonians $H_n$ do indeed converge to a Hamiltonian $H$, there is in general no guarantee that their spectra will be related in any simple way. In particular, it is not usually true that the ground energies of the $H_n$ will converge to the ground energy of $H$ [7]. Further theoretical analysis of the system is required to attain a complete understanding.

Any approach using numerical methods has to be applied paying attention to the assumptions needed in order to apply suitable convergence results. Such assumptions may not be suggested by the numerical results and, even if they do, its physical consequences may not be fully realized. For instance, the numerically evaluated probability density may suggest the use of the Dirichlet condition $\psi(0) = 0$ though not the full consequences of the symmetry breakdown that arises from choosing such boundary condition. In fact, the results obtained from numerical approaches applied to the regularized 1D Coulomb potential (2) do not provide information about the 1D Coulomb problem whose properties have been carefully proved in [7, 22, 23, 32]. Any attempt to find the ground state energy of the 1D Coulomb problem using numerically calculated ground state energies of regularized Hamiltonians is futile unless supported by appropriate convergence results. The same can be said on the evidence presented about the existence of parity eigenstates. The methods used either to support or to disprove any claim regarding the spectrum of a singular system cannot be purely numerical. In a way of speaking, such spectral features are non-perturbative properties of

 

the 1D hydrogen atom.

## V. CONCLUSIONS.

Concerning the 1D Coulomb problem, it should be regarded as firmly established and completely proved that

A. There cannot be any relation between the right ($x > 0$) and the left ($x < 0$) sides of the singularity and, as it was convincingly argued for the first time in [4], not even for positive energies there can be any transmision from one side of the singularity to the other [11, 16] since a superselection rules operates on the system [12, 32, 42].

B. The controversy about the parity of the eigenfunctions is actually settled due to the superselection rule mentioned in [A] which, among other things, prevents the 1D Coulomb problem eigenstates to have a well defined parity [10, 12, 16, 32, 42].

C. The ground state energy of the 1D Coulomb problem corresponds to $E_{gs} = -1/2$. The supposed infinite energy ground state does not exist [10, 11, 32].

However, it should be taken into account that the conclusions listed above were obtained under the hypothesis of a Dirichlet boundary condition $\psi(0) = 0$ which was also employed, although not explicitly, in [34, 36, 37]. Other boundary conditions, that should be chosen according to the physics of the problem being analysed, could lead to different conclusions [23, 41].

The type of mistakes induced by numerical data that we have discussed in this paper may not only arise in the study of singular quantum problems like the 1D hydrogen atom, but they may also occur while examining other stiff problems. We should be well aware of such complications and remember that a careful analysis bolstered in solid physical and mathematical grounds is required in order to validate any numerical evidence. In summary, we cannot deduce the features of the singular Coulomb Hamiltonian $H_C$ only from analysing numerical data extracted from the solutions of the regularized Hamiltonians that approach $H_C$ through a sort of limiting process. This limitation stems from the basic differences that usually exist between the spectral features of regular and singular potentials. Such general conclusion is applicable to many other stiff systems. We also consider that the numerical investigations has established that not only the odd states but also the even ones have to be taken into account when studying the interaction of a *regularized* 1D hydrogen atom with a radiation field but that this is not true for the singular Coulomb potential with Hamiltonian $H_C$ [35, 37].

 

## VI. ACKNOWLEDGEMENTS

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### Appendix A. Spectral pollution from a sequence of Hamiltonians

It can be shown that if an arbitrary sequence of operators $H_n\,(n = 1, 2, 3, ...)$ does indeed converge to an operator $H$, then the spectra of the $H_n$ is usually not related, in any direct way, to the spectrum of $H$. In particular, it may well be the case that a sequence of eigenvalues $\lambda_n$ of $H_n$ converges to a $\lambda$ which is not in the spectrum of the limit operator $H$. The ocurrence of such spurious "eigenvalues" $\lambda$ had been termed *spectral pollution* and it occurs in a variety of contexts, than ranges from the theory of Schrödinger and Sturm-Liouville operators to elasticity and hydrodynamics. For a good account on the topic, see [48, 52, 53] and the references therein.

In fact, it can be shown that if a sequence of self-adjoint operators $H_n$ converges to $H$ in the sense of strong resolvent convergence (also known as the strong graph limit), then for every $\lambda$ in the spectrum of $H$ there exist a sequence $\lambda_n$ in the spectrum of $H_n$ such that $\lambda_n \to \lambda$ [47], *but not the other way around*, as the following example illustrates [49]: consider in the space of real square integrable functions, $L^2(\mathbb{R})$, the sequence of operators

$$H_n(x) = -\frac{1}{2}\frac{d^2}{dx^2} + V_n, \qquad n = 1, 2, 3, \ldots \tag{14}$$

where $V_n(x)$ is given by

$$V_n(x) = \begin{cases} -1 & \text{if } n \leq x \leq n+1, \\ 0 & \text{otherwise;} \end{cases} \tag{15}$$

thus the operator $H = -\frac{1}{2}\frac{d^2}{dx^2}$ is the strong graph limit of the sequence (14). However, the spectrum of $H$ is purely continuous spanning the whole non-negative axis, $0 \leq x < \infty$, whereas the spectrum of each $H_n$ includes also a simple eigenvalue, $\mu$, with a value between $-1$ and 0. As the above example suggest, we cannot conclude without further analysis that the ground energies of the sequence of Hamiltonian operators will end converging to the ground state of $H$. On the other

 

hand, if $H_n$ converges to $H$ strongly in norm then spectral pollution never takes place, that is, every converging sequence of eigenvalues $\lambda_n$ of $H_n$ converges to an eigenvalue $\lambda$ of $H$ [47].

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[55] The Friedrichs extension (FE) of the kinetic energy operator $p^2/2 = -(1/2)d^2/dx^2$ mantains the same functional form, $H_D = -(1/2)(d^2/dx^2)$, but has to be defined on the set of functions $f$ such that $f(0) = 0$ —the Dirichlet condition— and under the assumption that the triplet $f$, $f'$, and $f''$ are all square integrable and absolutely continuous excepting at $x = 0$, that is, the FE redefines the domain of the operator [54].

[56] When dealing with unbounded operators $H$, convergence is usually stated in terms of the resolvents $R(H, z) = (H - z)^{-1}$, $z \in \mathbb{C} - \mathbb{R}$. A sequence of operators $H_n$ is said to converge in the sense of strong norm convergence to $H$ if their resolvents converge in norm, that is, if $\|R(H_n, z) - R(H, z)\| \to 0$.

[57] An operator $H$ is the strong graph limit of a sequence of operators if their resolvents converge pointwise, that is, if $R(H_n, z) \to R(H, z)$. It is clear then that strong norm convergence implies strong ghaph convergence.

 