The bound-state solutions of the one-dimensional hydrogen atom

Rufus Boyack and Frank Marsiglio

Department of Physics and Theoretical Physics Institute,
University of Alberta, Edmonton, Alberta T6G 2E1, Canada

The one-dimensional hydrogen atom is an intriguing quantum mechanics problem that exhibits several properties which have been continually debated. In particular, there has been variance as to whether or not even-parity solutions exist, and specifically whether or not the ground state is an even-parity state with infinite negative energy. We study a “regularized” version of this system, where the potential is a constant in the vicinity of the origin, and we discuss the even- and odd-parity solutions for this regularized one-dimensional hydrogen atom. We show how the even-parity states, with the exception of the ground state, converge to the same functional form and become degenerate for \( x > 0 \) with the odd-parity solutions as the cutoff approaches zero. This differs with conclusions derived from analysis of the singular (i.e., without regularization) one-dimensional Coulomb potential, where even-parity solutions are absent from the spectrum.

I. INTRODUCTION

The one-dimensional (1D) hydrogen atom, described by the potential \( V(x) \sim 1/|x| \), has long been a quantum mechanics problem of theoretical interest, in part due to a lack of consensus as to whether or not even-parity solutions are admissible. There is a bevy of literature on this subject, and for our purposes we highlight only several pertinent articles which can be further investigated. The first study of the odd-parity solutions of the 1D hydrogen atom was performed in Ref. [1], where the usual hydrogen spectrum was derived. Following this initial study, a seminal investigation by Loudon\(^{23}\) used a regularization procedure to derive both odd-parity and even-parity solutions; in particular, Loudon found that the ground-state solution of the 1D hydrogen atom is an even-parity function with infinite negative energy, whose square modulus limits to a delta function as the regularization parameter goes to zero. Moreover, apart from his proposed ground-state solution, Loudon found that all the other states are two-fold degenerate, having either even or odd parity. There are two fundamental questions related to Loudon’s results which have caused disagreement in the literature – (i) are the solutions to the 1D hydrogen atom degenerate? (ii) if even-parity solutions are permissible, is the ground-state solution the same as that given by Loudon, which has the peculiarity that its square modulus limits to a delta function? Standard texts\(^4\) in quantum mechanics argue that the bound-state solutions of a 1D potential are non-degenerate; whether this result remains valid for singular potentials requires a more elaborate analysis.

In Ref. [5], Andrews further investigated Loudon’s ground-state solution, and there he showed that its scalar product with any square-integrable function vanishes, upon which he concluded that this solution is not observable and therefore presumably does not exist. In this mathematical analysis it was important to take the limiting form of Loudon’s ground-state solution after performing the integration. This conclusion was similarly obtained by Núñez-Yépez and Salas-Brito,\(^6\) who argued that the discrepancy with Ref. [2] is because Loudon computed the limiting probability distribution as opposed to the limiting wave function. Their conclusion was that the ground-state solution therefore does not exist. Haines and Roberts\(^7\) used the same regularized potential as Loudon and reached similar conclusions for this variant of the problem. However, for the singular Coulomb potential, they showed that only the odd-parity solutions are admissible. As a result, this ruled out any possible degeneracy in the bound-state solutions. In addition, these authors also claimed that there are a continuum of negative energy states.

Andrews\(^8\) later investigated the notion of degeneracy in singular potentials and provided a more encompassing analysis than that usually given in textbooks. Three types of potentials were defined by Andrews – mildly singular (MS), singular (S), and extremely singular (XS). An MS potential is one which is continuous, infinitely large at the origin, but integrable: \( \int_0^L |V(x)| \, dx < \infty \). An S potential is continuous, infinitely large at the origin, and nonintegrable near the origin: \( \int_0^L x |V(x)| \, dx < \infty \) but \( \int_0^L x |V(y)| \, dy \to \infty \) as \( x \to 0 \). An XS potential is continuous with \( \int_0^L x |V(x)| \, dx \) being divergent. Andrews showed that MS potentials behave in the same manner as non-singular potentials – their wave functions and the first derivatives of the wave functions are continuous. However, he argued that for class S potentials the potential acts as an impenetrable barrier and hence there is no reason to try to match the wave functions at boundaries. As a result, the even-parity bound state solutions, which Haines and Roberts deemed inadmissible based on a rigorous continuity condition derived from the Schrödinger equation, were argued by Andrews to be admissible; the reason being that whilst such solutions add a delta function at the origin, it is claimed that this does not affect any matrix elements of the Hamiltonian. In addition, Andrews argued that the continuum of negative energy states discussed by Haines and Roberts is incorrect. A similar conclusion about the invalidity of Haines and
Roberts’ continuum solutions, and the absence of even-parity solutions, was reached by Gomes and Zimerman in Ref. [9]; moreover, these latter authors asserted that the impenetrable boundary idea of Andrews is incorrect; see Refs. [10–13].

More recently, Xianxi et al.14 revisited the 1D hydrogen atom, deriving a continuity condition for the derivative of the wave function and showing that only odd-parity solutions therein satisfy this condition. These authors also considered a similar argument to that of Andrews5 as to the reason for the invalidity of Loudon’s ground-state solution. Palma and Raff15 argued that there is no degeneracy in the 1D hydrogen atom – all of the bound-state solutions have odd parity – and moreover they asserted that Loudon’s ground-state wave function does not satisfy the Schrödinger equation. This resolves the disputes in the literature, providing definitive answers to the two questions posed earlier in the introduction, and disproves the claim by Andrews that the (singular) 1D hydrogen atom acts as an impenetrable barrier. Further references on methods of solution to the 1D hydrogen atom can be found in Ref. [15] and a detailed collection of additional references is in Ref. [16]. Another collection of recent literature17,18 has claimed that there are neither even nor odd-parity eigenstates, the argument19 being that the odd-parity states would necessarily have vanishing expectation values for both the position and momentum operators. However, this is not a mathematical justification for discarding the odd-parity solutions.

Other approaches to studying the one-dimensional Coulomb potential include the use of symmetry arguments,20,21 the Laplace transform,22 and the theory of distributions.16,23–26 The d-dimensional hydrogen atom has been studied also,27,28 although the problems associated with the even-parity solutions in the d = 1 case were not fully addressed.

The 1D hydrogen atom system has also garnered interest29,30 in its application to the explanation of why electrons “float” above the surface of liquid helium – in one of the simplest models, the bulk of the inert helium acts as an infinite barrier while in the region outside the helium the electron experiences an attractive force with an image charge created in the dielectric medium. The resulting calculation of the mean distance an electron floats above the liquid helium surface is in reasonable agreement with the results quoted here come primarily from Andrews5,8 and Palma and Raff.15 The essential point is that our regularized calculations always have the ground state and the ensuing excited even states. The existence of such a ground state acts as a (penetrable) barrier for the remaining eigenstates, and indeed, for any function constructed from them.31

The outline of the paper is as follows. In Sec. II we study our particular regularized Coulomb potential. The energy eigenvalue equations for both the even and odd-parity solutions are investigated in Sec. III, and, following this, in Sec. IV we provide analytical expressions for the energy eigenvalues in the limit that the regularized potential approaches the singular potential. The wave functions are investigated in Sec. V and finally we conclude in Sec. VI.

II. REGULARIZED COULOMB POTENTIAL

FORMALISM

In this section we consider a regularized one-dimensional hydrogen atom potential given by

\[
V(x) = \begin{cases} 
-V_0 \frac{a_0 \delta}{|x|}, & |x| \geq \delta a_0 \\
-V_0, & |x| \leq \delta a_0.
\end{cases}
\] (2.1)

Here \(a_0 = \frac{4\pi \epsilon_0 k^2}{m e^2}\) is the Bohr radius and \(\delta > 0\) is a positive constant. The constant \(V_0\) is defined by

\[
V_0 = \frac{e^2}{4\pi \epsilon_0 a_0 \delta}.
\] (2.2)

Loudon2 studied a different regularization, but he provided some brief comments and calculations for this potential as well. Here we provide a more in-depth analysis of the potential in Eq. (2.1), and in particular we follow the method of analysis of Ref. [32], which highlighted how to solve the conventional hydrogen atom in a more symmetric fashion when considering the boundary conditions near the origin and near infinity. Since the potential is parity-invariant, the solutions to the Schrödinger equation have definite parity. Let region I be defined by \(|x| \leq \delta a_0\) whereas region II is \(|x| \geq a_0 \delta\). The Schrödinger
The equation in region I is then
\[ -\frac{\hbar^2}{2m} \psi''(x) - V_0 \psi(x) = E \psi(x). \] (2.3)

In what follows we focus on the bound-state solutions only. Define the wave vector \( q \), the energy \( E \), and the coordinate \( y \) by
\[ q = \sqrt{\frac{2m}{\hbar^2}} (E + V_0), \quad E = -\frac{\hbar^2}{2ma_0^2\beta^2}, \quad y = \frac{x}{a_0\beta}. \] (2.4)

Note that
\[ q = \frac{1}{a_0} \sqrt{\frac{2}{\delta} - \frac{1}{\beta^2}}. \] (2.5)

Thus, Eq. (2.3) now becomes
\[ \psi''(x) + q^2 \psi(x) = 0. \] (2.6)

The general solution to this differential equation is
\[ \psi(x) = A_1 \cos(qx) + B_1 \sin(qx). \] (2.7)

The even-parity solution has \( B_1 = 0 \) whereas the odd-parity solution has \( A_1 = 0 \). In region II, the Schrödinger equation is
\[ -\frac{\hbar^2}{2m} \psi''(x) - \frac{e^2}{4\pi\epsilon_0 |x|} \psi(x) = E \psi(x). \] (2.8)

Rewriting Eq. (2.8) in terms of the variables introduced in Eq. (2.4) gives
\[ \psi''(y) + \frac{2 \beta}{y} \psi(y) - \psi(y) = 0. \] (2.9)

Consider the region \( y \geq 0 \); let \( \psi(y) = y e^{-y} f(y) \) and substitute this into the above differential equation to obtain
\[ y f'' + 2(1 - y) f' - 2(1 - \beta) f = 0. \] (2.10)

The Kummer equation is given by\(^{33}\)
\[ yw'' + (b - y) w' - aw = 0, \] (2.11)
and its solutions are\(^{33}\)
\[ w(y) = c M(a, b; y) + d U(a, b; y). \] (2.12)

In Appendix B we provide a brief overview of the Kummer function \( M \) and the Tricomi function \( U \). The general solution to Eq. (2.10) is thus
\[ f(y) = A_{11} M(1 - \beta, 2; 2y) + B_{11} U(1 - \beta, 2; 2y). \] (2.13)

As \( y \to \infty \), \( M(a, b; y) \to [\Gamma(b) / \Gamma(a)] y^{a-b} e^y \), assuming that \( a \) is not a negative integer; in the case that it is, the solution truncates to a power series. Proceeding under the assumption that \( 1 - \beta \) is not a negative integer, which will turn out to be the case, then normalizability of the wave function requires \( A_{11} = 0 \).

### III. ENERGY EIGENVALUES

#### A. Even-parity solutions

Consider the even-parity solution: \( B_1 = 0 \). Only the domain \( x \geq 0 \) then needs to be investigated, and the solution for negative \( x \) can be determined from \( \psi(x) = \psi(-x) \). The wave function is thus
\[ \psi(x) = \begin{cases} A_1 \cos(qx), & x \leq \delta a_0 \\ B_{11} \frac{x}{a_0\beta} e^{-(x/(a_0\beta))} U(1 - \beta, 2; \frac{2x}{a_0\beta}), & x \geq \delta a_0. \end{cases} \] (3.1)

To determine the eigenvalue condition we match \( \psi \) and \( \psi' \) at \( x = \delta a_0 \). In region I, \( \psi' / \psi \) at \( x = \delta a_0 \) is given by
\[ \frac{\psi'_I}{\psi_I} = -q \frac{\sin(q \delta a_0)}{\cos(q \delta a_0)}. \] (3.2)

In the small \( \delta \) limit this reduces to \(-q^2 \delta a_0 = -2/a_0\), which agrees with Eq. (3.36) in Ref. [2]. To evaluate the derivatives of \( \psi \) in region II, a useful identity is\(^{33}\)
\[ \frac{d}{dx} U(a, b; x) = -a U(a + 1, b + 1; x). \] (3.3)

Using this relation, in region II we find that \( \psi' / \psi \) at \( x = \delta a_0 \) is given by
\[ \frac{\psi'_I}{\psi_I} = \frac{1}{a_0 \delta} \left[ 1 - \frac{\delta}{\beta} - \frac{2 \delta}{\beta} (1 - \beta) U \left( 2 - \beta, 3; \frac{2 \delta}{\beta} \right) \right]. \] (3.4)

Matching Eq. (3.2) and Eq. (3.4), for a given \( \delta \), then determines the eigenvalue condition for \( \beta \) and thus \( E \). The result is the following transcendental equation for \( \beta \):
\[ -qa_0 \tan(qa_0 \delta) = 1 - \frac{\delta}{\beta} - \frac{2 \delta}{\beta} U \left( 2 - \beta, 3; \frac{2 \delta}{\beta} \right) \] (3.5)

where \( q \) is defined in Eq. (2.4). This can be rewritten in a simplified manner by using the recurrence relations for the \( U \) function. In particular, by using Eqs. (B.6) and (B.7) in Appendix B, we find that
\[ \frac{2 \delta}{\beta} U \left( 2 - \beta, 3; \frac{2 \delta}{\beta} \right) = U \left( 1 - \beta, 2; \frac{2 \delta}{\beta} \right) + \beta U \left( 2 - \beta, 2; \frac{2 \delta}{\beta} \right) = \frac{1}{1 - \beta} \left[ U \left( 1 - \beta, 2; \frac{2 \delta}{\beta} \right) - \beta U \left( 1 - \beta, 1; \frac{2 \delta}{\beta} \right) \right]. \] (3.6)

Inserting this identity into Eq. (3.5) then simplifies the even-parity eigenvalue equation to
\[ qa_0 \tan(qa_0 \delta) = \frac{1}{\beta} \left[ 1 - \frac{\beta^2 U \left( 1 - \beta, 1; \frac{2 \delta}{\beta} \right)}{\delta U \left( 1 - \beta, 2; \frac{2 \delta}{\beta} \right)} \right]. \] (3.7)
For the odd-parity solution: \( A_1 = 0 \). Only the domain \( x \geq 0 \) then needs to be investigated, and the solution for negative \( x \) can be determined from \( \psi(x) = -\psi(-x) \). The wave function is thus

\[
\psi(x) = \begin{cases} 
B_1 \sin(qx), & x \leq \delta a_0 \\
B_1 \frac{x}{a_0^3} e^{-x/(a_0^3)} \left( 1 - \beta, 2; \frac{2x}{a_0^3} \right), & x \geq \delta a_0.
\end{cases}
\]

In region \( I \), \( \psi'/\psi \) at \( x = \delta a_0 \) is given by

\[
\frac{\psi'}{\psi} = q \frac{\cos(q\delta a_0)}{\sin(q\delta a_0)}.
\]

Using the identity in Eq. (3.6), the odd-parity eigenvalue equation then becomes

\[
-q a_0 \cot(qa_0 \delta) = \frac{1}{\beta^2} \left[ 1 - \frac{\beta^2}{\delta} \frac{U(1 - \beta, 1; 2 \frac{\pi}{\beta})}{U(1 - \beta, 2; 2 \frac{\pi}{\beta})} \right].
\]

A full numerical solution of Eq. (3.7) and Eq. (3.10) for the even and odd-parity cases, respectively, is given in the figures below. First, however, we explore some analytical results in the limit \( \delta \to 0 \).

**IV. ANALYTICAL RESULTS IN THE LIMIT \( \delta \to 0 \)**

**A. Even-parity solutions**

Let us now investigate the limit of small values of \( \delta \). First consider the case \( \beta \neq 0 \). For the even-parity solution, after taking the limit \( \delta \to 0 \) in Eq. (3.7) and then simplifying, the result is

\[
2 = \frac{1}{\beta^2} + 2 \left[ 2 \gamma + \ln \left( \frac{2 \delta}{\beta^2} \right) + \Psi(1 - \beta) \right].
\]

Here \( \Psi \) denotes the digamma function, which is discussed in Appendix A. Note that, throughout the paper we use \( \psi \) to denote a wave function whereas \( \Psi \) is the digamma function. As \( \delta \to 0 \) the logarithmic term diverges, and thus, to ensure that the right-hand side of this equation is finite for any \( \delta \), the digamma function must also diverge, and as a result \( \beta \to n \in \mathbb{N} \). We define the energy scale \( E_0 = -\frac{\hbar^2}{2ma_c^2} \), which is the same energy scale appearing in the 3D hydrogen atom, so that the even-parity energy eigenvalues limit to

\[
E \to -\frac{E_0}{n^2}, \quad n \in \mathbb{N}, \quad \text{as} \quad \delta \to 0.
\]

In Fig. 1 we plot \( \beta \equiv (-E_0/E)^{\frac{1}{2}} \), as computed from Eq. (3.7) and Eq. (3.10), as a function of \( x \equiv 1/\ln \left( \frac{1}{\delta^2} \right) \), and as can be observed the parameter \( \beta \) does indeed converge to an integer \( n \) in the limit \( \delta \to 0 \).

To study the deviation of the parameter \( \beta \) from an integer \( n \) we define \( \rho_n = \beta - n \) (Loudon\(^2\) calls these “quantum defects”), which obeys \( \rho_n \to 0 \) as \( \delta \to 0 \). The dependence of \( \rho_n \) on \( x \) can be deduced from Eq. (4.1) as follows. First, using the identities in Eqs. (A.10) and (A.11) in Appendix A, we obtain \( \Psi(1 - \beta) = \Psi(\beta) + \pi \cot(\pi \beta) = \Psi(\beta + 1) - \frac{1}{\beta} + \pi \cot(\pi \beta) \). Thus, as \( \beta \to n \), we find that \( \Psi(1 - \beta) \to \Psi(n + 1) - \frac{1}{n} + \frac{1}{\rho_n} \). In Eq. (A.12), it is proved that \( \Psi(n + 1) = \sum_{k=1}^{n} \frac{1}{k} - \gamma \). If we define the constant \( c_n \) by

\[
c_n = \gamma - 1 - \frac{1}{2n} + \ln 2 + \left( \sum_{k=1}^{n} \frac{1}{k} - \ln n \right),
\]

then Eq. (4.1) becomes \( \frac{1}{\rho_n} = \frac{1}{x} \left( 1 - xc_n \right) \). This is a more accurate version of Eq. (3.26) in Ref. [2], which, in our notation, is given by \( \frac{1}{\rho_n} = \frac{1}{x} - (\ln 2 - \ln n) \). Inverting

![FIG. 1. The energy eigenvalues, \( E_n \), for both even-parity (blue squares) and odd-parity (red circles) eigenstates as a function of the cutoff, \( \delta a_0 \), for the Coulomb potential. Motivated by Eq. (4.1), we plot \( \beta \equiv (-E_0/E)^{\frac{1}{2}} \) versus \( x \equiv 1/\ln \left( 1/\delta^2 \right) \), where \( E_0 = -\frac{\hbar^2}{2ma_c^2} \). An infinite spectrum of bound states arises, with all of the excited-state energies trending towards the positive integers as \( \delta \to 0 \). On the bottom axis, small arrows accompanied with labels indicate the actual value of \( \delta \); the integer value indicates the negative exponent of a power of 10 (e.g., the right-most set of points are calculated for \( \delta = 10^{-2} \) while the left-most set of points is for \( \delta = 10^{-7} \)). The energy eigenvalues for the odd-parity solutions converge to the integer values, even for “large” values of \( \delta \). However, the even-parity solutions are approaching the integer values more slowly as \( \delta \to 0 \). The even ground-state energy eigenvalue approaches \( \beta \to 0 \) as \( \delta \to 0 \). These trends will be examined more closely in subsequent figures.](image-url)
As \( n \to \infty \), the terms in brackets in Eq. (4.3) approach \( \gamma \); thus, \( c_n \approx 2 \gamma - 1 + \ln 2 \approx 0.8476 \) as \( n \to \infty \). Note that \( c_1 \approx 0.7704 \) and \( c_2 \approx 0.8272 \), and this number moves progressively closer to \( c_{\infty} \), so there is not a lot of variation of this constant with \( n \).

Now consider the case when \( \beta \to 0 \). Define \( \rho_0 = \beta \). In this limit, Eq. (4.1) becomes

\[
1 = \frac{1}{2 \rho_0} + \gamma + 2 - \frac{1}{x} + \ln \left( \frac{1}{\rho_0} \right),
\]

As \( \delta \to 0 \), i.e., as \( x \to 0 \), the lowest-order solution to this equation is \( \rho_0 = \frac{x}{2} \). If we define the constant \( c_0 \) by

\[
c_0 = \gamma + 2 \ln 2 - 1,
\]

then after inserting this result into Eq. (4.5), along with replacing the logarithm term by its lowest-order approximation, we find that

\[
\rho_0 = \frac{x}{2} \left[ 1 + x (c_0 - \ln x) \right], \quad \text{as } x \to 0.
\]

This is a more accurate version of Eq. (3.28) in Ref. [2]. As \( \delta \to 0 \), the energy for the \( n = 0 \) even state becomes increasingly large and negative. In Fig. 2 the deviation \( \rho_n = \beta - n \) is plotted as a function of \( x \). It is clear from the figure that Eq. (4.1) provides very accurate results in the range of \( \delta \) considered here, and iterative solution of the much more difficult Eq. (3.7) is not required.

### B. Odd-parity solutions

![Graph showing odd-parity solutions](image)

FIG. 3. The deviation of \( \beta \) with respect to integer values, defined as \( \rho_n \equiv \beta - n \), versus \( x \equiv 1 \left( \ln(1/\delta) \right) \) for the ground and excited states, respectively. The exact values are given by the squares – these are the same results as shown in Fig. 1. The solid curve corresponds to Eq. (4.1). The red curve is for the (even) bound state \( n = 0 \), while the green and blue curves correspond to \( n = 1 \) and \( n = 10 \) (effectively \( n \to \infty \)), respectively.

The deviations for all the excited even-parity states are almost identical. Also shown are the crude approximations, \( \rho_0 \approx x/2 \), for the ground state, and \( \rho_n \approx x \) for the (even) excited states indicated with dotted (black) curves. The latter is fairly accurate while the former is not accurate beyond extremely minute values of \( \delta \). Also shown are the more refined approximations given by Eq. (4.7) and Eq. (4.4) for the ground and excited states, respectively.
As will be shown, in order to determine the form of $\rho_n$ it is important to retain a portion of all of the terms appearing in the numerator and denominator. Following the previous section, we let $\beta = \rho_n + n$. Note that $\Psi (1 - \beta) = \Psi (\beta) + \pi \cot (\pi \beta)$. Thus, as $\rho_n \rightarrow 0$, for any $n \geq 1$, $\Psi (1 - \beta) \rightarrow \Psi (n) + 1/\rho_n$. Similarly, since $\Psi (2 - \beta) = \Psi (1 - \beta) + 1/\rho_n$, then, for any $n \geq 2$, $\Psi (2 - \beta) \rightarrow \Psi (n - 1) + 1/\rho_n$. Consider the case $n = 1$, and on the right-hand side of Eq. (4.8) keep only the singular terms. The result is then

$$-1 + \frac{2\delta}{3} - \frac{\delta}{\beta} = \frac{1}{\beta^3} - \ln \left(\frac{2\delta}{3} \right) + \frac{1}{\beta} \left[1 + (1 - n) \frac{2\delta}{3n}\right].$$

Equating both sides requires

$$\rho_n = \frac{2}{3} \delta^2.$$ 

V. WAVE FUNCTIONS

To determine the constants $A_I$, $B_I$, and $B_{II}$, the continuity condition along with the normalization constraint must be imposed. For the even and odd-parity solutions respectively, continuity of $\psi$ at $x = \delta a_0$ requires

$$A_I \cos (qa_0 \delta) = B_{II} \delta e^{-\frac{\delta}{\beta}} U \left(1 - \beta, 2; \frac{2\delta}{3\beta}\right),$$

$$B_I \sin (qa_0 \delta) = B_{II} \delta e^{-\frac{\delta}{\beta}} U \left(1 - \beta, 2; \frac{2\delta}{3\beta}\right).$$

Combining Eq. (5.1) and Eq. (5.2) with the normalization condition, $1 = \int_{-\infty}^{\infty} |\psi (x)|^2 dx$, then determines $A_I$ and $B_I$ for the even and odd-parity solutions respectively. Therefore, the coefficients $A_I$ and $B_I$ are deduced from

$$A_I^2 = \frac{1}{2 qa_0 \delta} \left(\int_0^1 \cos^2 \left(qa_0 \delta y\right) dy + \cos^2 \left(qa_0 \delta\right) \int_1^{\infty} \left[y e^{\frac{1}{3}(1-y)} U \left(1 - \beta, 2; \frac{2\delta}{3\beta}\right)\right]^2 dy\right),$$

$$B_I^2 = \frac{1}{2 qa_0 \delta} \left(\int_0^1 \sin^2 \left(qa_0 \delta y\right) dy + \sin^2 \left(qa_0 \delta\right) \int_1^{\infty} \left[y e^{\frac{1}{3}(1-y)} U \left(1 - \beta, 2; \frac{2\delta}{3\beta}\right)\right]^2 dy\right).$$

The even-parity and odd-parity solutions are now completely specified. In the even-parity case, the eigenvalue $\beta$ is determined from Eq. (3.7) and the wave function coefficients are obtained from Eqs. (5.1) and (5.3); in the odd-parity case, the eigenvalue $\beta$ is determined from Eq. (3.10) and the coefficients of the wave function are obtained from Eqs. (5.2) and (5.4).

In the limit that $\delta \rightarrow 0$, the expected form of the wave functions can be deduced as follows. Consider first the case of the odd-parity eigenstates. In Eq. (13.6.27) of Ref. [33], the following result is given: $U (-n, 1 + \alpha; x) = (-1)^n n! L_n^{(\alpha)} (x)$. Thus, the (normalized) odd-parity eigenstates limit to

$$\psi_{\text{odd}} (x) \cdot (-1)^n \left(\frac{2}{qa_0 n^3}\right)^{\frac{1}{2}} x \frac{\alpha}{a_0 n} e^{-\alpha (a_0 n) x} L_n^{(1)} \left(\frac{2|x|}{qa_0 n}\right),$$

where the proof of the normalization constant is provided in Appendix C. This result agrees with Eq. (A6) in Ref. [15] and with Eq. (3.29) in Ref. [2] (noting the difference in definitions of the associated Laguerre polynomials; see Appendix C).

Now consider the even-parity eigenstates. As $\delta \rightarrow 0$, for $n \geq 1$, the even-parity eigenstates limit to $\psi_{\text{even}} (x) \rightarrow \psi_{\text{odd}} (|x|)$. For the $n = 0$ even-parity eigenstate, we use
we plot the
solutions would have a discontinuous first derivative.
our notation, has no even-parity eigenstates, since such
form the normalized even-parity eigenstates have the limiting
U Eq. (B.4) in Appendix B:
clearly varies significantly with \( \delta \) we are zooming into domain near the origin. The ground state
given by Eq. (5.7). Note the scale of the horizontal scale —
\( \delta \) denoted by the squares for the smallest value of
has a continuous derivative at
the analytical result. This is to be expected, since the former
the numerical result is slightly different near the origin from
the points) The even-parity eigenstates, however, vary more
significantly with \( \delta \), and even for the smallest value of \( \delta \) the
numerical result is still slightly different from the analytical
result, as is clear from the plot for \( x > 0 \). Nonetheless, as \( \delta \) continues
to decrease, the numerical results will coincide with
the analytical result indicated by Eq. (5.6), and shown in the
figure for \( x > 0 \).

![Figure 4](image1.png)

**FIG. 4.** The even-parity ground state for \( \delta = 10^{-1} \) (red),
10^{-2} (green), 10^{-3} (blue), 10^{-4} (mauve), 10^{-5} (cyan), 10^{-6} (yellow), and 10^{-7} (black dash-dot). The analytical result,
denoted by the squares for the smallest value of \( \delta \), is
shown in the figure for \( x/a_0 \) close to the origin, whereas our regularized solutions (curves
in Fig. 4) do not. In fact, according to Ref. [15], the non-
regularized 1D Coulomb potential, which has \( \delta = 0 \) in
our notation, has no even-parity eigenstates, since such
solutions would have a discontinuous first derivative.

This observation is also hinted at in Figs. 5 and 6 where
we plot the \( n = 1 \) and \( n = 2 \) wave functions for the reg-
ularized 1D Coulomb potential along with the limiting
analytical form given in Eq. (5.5). We have plotted the
analytical form of only the odd solution, and as Eq. (5.6)
indicates, this coincides with the even analytical solution
for \( x > 0 \). The even analytical solution for \( x < 0 \) is
the mirror image of this solution (not shown), so that
here too a cusp is present at the origin for the analytical
even excited states. While the even results for non-zero
regularization parameter \( \delta \) trend towards the analytical
result, they also appear to have a cusp-like feature near
\( x = 0 \). Of course they do not, as the small \( x \) behavior is
given by the cosine function. This plot illustrates, in a
practical way, how finite-\( \delta \) results can nonetheless begin
to reproduce features of the \( \delta = 0 \) result. In the mean-
time, ignoring for the moment what is occurring very
close to the origin, the rest of the even wave function is
slowly approaching the expected analytical behavior
given by Eq. (5.6).

The situation with the odd-parity states is very differ-
ent. Over the 6 decades of variation of the regularization
parameter \( \delta \), the wave function has already converged to
the \( \delta = 0 \) solution given by Eq. (5.5); indeed, the differ-

![Figure 5](image2.png)

**FIG. 5.** The \( n = 1 \) even and odd-parity energy eigenstates for \( \delta = 10^{-1} \) (red), 10^{-2} (green), 10^{-3} (blue), 10^{-4} (mauve), 10^{-5} (cyan), 10^{-6} (yellow), and 10^{-7} (black dash-dot). The analytical results, denoted by the squares, are given by Eq. (5.5) and Eq. (5.6), and we have shown only the \( x > 0 \) half of Eq. (5.6) for clarity. For all values of \( \delta \), the odd-parity eigenstates cannot be distinguished from one another (all 7 different curves are shown in black and coincide with
the points) The even-parity eigenstates, however, vary more
significantly with \( \delta \), and even for the smallest value of \( \delta \) the
umerical result is still slightly different from the analytical
result, as is clear from the plot for \( x > 0 \). Nonetheless, as \( \delta \) continues
to decrease, the numerical results will coincide with
the analytical result indicated by Eq. (5.6), and shown in the
figure for \( x > 0 \).
VI. CONCLUSIONS

In this paper we have analyzed a regularized version of the one-dimensional hydrogen atom consisting of a potential that is constant in the vicinity of the origin, and Coulomb-like beyond. We have obtained results very much in agreement with those obtained by Loudon\textsuperscript{2} for a different regularization. This system has both even and odd-parity eigenstates, and moreover, for any finite cutoff, the eigenstates are nondegenerate. Nonetheless, as our regularization parameter representing the cutoff near the origin, \( \delta \), approaches zero, the even-parity eigenvalues approach those of their odd-parity counterparts. Their wave functions remain well-defined, and also approach their parity-adjusted odd-parity counterparts. The most intriguing feature of this model is the even-parity ground state, whose energy becomes increasingly negative as \( \delta \to 0 \). Concomitant with this behavior, the corresponding ground state becomes more localized near the origin, approaching a functional form whose square approaches that of a Dirac \( \delta \)-function. Because of the so-called pseudo-potential effect\textsuperscript{31} the presence of this state gives rise to an effective barrier for all other states, a property recognized by Andrews in Ref. \[8\]. This barrier serves to organize the remaining eigenstates into split even and odd doublets, as expected for a simple double well. The strength of this effective double well barrier is controlled by the regularization parameter \( \delta \).

ACKNOWLEDGMENTS

This work was supported in part by the Natural Sciences and Engineering Research Council of Canada (NSERC). R.B. acknowledges support from the Department of Physics and the Theoretical Physics Institute at the University of Alberta.
Appendix A: Gamma and Digamma functions

In the following appendices we provide a brief overview of the special functions and their pertinent identities used in the manuscript. The Gamma function was defined by Weierstrass (see Ch. 12 of Ref. [34] for example) by the equation

$$\frac{1}{\Gamma(z)} = ze^{\gamma z} \prod_{n=1}^{\infty} \left[ 1 + \frac{z}{n} \right] e^{-\frac{n}{z}}. \quad (A.1)$$

Here, $z$ is a complex number not equal to zero or a negative integer, and $\gamma$ is the Euler-Mascheroni constant, which approximates to $\gamma \approx 0.5772$, and is defined exactly by

$$\gamma = \lim_{n \to \infty} \left( \sum_{k=1}^{n} \frac{1}{k} - \ln(n) \right). \quad (A.2)$$

Using Eq. (A.1), along with its derivative with respect to $z$, after setting $z = 1$ we obtain

$$\Gamma(1) = 1. \quad (A.3)$$

$$\Gamma'(1) = -\lim_{n \to \infty} \sum_{k=1}^{n} \left( \frac{1}{k} - \ln \left( 1 + \frac{1}{k} \right) \right) = -\gamma. \quad (A.4)$$

An integral representation of the Gamma function, due to Euler, is

$$\Gamma(z) = \int_{0}^{\infty} dt t^{z-1} e^{-t}. \quad (A.5)$$

Two important properties of the Gamma function are given by

$$\Gamma(z+1) = z\Gamma(z). \quad (A.6)$$

$$\Gamma(1-z) \Gamma(z) = \frac{\pi}{\sin(\pi z)} \quad (A.7)$$

The first identity is easily proved using Eq. (A.5). The second identity, which is known as the reflection formula, can be proved using Eq. (A.1) and Eq. (A.6) and the Weierstrass factorization formula for the sine function. In the case where $z \in \mathbb{N}$, Eq. (A.6) becomes $\Gamma(n+1) = n!$. Another useful identity is known as the duplication formula, given by

$$\pi z \Gamma(2z) = 2^{2z-1} \Gamma(z) \frac{\Gamma \left( z + \frac{1}{2} \right)}{\Gamma(1/2)}. \quad (A.8)$$

The digamma function is defined by

$$\Psi(z) = \frac{d}{dz} \ln \Gamma(z). \quad (A.9)$$

By taking the logarithmic derivatives of Eq. (A.6) and Eq. (A.7), two recurrence relations for the digamma function are obtained:

$$\Psi(z+1) = \Psi(z) + \frac{1}{z}. \quad (A.10)$$

$$\Psi(1-z) - \Psi(z) = \pi \cot(\pi z). \quad (A.11)$$

The first identity above proves useful in evaluating the partial sums of the Harmonic series:

$$\sum_{k=1}^{n} \frac{1}{k} = \sum_{k=1}^{n} [\Psi(k+1) - \Psi(k)] = \Psi(n+1) - \Psi(1) = \Psi(n+1) + \gamma. \quad (A.12)$$

In addition, the limiting behavior of $\Psi(z)$, as $z \to -n$, where $n \in \mathbb{N}$, can be deduced from Eq. (A.11) as

$$\Psi(z) \to -\frac{1}{z+n}. \quad (A.13)$$

The asymptotic behavior of the digamma function is (see Eq. (6.3.18) in Ref. [33]):

$$\Psi(z) \to \ln(z) - \frac{1}{2z} - \frac{1}{12z^2} + O \left( z^{-4} \right). \quad (A.14)$$

Appendix B: Hypergeometric and Tricomi functions

The confluent hypergeometric differential equation, also known as Kummer’s equation, for the function $f(z)$ is given by (see Ch. 13 of Ref. [33] and Ch. 13 of Ref. [35]):

$$z \frac{d^2 f}{dz^2} + (b-z) \frac{df}{dz} - af = 0. \quad (B.1)$$

The differential equation has a regular singularity at $z = 0$ and an irregular singularity at $z = \infty$. The two linearly independent solutions of interest are known as Kummer’s function $M(a,b,z)$ and Tricomi’s function $U(a,b,z)$. The $M(a,b,z)$ power series representation about $z = 0$ is given by

$$M(a,b,z) = 1 + \frac{a}{b} z + \frac{(a)_2}{(b)_2} \frac{z^2}{2!} + \cdots + \frac{(a)_n}{(b)_n} \frac{z^n}{n!} + \cdots, \quad (B.2)$$

where $(a)_n = a(a+1)(a+2)\ldots(a+n-1)$, $(a)_0 = 1$. Similarly, for $U(a,b,z)$ we have

$$U(a,b,z) = \frac{\pi}{\sin(\pi b)} \left[ \frac{M(a,b,z)}{\Gamma(1+a-b) \Gamma(b)} - z^{1-b} \frac{M(1+a-b,2-b,z)}{\Gamma(a) \Gamma(2-b)} \right]. \quad (B.3)$$

The Tricomi function is a many-valued function, and its principal branch is given by $-\pi < \arg z \leq \pi$. The logarithmic series for $U$ is given in Eq. (13.2.9) of Ref. [35]:

$$U(a,n+1,z) = \frac{(-1)^{n+1}}{n!} \sum_{k=0}^{\infty} \frac{(a)_k z^k}{(n+1)_k k!} \left[ \ln z + \Psi(a+k) - \Psi(1+k) - \Psi(n+k+1) \right] + \frac{1}{\Gamma(a)} \sum_{k=1}^{n} \frac{(k-1)! (1-a+k)_{n-k} z^{-k}}{(n-k)!}. \quad (B.4)$$
The most pertinent recurrence relations for the $M$ and $U$ functions that were used in the main text are listed below; a more detailed collection of identities can be found in Refs. [33] and [35]. From Eq. (13.4.21) in Ref. [33], we have

$$
\frac{d}{dz} U(a, b, z) = -a U(a + 1, b + 1, z). \tag{B.5}
$$

In addition, Eqs. (13.4.17-18) in Ref. [33] are given by

$$
U(a, b, z) - a U(a + 1, b, z) - U(a, b - 1, z) = 0, \tag{B.6}
$$
$$
(b - a) U(a, b, z) + U(a - 1, b, z) - z U(a, b + 1, z) = 0. \tag{B.7}
$$

The asymptotic behavior of the $M$ and $U$ functions are written below. As $|z| \to \infty$,

$$
M(a, b, z) \to \frac{\Gamma(b)}{\Gamma(a)} e^z z^{-a} \left[ 1 + O \left( |z|^{-1} \right) \right], \quad \text{Re} \, z > 0, \tag{B.8}
$$
$$
M(a, b, z) \to \frac{\Gamma(b)}{\Gamma(b - a)} (-z)^{-a} \left[ 1 + O \left( |z|^{-1} \right) \right], \quad \text{Re} \, z < 0. \tag{B.9}
$$

These expressions assume that $a$ is not a negative integer, in that case the $M$ function truncates to a polynomial; this is discussed further in the next section. As $\text{Re} \, z \to \infty$,

$$
U(a, b, z) \to z^{-a} \left[ 1 + O \left( |z|^{-1} \right) \right]. \tag{B.10}
$$

**Appendix C: Laguerre polynomials**

Following Eq. (22.11.6) in Ref. [33], we define the associated Laguerre polynomials according to Rodrigues’ formula:

$$
L_n^{(\alpha)}(x) = \frac{1}{n!} e^x x^{-\alpha} \frac{d^n}{dx^n} \left( e^{-x} x^{n+\alpha} \right). \tag{C.1}
$$

This definition agrees with that used in Eq. (A5) of Ref. [15] (although that reference uses a calligraphic $\mathcal{L}$ whereas we use the italicized latin $L$). Note, however, this definition differs from the associated Laguerre polynomials defined in Ref. [36]. In certain special cases the $M$ and $U$ functions reduce to polynomial solutions. For the purposes of this paper, the pertinent case is when $M$ and $U$ reduce to the associated Laguerre polynomials (see Eqs. (13.6.9) and (13.6.27), respectively, of Ref. [33]):

$$
M(-n, \alpha + 1, x) = \frac{n!}{(\alpha + 1)_n} L_n^{(\alpha)}(x), \tag{C.2}
$$
$$
U(-n, \alpha + 1, x) = (-1)^n n! L_n^{(\alpha)}(x). \tag{C.3}
$$

As an example of the utility of these various identities, we prove that the wave function in Eq. (5.5) is normalized. The wave function is

$$
\psi_n(x) = \left( -1 \right)^{n-1} \left( \frac{2}{a_0 n^3} \right)^{\frac{1}{2}} \frac{|x|}{a_0 n} e^{-|x|/(a_0 n)} L_{n-1}^{(1)} \left( \frac{2|x|}{a_0 n} \right), \quad n \geq 1. \tag{C.4}
$$

The integral of the probability density is then

$$
N = \int_{-\infty}^{\infty} |\psi_n(x)|^2 \, dx = \frac{4}{a_0 n^3} \int_0^\infty \left( \frac{x}{a_0 n} \right)^2 e^{-2x/(a_0 n)} \left[ L_{n-1}^{(1)} \left( \frac{2|x|}{a_0 n} \right) \right]^2 \, dx = \frac{1}{2n^2} \int_0^\infty e^{-u} \left[ u L_{n-1}^{(1)}(u) \right]^2 \, du. \tag{C.5}
$$

To evaluate this integral, we need the following two identities, which correspond to Eq. (22.7.30) and Eq. (22.8.6), respectively, of Ref. [33]:

$$
L_n^{(a-1)}(x) = L_n^{(a)}(x) - L_{n-1}^{(a)}(x). \tag{C.6}
$$
$$
x \frac{d}{dx} L_n^{(a)}(x) = n L_n^{(a)}(x) - (n + \alpha) L_{n-1}^{(a)}(x). \tag{C.7}
$$

Combining these two results, we obtain $\frac{d}{du} u L_{n-1}^{(1)}(u) = n L_{n-1}^{(0)}(u)$. Using this identity, along with integration by parts, Eq. (C.5) then simplifies to

$$
N = \frac{1}{2n^2} \int_0^\infty e^{-u} \frac{d}{du} \left[ u L_{n-1}^{(1)}(u) \right]^2 \, du = \frac{1}{n} \int_0^\infty e^{-u} u L_{n-1}^{(1)}(u) L_{n-1}^{(0)}(u) \, du. \tag{C.8}
$$

To evaluate this integral, another recurrence relation is needed (see Eq. (22.7.32) in Ref. [33]):

$$
L_n^{(a-1)}(x) = \frac{1}{n + \alpha} \left[ (n + 1) L_{n+1}^{(a)}(x) - (n + 1 - x) L_n^{(a)}(x) \right]. \tag{C.9}
$$

Rewriting this equation with $\alpha = 1$ and $n \to n - 1$, and then isolating the last term containing $x L_{n-1}^{(1)}(x)$, results in

$$
x L_{n-1}^{(1)}(x) = n L_{n-1}^{(0)}(x) - n \left( L_n^{(1)}(x) - L_{n-1}^{(1)}(x) \right),
$$
$$
= n \left( L_{n-1}^{(0)}(x) - L_n^{(0)}(x) \right). \tag{C.10}
$$

The second line follows from using Eq. (C.6). Substituting this identity into (the second line of) Eq. (C.8) we obtain

$$
N = \int_0^\infty e^{-u} n L_{n-1}^{(0)}(u) \left[ L_{n-1}^{(0)}(u) - L_n^{(0)}(u) \right] \, du = 1. \tag{C.11}
$$

The last equality follows from the orthonormality condition of the associated Laguerre polynomials:

$$
\int_0^\infty dx x^\alpha e^{-x} L_n^{(\alpha)}(x) L_m^{(\alpha)}(x) = \frac{1}{n!} \delta_{nm} \Gamma(n + \alpha + 1). \tag{C.12}
$$
