

# Solutions of the Schroedinger equation for piecewise harmonic potentials: Remarks on the asymptotic behavior of the wave functions

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We discuss the solutions of the Schroedinger equation for piecewise potentials, given by the harmonic oscillator potential for  $|x| > a$  and by an arbitrary function for  $|x| < a$ , using elementary methods. The study of this problem sheds light on usual errors made in discussions of the asymptotic behavior of the eigenfunctions of the quantum harmonic oscillator and can also be used for the analysis of the eigenfunctions of the hydrogen atom. We present explicit results for the energy levels of a potential of this class, used to model the confinement of electrons in nanostructures. © 2017 American Association of Physics Teachers.

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## I. INTRODUCTION

The Schroedinger equation for the linear harmonic oscillator reads

$$\frac{d^2\psi}{dz^2} + \left( \mathcal{E} - \frac{z^2}{4} \right) \psi = 0, \quad (1)$$

where  $z = \sqrt{2m\omega/\hbar}x$ ,  $\mathcal{E} = E/(\hbar\omega)$ ,  $x$  is the coordinate of the oscillator, and  $m$  and  $\omega$  its mass and frequency, respectively. The traditional approach for solving this equation consists in proposing a solution of the form

$$\begin{aligned} \psi(z) &= e^{-z^2/4} \left[ \sum_{n \geq 0} a_{2n} z^{2n} + \sum_{n \geq 0} a_{2n+1} z^{2n+1} \right] \\ &\equiv e^{-z^2/4} [a_0 S_{\text{even}}(z) + a_1 S_{\text{odd}}(z)], \end{aligned} \quad (2)$$

and obtaining recurrence relations for the coefficients

$$a_{n+2} = \frac{n - \mathcal{E} + 1/2}{(n+1)(n+2)} a_n. \quad (3)$$

Note that these are two sets of independent recurrence relations for the even and odd coefficients, which are fully determined once one fixes  $a_0$  and  $a_1$ .

The energy eigenvalues are obtained by imposing the condition that  $|\psi(z)|^2$  should be integrable. In many textbooks,<sup>1-8</sup> it is remarked for large  $n$  that  $a_{2n+2}/a_{2n} \simeq a_{2n+3}/a_{2n+1} \simeq 1/(2n)$ , which is also the behavior for the coefficients of the series of  $e^{z^2/2}$ . Then, it is (incorrectly) argued<sup>1-4</sup> that, for large  $z$ ,

$$S_{\text{even}} \simeq S_{\text{odd}}/z \simeq e^{z^2/2}, \quad (4)$$

and therefore that  $|\psi(z)|^2$  would not be integrable, unless the series include only a finite number of terms. As a consequence, the allowed energy eigenvalues are  $\mathcal{E} = n + 1/2$ , for some nonnegative integer  $n$ .

A long time ago it had been pointed out that, although the conclusion for the eigenvalues is correct, the argument is wrong.<sup>9</sup> It is not true that, if two power series with

coefficients  $a_n$  and  $b_n$  are such that  $a_{n+1}/a_n \simeq b_{n+1}/b_n$  for large  $n$ , then they have the same behavior for large arguments. This is implicitly assumed in other textbooks,<sup>5-8</sup> where it is pointed out that  $a_{2n+2}/a_{2n} \simeq 1/(2n)$  is the behavior of the coefficients of the series of  $z^k e^{z^2/2}$  for any value of  $k$ . This property is used to argue that the asymptotic behavior of the odd and even series should be of this form for some particular values of  $k$ . Note that this claim is at least incomplete, since  $z^k e^{z^2/2}$  admits a representation in powers of  $z$  (for all  $z$ ) only if  $k$  is a natural number (or eventually an integer, if one considers also Laurent series). Moreover, in principle there could exist other functions with different asymptotic behavior and the same ratio  $a_{2n+2}/a_{2n}$  in the large  $n$  limit.

A correct reasoning is as follows.<sup>10</sup> If  $a_{n+1}/a_n > b_{n+1}/b_n$  and  $a_n, b_n > 0$  for  $n \geq N$ , then one can show that

$$\sum_{n \geq 0} a_n z^n \geq k \sum_{n \geq 0} b_n z^n + P(z), \quad (5)$$

where  $k$  is a positive constant and  $P(z)$  is a polynomial of degree  $N$ . One can use this bound to show that the odd and even series in Eq. (2) diverge faster than  $e^{\alpha z^2}$  with  $\alpha < 1/2$ , unless they contain a finite number of terms. From this property, one can derive the allowed eigenvalues for the harmonic oscillator.

In the present paper, we discuss a related problem: the Schroedinger equation in the presence of piecewise potentials that coincide with the harmonic oscillator potential for  $|x| > a$ . The analysis of this potential makes more evident the usual mistakes in the discussions of the asymptotic behavior of the wave functions, as the following (erroneous) argument shows: If  $\mathcal{E} - 1/2$  were not an integer, as the odd and even series cannot cancel each other for  $z \rightarrow +\infty$  [Eq. (4)], the wave function would not be quadratically integrable. Therefore,  $\mathcal{E} - 1/2$  must be a nonnegative integer, and the eigenvalues for the piecewise potentials would coincide with those of the harmonic oscillator, irrespective of the form of the potential for  $|x| < a$ . This is obviously nonsense. The error in the argument goes back to the assumed asymptotic behavior in Eq. (4). As we will see,  $S_{\text{even}}/S_{\text{odd}} \rightarrow \text{const}$  as  $z \rightarrow +\infty$ , for any value of  $\mathcal{E}$  such that  $\mathcal{E} - 1/2 \neq 0, 1, 2, \dots$

It is worth noting that for solving this problem it is not enough to obtain a lower bound for the series: the leading behavior of both series is needed. As this behavior is not difficult to obtain, it will be useful even when discussing the usual quantum harmonic oscillator. Moreover, when considering the radial Schroedinger equation for the hydrogen atom, one also encounters vague arguments in the analysis of the asymptotic behavior of the solutions. Our results shed light on the discussion on this and related problems.

Piecewise potentials involving the harmonic potential have been considered before by other authors.<sup>11–15</sup> In some works,<sup>11–13</sup> the harmonic part of the potential is restricted to a bounded region ( $|x| < a$  in our notation), the opposite situation of the one considered here, and therefore the discussion of the asymptotic behavior of the series Eq. (2) is not relevant there. In other works,<sup>14,15</sup> the authors consider the combination of a harmonic potential for  $x > a$  and a finite potential step for  $x < a$ . In this case, the analysis of the large- $x$  behavior of the solutions is relevant, and could be discussed using the elementary methods proposed below. Alternatively, in Ref. 14 the problem is tackled by solving the Schroedinger equation in terms of special functions, while in Ref. 15 the eigenvalue equation is solved using an integral representation method.

## II. SCHROEDINGER EQUATION WITH PIECEWISE HARMONIC POTENTIALS

Let us now consider the Schroedinger equation

$$\frac{d^2\psi}{dz^2} + (\mathcal{E} - V(z))\psi = 0, \quad (6)$$

with

$$V(z) = \begin{cases} \frac{1}{4}(z+l)^2 & z < -l, \\ f(z) & -l < z < l, \\ \frac{1}{4}(z-l)^2 & z > l, \end{cases} \quad (7)$$

where  $f(z)$  is an arbitrary function and  $l = \sqrt{2m\omega/\hbar} a$ . The potential is harmonic for  $|z| > l$  and arbitrary otherwise.

Let us first analyze the asymptotic behavior of the solutions of Eq. (6). As the potential is defined in three different regions, one can study the behavior for  $z < -l$  and  $z > l$  separately. It will be enough to analyze the asymptotic behavior in the region  $z > l$ . We introduce the notation  $y = z - l$ . Given the form of the potential, one expects that, for  $y \rightarrow +\infty$

$$\psi(y) \simeq y^\gamma e^{\beta y^2}, \quad (8)$$

for some constants  $\beta$  and  $\gamma$ . Indeed, inserting this ansatz into Eq. (6) we obtain

$$4\beta^2 - \frac{1}{4} + y^{-2}(\mathcal{E} + 2\beta(1 + 2\gamma)) + O(y^{-4}) = 0, \quad (9)$$

that is satisfied, in the limit  $y \gg 1$ , when

$$\beta^2 = \frac{1}{16} \quad \gamma = -\frac{1}{4\beta}(\mathcal{E} + 2\beta). \quad (10)$$

We conclude that the Schroedinger equation has a solution that converges at  $y \rightarrow +\infty$  ( $\beta = -1/4, \gamma = \mathcal{E} - 1/2$ ) and a linearly independent solution that diverges in the same limit ( $\beta = 1/4, \gamma = -\mathcal{E} - 1/2$ ). The analysis could be pursued systematically by assuming

$$\psi(y) \simeq y^\gamma e^{\beta y^2} \left( 1 + \frac{\gamma_1}{y} + \frac{\gamma_2}{y^2} + \dots \right), \quad (11)$$

but this will not be necessary for what follows.

In the usual discussions of the asymptotic behavior of the solutions of the harmonic oscillator, only the leading term is kept in Eq. (9). This gives  $\beta = \pm 1/4$ , and no information on  $\gamma$ .

We now propose a solution of Eq. (6) for  $y > 0$  ( $z > l$ ) of the form given in Eq. (2), with  $y$  instead of  $z$ . As we expect that the eigenvalues for the piecewise potentials will differ from those of the usual harmonic oscillator, in what follows we will assume that  $\mathcal{E} - 1/2 \neq 0, 1, 2, \dots$ . The usual eigenvalues will be obtained in the limiting case  $l \rightarrow 0$ .

The bounds in Eq. (5) on the odd and even series imply that both  $e^{-y^2/4}S_{\text{even}}(y)$  and  $e^{-y^2/4}S_{\text{odd}}(y)$  diverge as  $y \rightarrow +\infty$ . However, the existence of solutions with the asymptotic behavior given in Eq. (8) with  $\beta = -1/4$  implies that there should be a *unique choice* of  $a_1/a_0$  such that the combination

$$\psi(y) = e^{-y^2/4}[a_0S_{\text{even}}(y) + a_1S_{\text{odd}}(y)] \quad (12)$$

converges as  $y \rightarrow +\infty$ . When  $a_1/a_0 \equiv a_*$  is properly chosen, the linear combination of the two divergent series becomes convergent. It is important to remark that this should happen for any value of  $\mathcal{E}$ . The value of  $a_*$  is clearly unique, otherwise one would obtain two convergent, linearly independent solutions of the differential equation, and the divergent solutions would not exist.

In Sec. II A, we will obtain the precise value of  $a_*$ . Assuming that this value is known, it is easy to find the set of equations that determines the energy eigenvalues. We introduce the notation

$$D_{\mathcal{E}-1/2}(y) = S_{\text{even}}(y) + a_*S_{\text{odd}}(y). \quad (13)$$

In terms of this function, the quadratically integrable solution of Eq. (6) can be written as

$$\psi(z) = \begin{cases} Ae^{-(z+l)^2/4}D_{\mathcal{E}-1/2}(-(z+l)) & z < -l, \\ B\psi_1(z) + C\psi_2(z) & -l < z < l, \\ Fe^{-(z-l)^2/4}D_{\mathcal{E}-1/2}(z-l) & z > l, \end{cases} \quad (14)$$

where  $\psi_1$  and  $\psi_2$  are two linearly independent solutions in the region  $|z| < l$ , while  $A, B, C$ , and  $F$  are constants. The wavefunction  $\psi$  and its first derivative should both be continuous at  $z = \pm l$ . These four conditions and the normalization of the wavefunction determine the four constants and the allowed values of the energy.

### A. Calculation of $a_*$

From the recurrence relation Eq. (3) one can see that

$$\begin{aligned}
a_2 &= \frac{a_0(-\mathcal{E} + 1/2)}{2} = \frac{a_0(-\mathcal{E}/2 + 1/4)}{2 \times 1/2}, \\
a_4 &= \frac{a_0(-\mathcal{E} + 1/2) \times (-\mathcal{E} + 1/2 + 2)}{2 \times 3 \times 4} = \frac{a_0(-\mathcal{E}/2 + 1/4) \times (-\mathcal{E}/2 + 1/4 + 1)}{2^2 \times 1/2 \times 3/2 \times 2}, \\
a_6 &= \frac{a_0(-\mathcal{E}/2 + 1/4) \times (-\mathcal{E}/2 + 1/4 + 1) \times (-\mathcal{E}/2 + 1/4 + 2)}{2^3 \times 1/2 \times 3/2 \times 5/2 \times 2 \times 3}, \tag{15}
\end{aligned}$$

and, in general,

$$\begin{aligned}
a_{2n} &= \frac{a_0}{2^n n!} \frac{(-\mathcal{E}/2 + 1/4) \times \dots \times (-\mathcal{E}/2 + 1/4 + n - 1)}{1/2 \times 3/2 \times \dots \times (1/2 + n - 1)} \\
&= \frac{a_0}{2^n n!} \frac{\Gamma[1/2]}{\Gamma[-\mathcal{E}/2 + 1/4]} \frac{\Gamma[-\mathcal{E}/2 + 1/4 + n]}{\Gamma[1/2 + n]}, \tag{16}
\end{aligned}$$

where  $\Gamma[z]$  denotes the Gamma function. Note that in the last equality we have made repeated use of the well known identity  $\Gamma[z + 1] = z\Gamma[z]$ . Following similar steps, we can verify that

$$a_{2n+1} = \frac{a_1}{2^n n!} \frac{\Gamma[3/2]}{\Gamma[-\mathcal{E}/2 + 3/4]} \frac{\Gamma[-\mathcal{E}/2 + 3/4 + n]}{\Gamma[3/2 + n]}. \tag{17}$$

The large- $n$  behavior of the coefficients  $a_n$  can be analyzed using Stirling's approximation for the Gamma function at large arguments<sup>16</sup>

$$\Gamma[z + 1] \simeq z^z e^{-z} \sqrt{2\pi z}, \tag{18}$$

from which we obtain

$$\frac{\Gamma[n + b]}{\Gamma[n + c]} \simeq n^{b-c}. \tag{19}$$

Inserting this approximation into Eqs. (16) and (17) we obtain, for large  $n$ ,

$$a_{2n} \simeq \frac{a_0}{2^n n!} \frac{\Gamma[1/2]}{\Gamma[-\mathcal{E}/2 + 1/4]} n^{-\mathcal{E}/2 - 1/4}, \tag{20}$$

$$a_{2n+1} \simeq \frac{a_1}{2^n n!} \frac{\Gamma[3/2]}{\Gamma[-\mathcal{E}/2 + 3/4]} n^{-\mathcal{E}/2 - 3/4}. \tag{21}$$

From Eqs. (20) and (21), we see that the asymptotic behavior of  $S_{even}$  and  $S_{odd}$  can be studied by considering the series

$$S(\omega) = \sum_{n=1}^{\infty} \frac{n^{-r} \omega^n}{n!}. \tag{22}$$

Indeed, if two power series with positive coefficients  $A_n$  and  $B_n$  are such that  $A_n/B_n \rightarrow 1$  for  $n \rightarrow \infty$ , then they have the same asymptotic behavior. Hence, by virtue of Eq. (20), putting  $\omega = y^2/2$ ,  $r = \mathcal{E}/2 + 1/4$  and multiplying by  $a_0 \Gamma[1/2]/\Gamma[-\mathcal{E}/2 + 1/4]$  on both sides of Eq. (22), we see that

$$S_{even}(y) \simeq \frac{\Gamma[1/2]}{\Gamma[-\mathcal{E}/2 + 1/4]} S\left(\frac{y^2}{2}\right) \tag{23}$$

for large values of  $y$ . If, instead, we put  $r = \mathcal{E}/2 + 3/4$  and multiply by  $a_1 \Gamma[3/2]/\Gamma[-\mathcal{E}/2 + 3/4]$  on both sides of Eq. (22), we obtain

$$S_{odd}(y) \simeq \frac{y \Gamma[3/2]}{\Gamma[-\mathcal{E}/2 + 3/4]} S\left(\frac{y^2}{2}\right) \tag{24}$$

for large  $y$ .

In order to study the asymptotic behavior of  $S(\omega)$ , the key observation is that, for a fixed large value of  $\omega$ , the coefficients

$$c_n(\omega) = \frac{\omega^n}{n!}, \tag{25}$$

have, as a function of  $n$ , a peak at  $n = \omega$ . Moreover, the width of the peak is much smaller than  $\omega$ . It is an interesting exercise to verify these properties by plotting  $c_n(\omega)$  as a function of  $n$  for large values of  $\omega$ . We can prove them analytically using Stirling's approximation Eq. (18) for the factorial  $n! = \Gamma[n + 1]$ , and evaluating for  $n \simeq \omega$ . We obtain

$$n! \simeq \sqrt{2\pi\omega} e^{-n} \omega^n e^{n \ln\left(1 + \frac{n-\omega}{\omega}\right)}. \tag{26}$$

Expanding the logarithm in the exponential in powers of  $(n-\omega)/\omega$  we get

$$c_n(\omega) \simeq \frac{e^\omega}{\sqrt{2\pi\omega}} e^{-\frac{(n-\omega)^2}{2\omega}}. \tag{27}$$

Therefore, for large (fixed)  $\omega$ ,  $c_n(\omega)$  is a Gaussian function of  $n$ , with a peak at  $n = \omega$  and width  $\sqrt{\omega}$ . Thus, for the relevant values of  $n$  we can approximate  $n^{-r}$  by  $\omega^{-r}$  in  $S(\omega)$  obtaining, for large  $\omega$ ,

$$S(\omega) \simeq \omega^{-r} \sum_{n=1}^{\infty} \frac{\omega^n}{n!} \simeq \omega^{-r} e^\omega. \tag{28}$$

We present a more rigorous proof of this asymptotic behavior in the [Appendix](#).

Taking into account Eqs. (23), (24), and (28) and we obtain, for large  $y$ ,

$$S_{even}(y) \simeq \frac{\Gamma[1/2]}{\Gamma[-\mathcal{E}/2 + 1/4]} \left[\frac{y^2}{2}\right]^{-\frac{\mathcal{E}}{2} - \frac{1}{4}} e^{\frac{y^2}{2}}, \tag{29}$$

$$S_{odd}(y) \simeq \frac{\sqrt{2}\Gamma[3/2]}{\Gamma[-\mathcal{E}/2 + 3/4]} \left[\frac{y^2}{2}\right]^{-\frac{\mathcal{E}}{2} - \frac{1}{4}} e^{\frac{y^2}{2}}. \tag{30}$$

This calculation reproduces the asymptotic behavior of the solutions anticipated in Eqs. (8) and (10). Both series lead to linearly independent solutions to the Schroedinger equation

that have the same asymptotic behavior with  $\beta = +1/4$  and  $\gamma = -\mathcal{E} - 1/2$  [see Eqs. (8) and (10)].

These two linearly independent solutions of the Schroedinger equation are not quadratically integrable, and therefore physically unacceptable. However, we know that a linear combination of them should produce a solution with the adequate behavior ( $\beta = -1/4$ ). A necessary condition for this to happen is that the exponentially growing behavior of both series should cancel each other. Therefore, using Eqs. (12), (29), and (30) we obtain

$$a_* = \frac{a_1}{a_0} = -\sqrt{2} \frac{\Gamma[-\mathcal{E}/2 + 3/4]}{\Gamma[-\mathcal{E}/2 + 1/4]}. \quad (31)$$

With this result we can construct the function  $D_{\mathcal{E}-1/2}(y)$  in Eq. (13), and obtain the formal solution of the Schroedinger equation Eq. (14).

We point out, for the advanced reader, that for this particular value of  $a_*$  Eq. (12) reproduces the series expansion of the parabolic Weber function  $D_\sigma(y)$ ,<sup>14,17</sup> which is the unique solution of Eq. (6) that tends to zero as  $y \rightarrow +\infty$ .

### III. EXAMPLE: A PARTICLE IN A “BATHTUB” POTENTIAL

In order to illustrate the usefulness of the previous results, we will consider the particular case of a particle in a box bounded by harmonic walls, i.e., we will analyze the Schroedinger equation with the potential given in Eq. (7) with  $f(z) = 0$ . These so called “bathtub” potentials have been used as confining potentials for electrons in nanostructures, in particular when analyzing the quantum Hall effect.<sup>18–23</sup>

As the potential is an even function, it is convenient to take as independent solutions in the region  $-l < z < l$

$$\begin{aligned} \psi_1(z) &= \cos \sqrt{\mathcal{E}}z, \\ \psi_2(z) &= \sin \sqrt{\mathcal{E}}z, \end{aligned} \quad (32)$$

and look for solutions of the Schroedinger equation which are either even or odd. For the even solutions we take  $C = 0$  in Eq. (14) and impose continuity of the function and its first derivative at  $z = l$ . The transcendental equation that determines the energy eigenvalues is

$$\sqrt{\mathcal{E}} \tan \sqrt{\mathcal{E}}l = -\frac{D'_{\mathcal{E}-1/2}(0)}{D_{\mathcal{E}-1/2}(0)} = -a_*. \quad (33)$$

Similarly, for the odd solutions ( $B = 0$ ) the condition reads

$$\sqrt{\mathcal{E}} \cot \sqrt{\mathcal{E}}l = \frac{D'_{\mathcal{E}-1/2}(0)}{D_{\mathcal{E}-1/2}(0)} = a_*. \quad (34)$$

In the limit  $l \rightarrow 0$  one recovers the eigenvalues of the harmonic oscillator. On the one hand, for the even solutions, in this limit the condition Eq. (33) reads  $a_* = 0$ . As the Gamma function does not have zeros for real arguments, and has poles on the non-positive integers, from Eq. (31) we see that the argument of the Gamma function in the denominator must be a non-positive integer  $-n$ , and therefore  $\mathcal{E} = 2n + 1/2$ , the usual eigenvalues for even eigenfunctions. On the other hand, for the odd solutions the condition Eq. (34) is

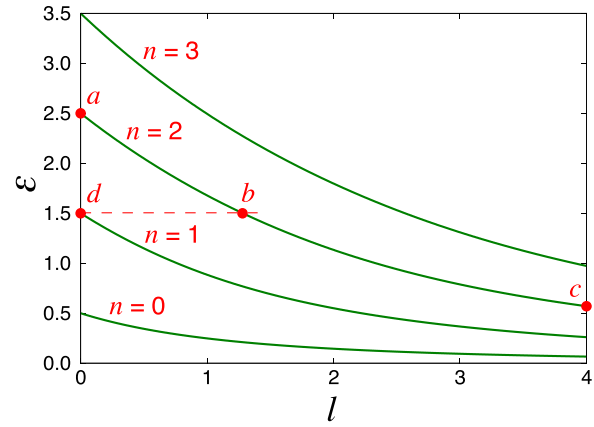


Fig. 1. Eigenvalues for the “bathtub” potential, as a function of  $l$ . According to the uncertainty principle, the eigenvalues are decreasing functions of  $l$ . The wave functions associated with the particular values (a), (b), (c), and (d) are plotted in Figs. 2 and 4.

$a_* = \infty$ , which is satisfied for  $\mathcal{E} = 2n + 1 + 1/2$ , i.e., the usual energy levels for odd wave functions.

In Fig. 1, we plot the eigenvalues of the energy  $\mathcal{E}$  as a function of  $l$ . The eigenvalues start at the harmonic oscillator values  $n + 1/2$  for  $l = 0$ , and are decreasing functions of  $l$ , as suggested by the Heisenberg uncertainty principle. In Fig. 2, we plot the wave function of the second excited state for increasing values of  $l$ . At  $l = 0$  the wave function is the usual solution for the harmonic oscillator with energy  $\mathcal{E} = 5/2$ . The wave function has two nodes for all values of  $l$ . They are located in the harmonic region for  $0 < l < 1.28$ , and in the flat region for  $l > 1.28$ . For this critical value of  $l$ , the eigenvalue of the second excited state equals  $\mathcal{E} = 3/2$ , i.e., the value of the first excited state of the usual harmonic oscillator (point (b) in Fig. 1).

An interesting property of the eigenvalues is their behavior in the limit  $l \gg 1$ . When  $a \gg \sqrt{\hbar/2m\omega}$ , the scale of variation of the harmonic potential is much shorter than the size of the flat bottom of the potential. Therefore, the harmonic walls act as infinite potential barriers, and we expect the spectrum of a particle in a box, that is,  $\mathcal{E}_n/\mathcal{E}_0 \simeq (n + 1)^2$ . This behavior is illustrated in Fig. 3.

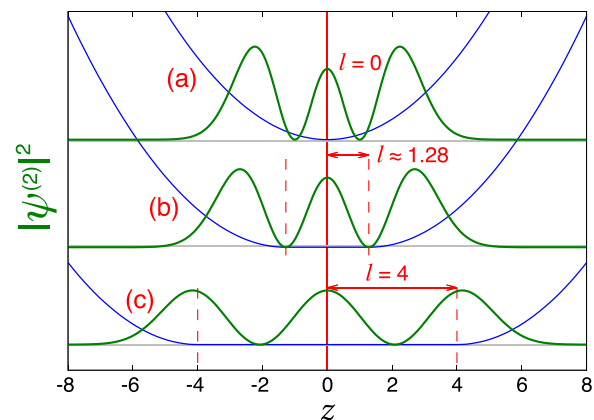


Fig. 2. Plots of the normalized wave function for the second excited state,  $\psi^{(2)}$ , for different values of  $l$ . As expected, the wave function has two nodes. Note that the nodes are located in the harmonic region for  $0 < l < 1.28$ , at  $z = l$  for  $l = 1.28$  and in the flat bottom for  $l > 1.28$ . The corresponding eigenvalues are given by the points (a), (b), and (c) in Fig. 1.



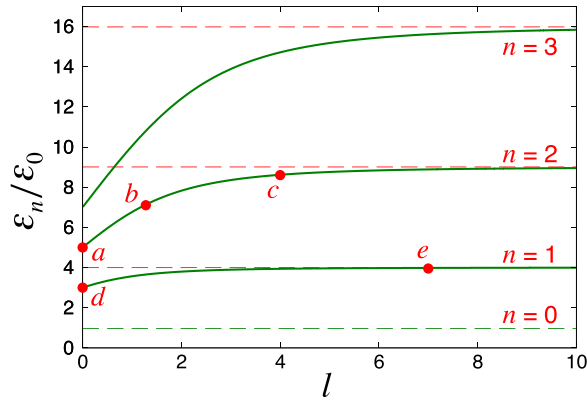


Fig. 3. Eigenvalues for the “bathtub” potential, normalized to the ground state, as a function of  $l$ . At large values of  $l$  the spectrum coincides with that of an infinite square well. The wave functions associated to the particular values (a), (b), (c), (d), and (e) are plotted in Figs. 2 and 4.

We also expect the wave functions to evolve from those of the usual harmonic oscillator at  $l=0$  to those of the infinite square well for  $l \gg 1$ . This fact is illustrated in Fig. 4, where we plotted the first excited state for different values of  $l$ . Note that for large values of  $l$  the wave function tends to zero in the harmonic region, on a spatial scale much shorter than the size of the flat bottom.

#### IV. THE HYDROGEN ATOM

The remarks about the behavior of the series for the harmonic oscillator also apply to the solutions of the Schrodinger equation for the hydrogen atom. The radial wave function is usually written as

$$\psi(\rho) = \rho^{L+1} e^{-\rho} F(\rho), \quad (35)$$

where  $\rho$  is a dimensionless radius,  $L$  is the angular momentum, and

$$F(\rho) = \sum_{n \geq 0} c_n \rho^n. \quad (36)$$

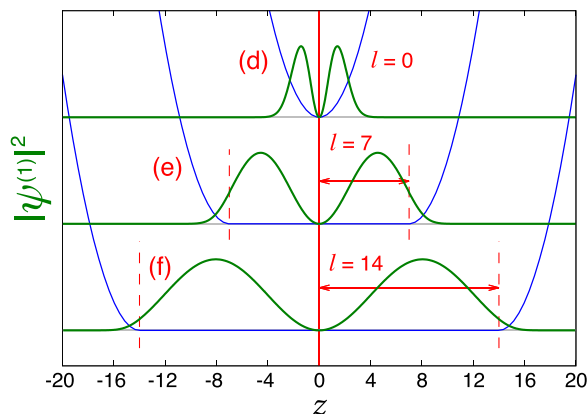


Fig. 4. Plots of the wave function for the first excited state,  $\psi^{(1)}$ , for different values of  $l$ . This wave function has only one node at  $z=0$  for all values of  $l$ . The figure illustrates the fact that the wave function for the piecewise potential tends to that of a particle in a box, and therefore vanishes in the harmonic region in the large  $l$  limit. The corresponding eigenvalues are given by the points (d) and (e) in Fig. 3. Point (f) is out of scale in Fig. 3, being at the right of point (e), on the curve  $n=1$ . For the sake of clarity, in this figure we normalized each wave function to its maximum value.

The coefficients of the power series satisfy the recurrence relation

$$c_{n+1} = \frac{(-\xi + 2L + 2 + 2n)}{(n+1)(2L + 2 + n)} c_n, \quad (37)$$

where  $\xi$  is the inverse of the (dimensionless) energy. Note that, once again, for large  $n$  we have  $c_{n+1}/c_n \simeq 2/n$ , and one would be tempted to conclude that, if the series does not have a finite number of terms,  $F(\rho) \simeq e^{2\rho}$  as  $\rho \rightarrow \infty$ . However, a more careful analysis along the lines of Secs. II–III shows that this is not the case. Indeed, the coefficients are given by

$$c_n = c_0 \frac{2^n}{n!} \frac{\Gamma(2L + 2)}{\Gamma(-\xi/2 + L + 1)} \frac{\Gamma(-\xi/2 + L + n + 1)}{\Gamma(2L + n + 2)}, \quad (38)$$

and tend to

$$c_n \simeq c_0 \frac{2^n}{n!} n^{-\xi/2 - L - 1} \quad (39)$$

for large  $n$ . Therefore

$$F(\rho) \simeq c_0 e^{2\rho} (2\rho)^{-\xi/2 - L - 1} \quad (40)$$

for large  $\rho$ . This is the correct behavior of the series that of course leads to an unacceptable wave function, unless the series has a finite number of non-vanishing terms. We leave the details for the reader. She/he could also address the problem of a particle in a piecewise Coulomb potential given by

$$V(r) = \begin{cases} -\frac{k}{R} & 0 < r < R, \\ -\frac{k}{r} & r > R, \end{cases} \quad (41)$$

following the procedure described for the piecewise harmonic oscillator.

#### V. CONCLUSIONS

We have discussed in detail the asymptotic behavior of the solutions of the Schrodinger equation with harmonic-like potentials. Following the standard approach, we looked for solutions of the form given in Eq. (2). We have shown that when the even and odd series contain an infinite number of terms, they have, up to a constant, the same divergent asymptotic behavior as  $z \rightarrow +\infty$ , contrary to previous claims in many textbooks. This is a necessary property, given that there should be a linear combination of the odd and even series that produce a solution that is convergent for  $z \rightarrow +\infty$ , for any value of  $\mathcal{E}$ .

For the usual harmonic oscillator, Eq. (2) should be the solution to the Schrodinger equation for all values of  $z$ . If we choose  $a_*$  such that the wave function converges at  $z \rightarrow +\infty$ , then it will diverge at  $z \rightarrow -\infty$  (and viceversa). Therefore, the physically acceptable solutions are those for which both series contain a finite number of terms, and  $\mathcal{E} = n + 1/2$ . However, for piecewise potentials, we can consider independent linear combinations of the even and odd series in the regions  $z < -l$  and  $z > l$ , such that  $|\psi(z)|^2$  is

integrable. The continuity conditions of the wave function and its first derivative at  $z = \pm l$  fix the allowed energy eigenvalues. We illustrated the procedure by computing the eigenvalues of a potential with a “bathtub” shape.

The main mathematical result in our discussion is the large- $\omega$  behavior of the series

$$S(\omega) = \sum_{n=1}^{\infty} \frac{n^{-r} \omega^n}{n!} \simeq \omega^{-r} e^{\omega} \quad (42)$$

that can be derived as described above and in the [Appendix](#). It can be even checked numerically by the students using MATHEMATICA or similar programs, by plotting  $S(\omega)\omega^r e^{-\omega}$  as a function of  $\omega$ , for different values of  $r$ .

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## APPENDIX: ASYMPTOTIC BEHAVIOR OF THE SERIES $S(\omega)$

In this [Appendix](#), we provide an alternative and more rigorous proof of Eq. (28), which is the main mathematical ingredient in our work. The derivation is somewhat cumbersome, but only uses elementary bounds for different series.

For simplicity, we will assume  $r > 0$  (the case  $r < 0$  can be treated using similar arguments). Let us consider

$$e^{-\omega} \omega^r S(\omega) = e^{-\omega} \sum_{n=1}^{\infty} \left(\frac{\omega}{n}\right)^r \frac{\omega^n}{n!} \quad (A1)$$

and introduce the notation

$$T(\omega, n_1, n_2) = e^{-\omega} \sum_{n=n_1}^{n_2} \left(\frac{\omega}{n}\right)^r \frac{\omega^n}{n!}. \quad (A2)$$

We would like to see that  $T(\omega, 1, \infty) \rightarrow 1$  as  $\omega \rightarrow \infty$ .

On one hand, given any  $0 < \lambda < 1$ , we split the series as

$$T(\omega, 1, \infty) = T(\omega, 1, [\lambda\omega]) + T(\omega, [\lambda\omega] + 1, \infty), \quad (A3)$$

where the brackets denote integer part. As  $\omega/n \leq \omega$ , the first term can be bounded by

$$T(\omega, 1, [\lambda\omega]) \leq e^{-\omega} \omega^r \sum_{n=1}^{[\lambda\omega]} \frac{\omega^n}{n!}. \quad (A4)$$

Noting that  $\omega^n/n!$  is an increasing function of  $n$  for  $n \leq [\omega]$ , we see that the series on the right hand side of Eq. (A4) satisfies

$$\sum_{n=1}^{[\lambda\omega]} \frac{\omega^n}{n!} \leq \sum_{n=1}^{[\lambda\omega]} \frac{\omega^{[\lambda\omega]}}{[\lambda\omega]!} = [\lambda\omega] \frac{\omega^{[\lambda\omega]}}{[\lambda\omega]!} \leq \lambda\omega \frac{\omega^{[\lambda\omega]}}{[\lambda\omega]!} \quad (A5)$$

and, hence, putting Eqs. (A4) and (A5) together we obtain  $T(\omega, 1, [\lambda\omega]) \leq \lambda e^{-\omega} \omega^{r+1} \omega^{[\lambda\omega]}/[\lambda\omega]!$ . Let us show that

$\lambda e^{-\omega} \omega^{r+1} \omega^{[\lambda\omega]}/[\lambda\omega]!$  and, hence,  $T(\omega, 1, [\lambda\omega])$ , vanishes as  $\omega \rightarrow \infty$ . Using Stirling’s approximation we see that, for large  $\omega$ ,

$$e^{-\omega} \frac{\omega^{[\lambda\omega]}}{[\lambda\omega]!} \simeq e^{-\omega} \frac{\omega^{[\lambda\omega]}}{\sqrt{2\pi[\lambda\omega]} \left(\frac{e}{[\lambda\omega]}\right)^{[\lambda\omega]}}. \quad (A6)$$

Then, observing that

$$\left(\frac{\omega}{[\lambda\omega]}\right)^{[\lambda\omega]} \leq \left(\frac{1}{\lambda}\right)^{\lambda\omega} \quad (A7)$$

and  $\sqrt{2\pi[\lambda\omega]} \simeq \sqrt{2\pi\lambda\omega}$ , we obtain

$$e^{-\omega} \frac{\omega^{[\lambda\omega]}}{[\lambda\omega]!} \leq \frac{e^{-\omega}}{\sqrt{2\pi\lambda\omega}} \left(\frac{e}{\lambda}\right)^{\lambda\omega} \quad (A8)$$

and, since  $(e/\lambda)^\lambda < e$  for  $0 < \lambda < 1$ , we deduce from Eq. (A8) that  $e^{-\omega} \omega^{[\lambda\omega]}/[\lambda\omega]!$  goes to zero exponentially as  $\omega \rightarrow \infty$ . This proves that  $\lambda e^{-\omega} \omega^{r+1} \omega^{[\lambda\omega]}/[\lambda\omega]!$  vanishes as  $\omega \rightarrow \infty$ . Therefore, the first term in Eq. (A3) also vanishes.

The second term in Eq. (A3) can be bounded by

$$T(\omega, [\lambda\omega] + 1, \infty) \leq e^{-\omega} \left(\frac{\omega}{[\lambda\omega] + 1}\right)^r \sum_{n=[\lambda\omega]+1}^{\infty} \frac{\omega^n}{n!} \quad (A9)$$

by simply noting that  $\omega/n \leq \omega/([\lambda\omega] + 1)$ . Since  $\omega/([\lambda\omega] + 1) \leq 1/\lambda$  and

$$\sum_{n=[\lambda\omega]+1}^{\infty} \frac{\omega^n}{n!} \leq e^{\omega}, \quad (A10)$$

we deduce that  $T(\omega, [\lambda\omega] + 1, \infty) \leq (1/\lambda)^r$  and, therefore, that

$$T(\omega, 1, \infty) \leq T(\omega, 1, [\lambda\omega]) + \left(\frac{1}{\lambda}\right)^r \xrightarrow{\omega \rightarrow \infty} \left(\frac{1}{\lambda}\right)^r. \quad (A11)$$

On the other hand, given any  $\sigma > 1$  we have

$$T(\omega, 1, \infty) \geq T(\omega, 1, [\sigma\omega]) \geq e^{-\omega} \left(\frac{\omega}{[\sigma\omega]}\right)^r \sum_{n=1}^{[\sigma\omega]} \frac{\omega^n}{n!}. \quad (A12)$$

We will see that  $e^{-\omega} \sum_{n=1}^{[\sigma\omega]} \omega^n/n!$  tends to unity as  $\omega \rightarrow \infty$ . Given that

$$\begin{aligned} e^{-\omega} \sum_{n=1}^{[\sigma\omega]} \frac{\omega^n}{n!} &= e^{-\omega} \left( e^{\omega} - 1 - \sum_{n=[\sigma\omega]+1}^{\infty} \frac{\omega^n}{n!} \right) \\ &= 1 - e^{-\omega} - e^{-\omega} \sum_{n=[\sigma\omega]+1}^{\infty} \frac{\omega^n}{n!}, \end{aligned} \quad (A13)$$

it suffices to show that  $e^{-\omega} \sum_{n=[\sigma\omega]+1}^{\infty} \omega^n/n!$  vanishes as  $\omega \rightarrow \infty$ . Now, since

$$\begin{aligned} \sum_{[\sigma\omega]+1}^{\infty} \frac{\omega^n}{n!} &= \frac{\omega^{[\sigma\omega]+1}}{([\sigma\omega]+1)!} \left( 1 + \frac{\omega}{[\sigma\omega]+2} \right. \\ &\quad \left. + \frac{\omega^2}{([\sigma\omega]+3)([\sigma\omega]+2)} + \dots \right) \\ &\leq \frac{\omega^{[\sigma\omega]+1}}{([\sigma\omega]+1)!} \left( 1 + \frac{\omega}{[\sigma\omega]+1} \right. \\ &\quad \left. + \frac{\omega^2}{([\sigma\omega]+1)^2} + \dots \right) \end{aligned} \quad (\text{A14})$$

and  $\omega/([\sigma\omega]+1) \leq 1/\sigma$ , we deduce

$$\begin{aligned} e^{-\omega} \sum_{[\sigma\omega]+1}^{\infty} \frac{\omega^n}{n!} &\leq e^{-\omega} \frac{\omega^{[\sigma\omega]+1}}{([\sigma\omega]+1)!} \sum_{k \geq 0} \left( \frac{1}{\sigma} \right)^k \\ &= e^{-\omega} \frac{\sigma}{\sigma-1} \frac{\omega^{[\sigma\omega]+1}}{([\sigma\omega]+1)!}. \end{aligned} \quad (\text{A15})$$

Once more, one can check that this last term vanishes as  $\omega \rightarrow \infty$ . Then, the left hand side of Eq. (A13) tends to unity as  $\omega \rightarrow \infty$  and, therefore, from Eq. (A12) we see that

$$T(\omega, 1, \infty) \geq e^{-\omega} \left( \frac{\omega}{[\sigma\omega]} \right)^r \sum_{n=1}^{[\sigma\omega]} \frac{\omega^n}{n!} \xrightarrow{\omega \rightarrow \infty} \left( \frac{1}{\sigma} \right)^r. \quad (\text{A16})$$

Now, since  $\lambda$  and  $\sigma$  were arbitrarily close to 1 (from below and above, respectively), Eqs. (A11) and (A16) imply that  $\lim_{\omega \rightarrow \infty} T(\omega, 1, \infty) = 1$ , which is the desired statement.

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