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# Solution of the quantum harmonic oscillator plus a delta-function potential at the origin: the *oddness* of its even-parity solutions

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**Abstract**

We derive the energy levels associated with the even-parity wavefunctions of the harmonic oscillator with an additional delta-function potential at the origin. Our results bring to the attention of students a non-trivial and analytical example of a modification of the usual harmonic oscillator potential, with emphasis on the modification of the boundary conditions at the origin. This problem calls the attention of the students to an inaccurate statement in quantum mechanics textbooks often found in the context of the solution of the harmonic oscillator problem.

(Some figures in this article are in colour only in the electronic version)

## 1. Introduction

Every single book on quantum mechanics gives the solution of the harmonic oscillator problem. The reasons for that are, at least, two. (i) It is a simple problem, amenable to different methods of solution, such as the Frobenius method for solving differential equations [1, 2] and the algebraic method leading to the introduction of creation and annihilation operators [3]. This problem has therefore a natural pedagogical value. (ii) The system itself has immense applications in different fields of physics and chemistry [4, 5] and it will appear time and time again in the scientific life of a physicist.

Another problem often found in quantum mechanics textbooks is the calculation of the bound state (negative energy) of the potential $V(x) = \alpha\delta(x)$, with $\alpha < 0$. The latter example is instructive for the students because it cracks down the misconception that the continuity of the wavefunction and its first derivative at an interface is the only possible boundary condition in quantum problems. In fact, for this potential, the first derivative of the wavefunction is discontinuous at $x = 0$. To see the origin of this result, let us write the Schrödinger equation as

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + \alpha\delta(x)\psi(x) = E\psi(x). \tag{1}$$

Integrating equation (1) in an infinitesimal region around $x = 0$, we obtain [3]

$$\lim_{\epsilon\to 0}\frac{d\psi(x)}{dx}\bigg|_{-\epsilon}^{+\epsilon} - \frac{2m\alpha}{\hbar^2}\psi(0) = 0 \quad\Leftrightarrow\quad \psi'_>(0) - \psi'_<(0) = \frac{2m\alpha}{\hbar^2}\psi(0), \tag{2}$$

where $\psi_{\gtrless}(x)$ are the wavefunctions on each side of the delta potential and we have used Newton's notation for derivatives where the primes over functions denote the order of the derivative of that function. It is clear from equation (2) that the first derivative of the wavefunction is discontinuous. An explicit calculation gives the eigenstate of the system in the form

$$\psi(x) = \sqrt{\kappa}\,e^{-\kappa|x|}, \tag{3}$$

which has a kink at the origin as well as a characteristic length scale given by $\kappa = m\alpha/\hbar^2$. The eigenvalue associated with the wavefunction (3) is $E = -\hbar^2\kappa^2/(2m)$. When $E > 0$, the system has only scattering states for both positive and negative values of $\alpha$.

We now superimpose a harmonic potential on the already present delta-function potential. Due to the confining harmonic potential, the new system has only bound states, no matter what is the sign of $\alpha$ and $E$. Thus, the problem we want to address is the calculation of the eigenstates and eigenvalues of the potential

$$V(x) = \frac{m}{2}\omega^2 x^2 + \alpha\delta(x). \tag{4}$$

As we will see, this problem has both trivial and non-trivial solutions. Furthermore, it allows a little excursion into the world of special functions. Indeed, special functions play a prominent role in theoretical physics, to a point that the famous *Handbook of Mathematical Functions*, by Milton Abramowitz and Irene Stegun [6], would be one of the three texts (together with the *Bible* and Shakespeare's complete works) Michal Berry would take with him to a desert island [7]. In a time where symbolic computational software is becoming more and more the source of mathematical data, we hope with this problem to show that everything we need can be found in the good old text of Milton Abramowitz and Irene Stegun [6].

In addition, this problem will call the attention of students to an inaccurate statement in quantum mechanics textbooks often found in the context of the solution of the harmonic oscillator problem. Our approach is pedagogical, in the sense that it illuminates the role of boundary conditions imposed on the even-parity wavefunctions by the $\delta$-function potential. (We note that after the submission of this paper, the work by Busch *et al* [8] was brought to our attention; see *note added* at the end of the paper.)

## 2. Solution of the harmonic oscillator with a delta function

The Hamiltonian of the system is

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{m}{2}\omega^2 x^2 + \alpha\delta(x). \tag{5}$$

Following tradition, we introduce dimensionless variables using the intrinsic length scale of the problem $a_0^2 = \hbar/(m\omega)$. Substituting $y = x/a_0$ into equation (5), we can write the Schrödinger equation as

$$\frac{d^2\psi(y)}{dy^2} + (2\epsilon - y^2)\psi(y) + 2g\delta(y)\psi(y) = 0, \tag{6}$$

where $\epsilon = ma_0^2 E/\hbar^2$ and $g = \alpha a_0 m/\hbar^2$. With $g = 0$, equation (6) is recognized as the Weber–Hermite differential equation [1]. In quantum mechanics textbooks, the solution of equation (6) with $g = 0$ proceeds by making the substitution

$$\psi(y) = \mathrm{e}^{-y^2/2} w(y). \tag{7}$$

At the same time, it is a common practice to write $2\epsilon = 2\nu + 1$, where $\nu$ is a real number. This allows us to transform equation (6) into

$$w'' - 2yw' + 2\nu w - 2g\delta(y)w = 0, \tag{8}$$

which is Hermite's differential equation when $g = 0$; a further substitution, $z = y^2$, transforms equation (8) into Kummer's equation,

$$zw'' + (b - z)w' - a\nu w = 0 \quad \text{with} \quad a = -\frac{\nu}{2} \quad \text{and} \quad b = \frac{1}{2}, \tag{9}$$

which, obviously, has two linearly independent solutions: the confluent hypergeometric functions $M(a, b, z)$ and $U(a, b, z)$; these functions are also known as Kummer's functions (the latter solution is sometimes referred to as Tricomi's function)[1]. Thus, the general solution of equation (9) is

$$w(z) = A_\nu\, M\left(-\frac{\nu}{2}, \frac{1}{2}, z\right) + B_\nu\, U\left(-\frac{\nu}{2}, \frac{1}{2}, z\right), \tag{10}$$

where $A_\nu$ and $B_\nu$ are arbitrary complex constants and $\nu$ is an arbitrary real number. The $U(-\frac{\nu}{2}, \frac{1}{2}, z)$ function can also be written in terms of the functions $M(a, b, z)$ as [9(a)]

$$U\left(\frac{\nu}{2}, \frac{1}{2}, z\right) = \pi \left\{ \frac{M\left(-\frac{\nu}{2}, \frac{1}{2}, z\right)}{\Gamma\left(\frac{1}{2}\right)\Gamma\left(\frac{1}{2} - \frac{\nu}{2}\right)} - \sqrt{z}\frac{M\left(\frac{1}{2} - \frac{\nu}{2}, \frac{3}{2}, z\right)}{\Gamma\left(\frac{3}{2}\right)\Gamma\left(-\frac{\nu}{2}\right)} \right\}. \tag{11}$$

It is important to note that equation (11) is not a linear combination of two $M(a, b, z)$ functions. Using equation (11), it is possible to show that if $\nu$ is either zero or a positive integer number (denoted by $n$), the solution in equation (10) can be put in the following form ($z > 0$):[2]

$$w(z) \propto \begin{cases} M\left(-\frac{n}{2}, \frac{1}{2}, z\right) & \text{for } n \text{ even} \\ \sqrt{z}\, M\left(\frac{1}{2} - \frac{n}{2}, \frac{3}{2}, z\right) & \text{for } n \text{ odd,} \end{cases} \tag{12}$$

or more compactly [9(b), (c)], it can be written as $w(z) \propto H_n(\sqrt{z})$, with $H_n(z)$ the Hermite polynomial of order $n$; furthermore the product $w(z)\mathrm{e}^{-|z|}$ converges for all $z$. Then, the full wavefunction has the usual form

$$\psi_n(y) \propto \mathrm{e}^{-y^2/2} H_n(y),$$

with the corresponding eigenvalues being $\epsilon = n + \frac{1}{2}$. What we have detailed above condenses the typical solution of the quantum harmonic oscillator using special functions.

We now move to the solution of the quantum harmonic oscillator with a $\delta$-function potential at the origin. To that end, we have to review a few properties of the $M(a, b, z)$ functions. For non-integer values of $a$ and $b$, the $M(a, b, z)$ function is a convergent series for all finite given $z$ [9(a)], but diverges for $z \to +\infty$ as [9(d)]

$$M(a, b, z) = \frac{\Gamma(b)}{\Gamma(a)} \mathrm{e}^z z^{a-b} [1 + O(|z|^{-1})]. \tag{13}$$

[1] These functions may also be referred to as the confluent hypergeometric functions of the first and second kind, with the notation $M(a, b, z) = {}_1F_1(a; b; z)$ and $U(a, b, z) = z_2^{-a} F_0(a; 1 + a - b; -1/z)$. All these notations can be found when using computational methods and software.

[2] This is easy to see from equation (11) recalling that the Gamma function diverges at negative integer values.

In terms of the original variable $y^2$, function (13) diverges as $\mathrm{e}^{y^2}$, which implies that $\psi(y)$ also diverges at infinity as $\mathrm{e}^{y^2/2}$. Thus, $\psi(y)$ is not, in general, an acceptable wavefunction.

We noted in the introduction to this paper that it is many times referred to (erroneously) in most standard textbooks on quantum mechanics that the only mathematical solutions of the harmonic oscillator differential equation that do not blow up when $y \to +\infty$ are those having $\nu$ either zero or a positive integer.

On the contrary, however, the function $U(-\frac{\nu}{2}, \frac{1}{2}, y^2)$ with a non-integer $\nu$ does not blow up as $\mathrm{e}^{y^2}$ when $y \to +\infty$. Indeed, it is easy to see (using equations (11) and (13)) that $U(-\nu/2, 1/2, y^2) \to y^\nu$ [9(e)] as $y \to +\infty$. Thus, the function

$$\psi_\nu(y) = A\mathrm{e}^{-\frac{1}{2}y^2}\, U\left(-\frac{\nu}{2}, \frac{1}{2}, y^2\right) \tag{14}$$

could in principle be an acceptable wavefunction for any value of $\nu$, since it is both an even-parity function of $y$ and square integrable (therefore normalizable). Why is it then that this solution has been cast away from textbooks? The weaker answer would be because it does not provide quantized energy values, which are known to exist in any confined quantum system. The stronger answer is however that the function $\psi_\nu(y)$ violates the boundary condition $\psi'_<(0) = \psi'_>(0)$ for any non-integer $\nu$, which must be obeyed by the even-parity wavefunctions $\psi(y)$ when $g = 0$. We are now about to see that $\psi'_\nu(0^+) = -\psi'_\nu(0^-)$. It is the latter property of $\psi_\nu(y)$ which allows the solution of the quantum problem (8) with finite $g$.

We have now gathered all the information needed to find the solutions of the eigenvalue problem (8). Since Hamiltonian (5) is invariant over the parity transformation $x \to x$, their eigenstates $\psi_g(y)$ are either even- or odd-parity states. In the case of odd states, we have $\psi_g(0) = 0$ and therefore they do not see the presence of the delta function at the origin. Thus, the odd-parity wavefunctions $\psi_g^{\mathrm{odd}}(y)$ are the states $\psi_n(y)$ of the ordinary harmonic oscillator, with $\nu = n = 1, 3, 5, \ldots$, and the eigenvalues are $\epsilon = n + \frac{1}{2}$. To the latter result, we recall the 'trivial solution' of eigenproblem (8).

The solution of the even-parity eigenfunctions $\psi_g^{\mathrm{even}}(y)$ is not as simple, since these states feel the presence of the delta function at the origin. We need to find now the boundary condition the function $w(y)$ must obey at the origin. Proceeding as we did in the introductory section, we integrate equation (8) around $y = 0$ obtaining

$$w'_>(0^+) - w'_<(0^-) = 2gw(0). \tag{15}$$

Equation (15) enables us to find the quantized energies of the even-parity eigenstates we are seeking. Thus, the correct wavefunction for $\psi_g^{\mathrm{even}}(y)$ is $\psi_\nu(y)$ and not $\psi_n(y)$ with $n = 0, 2, 4, \ldots$, as in the case $g = 0$, for the latter wavefunction violates the boundary condition (15). Using the results [9(f)] [3]

$$\lim_{x\to 0^+} U(-\nu/2, 1/2, y^2) = \frac{\sqrt{\pi}}{\Gamma(1/2 - \nu/2)}, \tag{16}$$

$$\lim_{x\to 0^+} U'(-\nu/2, 1/2, y^2) = \frac{\nu\sqrt{\pi}}{\Gamma(1 - \nu/2)}, \tag{17}$$

the eigenvalues associated with even-parity eigenstates of equation (6) are given by the numerical solution of the transcendent equation

$$F(\nu) \equiv \nu - g\frac{\Gamma(1 - \nu/2)}{\Gamma(1/2 - \nu/2)} = 0, \tag{18}$$

[3] Here, the second identity can be derived from the first one using the fact that [9(g)] $U'(a, b, z) = -aU(a+1, b+1, z)$.

**Table 1.** Eigenvalues $\nu$ associated with the even-parity eigenstates $\psi_\nu(y)$ for several values of $g$; the leftmost column corresponds to the case where $g \to 0$, which coincides with the harmonic oscillator even-parity eigenvalues; the ensuing columns stand for $g = \pm 0.25$, $g = \pm 1.0$, $g = \pm 2.5$ and $g = \pm 5.0$. In between each pair of eigenvalues, we also have the states associated with the odd-parity eigenstates, which have eigenvalues $\nu = 1, 3, 5, 7, \ldots$. The associated eigenenergies are given by $\epsilon_\nu = \nu + \frac{1}{2}$.

| $g \to 0$ | −0.25 | 0.25 | −1.0 | 1.0 | −2.5 | 2.5 | −5.0 | 5.0 |
|---|---|---|---|---|---|---|---|---|
| 0.0 | −0.1557 | 0.1281 | −0.8424 | 0.3927 | −3.5865 | 0.6434 | −12.9900 | 0.7961 |
| 2.0 | 1.9288 | 2.0693 | 1.7208 | 2.2546 | 1.4285 | 2.5042 | 1.2305 | 2.7003 |
| 4.0 | 3.9469 | 4.0525 | 3.7912 | 4.2002 | 3.5420 | 4.4274 | 3.3227 | 4.6364 |
| 6.0 | 5.9558 | 6.0439 | 5.8258 | 6.1699 | 5.6051 | 6.3772 | 5.3833 | 6.5887 |
| 8.0 | 7.9614 | 8.0384 | 7.8473 | 8.1501 | 7.6473 | 8.3412 | 7.4285 | 8.5509 |

which follows from the boundary condition (15). In figure 1, we give the graphical solution of equation (18) for $g = \pm 0.25$, $g = \pm 1.0$, $g = \pm 2.5$ and $g = \pm 5.0$, and in table 1, the corresponding numerical values of $\nu$, for the first five even-eigenstates. As expected, the effect of the potential is to shift the eigenenergies of the even-states of the ordinary harmonic oscillator up or down in energy for positive and negative values of $g$, respectively. This effect is stronger for the low-lying eigenvalues (as we can anticipate from perturbation theory) and shifts the eigenenergies of the states $\psi_\nu(x)$ towards those of their lower or higher neighbouring odd states, depending on the signal of $g$. This behaviour is plotted in figure 2. In the problem we are dealing with, and contrary to the simple case of the ordinary harmonic oscillator, if $g < 0$, there is also a negative-energy eigenvalue, as we could have anticipated from the solution of the attractive $\delta$-function potential we have described in the introduction to this paper. The absolute value of this negative energy state increases with the strength of the $\delta$-function potential and, in the limit $g \to -\infty$, the confinement imposed by the harmonic potential becomes irrelevant and the wavefunction transforms into the bound state given by equation (3) and with the same eigenenergy. Indeed, using Stirling's formula [9(h)], it is easy to prove that as $z \to \infty$, $\Gamma\left(z + \frac{1}{2}\right)/\Gamma(z) \to \sqrt{z}$. For $z = 1 + \frac{1}{2}|\nu|$, this implies that as $g \to -\infty$, $g \sim \sqrt{2|\nu|}$. Since $E \sim -|\nu|\hbar\omega$[4], the former result implies that

$$E_\nu = -g^2\frac{1}{2}\hbar\omega = -\frac{\alpha^2 m}{2\hbar^2},$$

which is the energy value we have obtained before for the simple case of an isolated attractive $\delta$-function potential.

Finally, in figure 3 we plot in solid lines $|\psi_n(y)|^2$ as a function of $y$ for $n = 1, 2, 3$. In panels (a), (b) and (c) of the same figure, we also plot, in dashed lines, $|\psi_n(y)|^2$ for the wavefunctions that would correspond to the harmonic oscillator with $n = 2$ for different positive and negative values of $g$. As $g$ increases in positive (negative) values, the corresponding value of $\nu$ approaches $\nu = 3$ ($\nu = 2$) making the absolute square of the wavefunction, $|\psi_\nu(x)|^2$, look like the absolute square of the wavefunction of its odd-parity state neighbour, $|\psi_{n\pm 1}(x)|^2$. This does not mean however that the two types of wavefunctions are the same, since they refer to orthogonal eigenstates. To make this point evident, we plot both types of states in panel (d) of figure 3.

The behaviour $\psi_\nu'(0^+) \neq 0$ (the number of nodes defines the order of the state) is clear from figure 3. When $g \gg 1$, pairs of states (odd and even) of the harmonic oscillator with a

[4] Note that here, the harmonic oscillator frequency appears just as a by-pass between the $\alpha$ and $g$ coupling constants: at the end, the harmonic potential, too shallow compared with the delta, plays no role in obtaining the result.

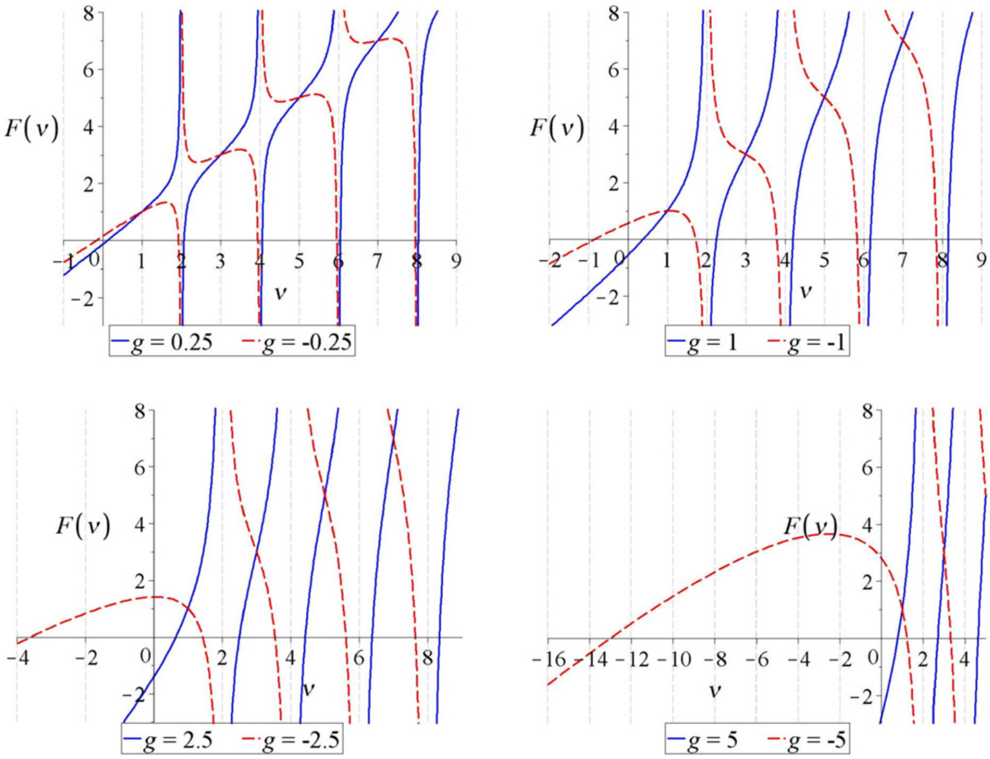


**Figure 1.** Graphical solution of equation (18), for several positive and negative values of $g$. The numerical values of $\nu$ are given in table 1. The eigenvalues for the energy $E_\nu$ are given by $\nu + \frac{1}{2}$ with $\nu$ the intercepts of the graphs with the $x$-axis (the dashed lines refer to negative $g$, whereas the solid lines refer to positive $g$).

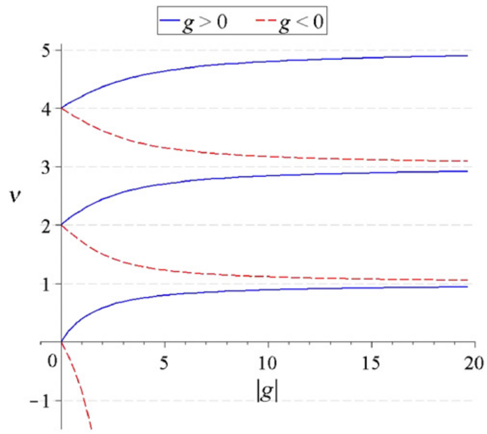


**Figure 2.** Graphical solution of equation (18), for several positive and negative values of $g$. The numerical values of $\nu$ are given in table 1.

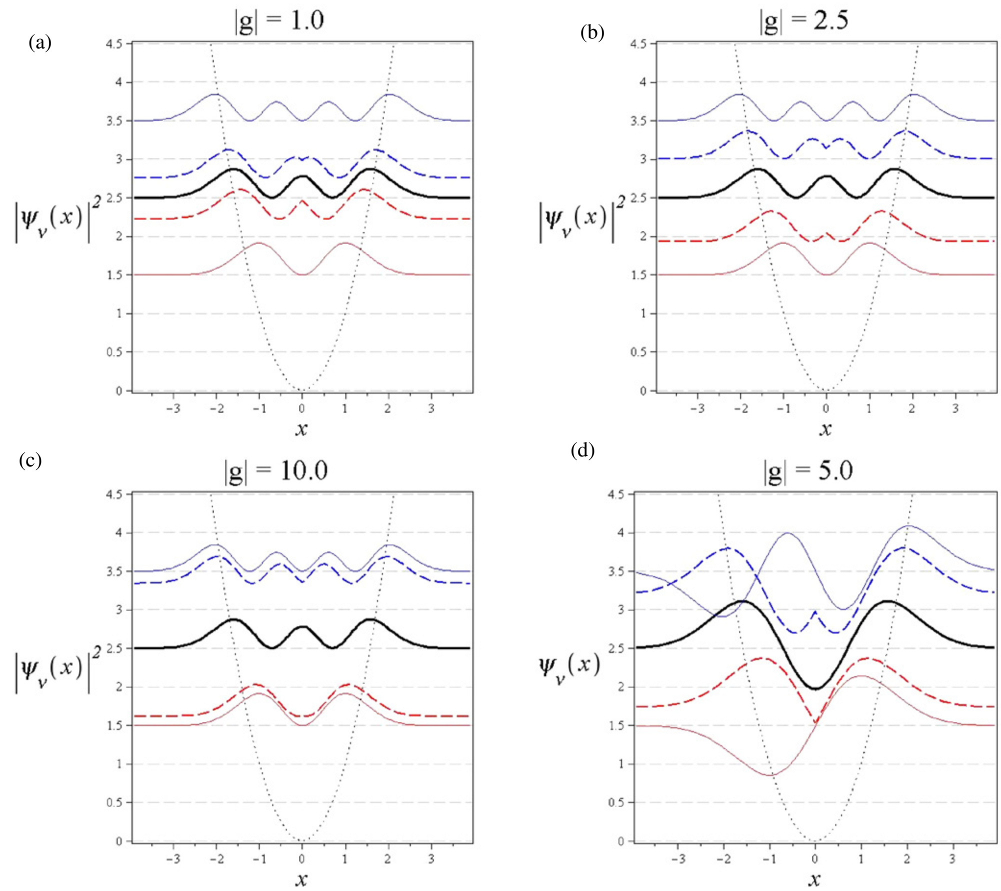


**Figure 3.** Panels (a), (b) and (c): absolute square values of the wavefunctions of the harmonic oscillator (solid lines) for (from top to bottom) $\nu = n = 3, 2, 1$ (plotted, respectively, in blue, black and red) and for $\psi_\nu(x)$ (dashed lines) with $\nu$ corresponding to values of $g$ that vary from 1 to 10, for positive and negative values (top and bottom curves, respectively). These plots show that the $|\psi_\nu(x)|^2$ curves approach the neighbouring odd states. However, as is shown in panel (d), the wavefunctions are quite different since the $\psi_\nu(x)$ are symmetrical with respect to $x$, presenting always a kink at $x = 0$.

delta function become quasi-degenerate. Indeed, in this regime the dip of the wavefunction $\psi_\nu(y)$ at $y = 0$ approaches zero, but looking at figure 3 it is seen by the naked eye that the two functions are orthogonal (one is even and the other is odd; this is not self-evident from the density probability graphs). The enhancement of the curvature of the wavefunction around $y = 0$ leads to an increase in the kinetic energy and therefore to an increase in the energy of the even-parity eigenstates.

## 3. Conclusions

We have discussed the solution of the Schrödinger equation for the one-dimensional harmonic potential with a Dirac delta function at the origin. The odd-parity eigenstates are given by the wavefunctions of the ordinary harmonic oscillator. This is obvious since the states of the latter system are zero at the origin and therefore do not feel the presence of the delta function. For the even-parity states, the solution is non-trivial. We have shown the existence of a solution of the differential equation of the harmonic oscillator that does not blow up at infinity as $e^{x^2/2}$ for non-integer values of $\nu$. As is well known, this solution is never mentioned in quantum mechanics textbooks for a good reason, but unfortunately that reason is, as far as we know, never discussed. Here we have shown that the reason lies in the fact that its derivative at $x = 0$ is finite, violating the boundary conditions imposed on the simple harmonic oscillator problem, that is, without the $\delta$-function at the origin. Nevertheless, the wavefunction (14) is the one we need for solving problem (8). In our work, we have computed the eigenvalues and eigenfunctions of the even-parity states and made, at the same time, a little excursion into the famous *Handbook of Mathematical Functions* [6].

*Note added.* After the submission of this paper, the work by Busch et al [8] was brought to our attention; the latter work elaborates on top of another paper by Janev and Marić [10] and, although focused on the three-dimensional harmonic oscillator with a delta function at the origin, one of the figures in [8] (figure 2) has the same information as our figure 2, albeit presented in a different form. Furthermore, the energy eigenvalues of the zero angular momentum states are given by an equation identical to our equation (18) but with $1/2$ replaced by $3/2$ (for obvious reasons).

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