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# On the harmonic oscillator inside an infinite potential well

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The exact solution to Schrödinger's equation for a three-dimensional harmonic oscillator confined by two impenetrable walls is presented. The energy levels of this system are obtained as a function of wall separation as well as distance of the center of the oscillator to the walls. The force exerted by the walls on the oscillator is also evaluated, showing a classical behavior.

## I. INTRODUCTION

The harmonic oscillator is perhaps one of the simplest systems that has been extensively studied both classically as well as quantically. At the undergraduate level, the student learns that the quantum oscillator problem allows for exact solutions to Schrödinger's equation, providing us with a complete set of basis functions useful in the treatment of a great variety of problems in modern physics.[1] Being one of the few exactly solvable problems in quantum physics, we consider it instructive to introduce the student to the properties of bounded quantum systems by solving Schrödinger's equation for a three-dimensional harmonic oscillator confined within two infinite potential walls. In passing, we should mention that the study of bounded quantum systems has become increasingly important in recent years, mainly to understand the behavior of real systems, such as atoms under high pressure, electrons trapped in vacancies of crystals, tunneling of electrons and electron–hole pairs through multilayered crystalline structures, etc.

For clarity of presentation, we have divided this article into three sections. Section II deals with the mathematical details concerning the solution of Schrödinger's equation in cylindrical coordinates for the radial and angular parts. The eigenfunctions and eigenvalues for this part of the problem are explicitly obtained. In Sec. III the wavefunction and eigenvalues associated with the $z$ dependence of the wave equation are found. This part of the total wavefunction contains the information on the effect of the confinement on the oscillator states. In this section we also evaluate the force exerted by the walls on the oscillator by means of the Hellmann–Feynman theorem. Finally, in Sec. IV, a discussion of the results is presented.

## II. SEPARATION OF SCHRÖDINGER'S EQUATION

Let us assume a three-dimensional harmonic oscillator bounded by two impenetrable walls, as depicted in Fig. 1. The boundary condition makes it difficult to treat the problem in spherical coordinates, as would be the case for the free-oscillator. Making use of cylindrical coordinates ($\rho$, $\varphi$, $z$), Schrödiner's equation may be written as

$$[(-\hbar^2/2M)\nabla^2 + V(\rho,z) - E]\psi(\rho,\varphi,z) = 0, \quad (1)$$

where

$$V(\rho,z) = \begin{cases} (K/2)[\rho^2 + (z-a)^2] & (0<z<d), \\ \infty & (\text{otherwise}), \end{cases} \quad (2a)$$

where $d$ is the distance between the walls and $a$ is the position of the center of the oscillator well relative to one of the walls (see Fig. 1). The Laplacian operator in Eq. (1) in cylindrical coordinates reads explicitly as

$$\nabla^2 \equiv \frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\partial\frac{\partial}{\partial\rho}\right) + \frac{1}{\rho^2}\frac{\partial^2}{\partial\varphi^2} + \frac{\partial^2}{\partial z^2}. \quad (2b)$$

Setting $M = \hbar = K = 1$ and writing $\psi(\rho,\varphi,z)$ as the product:

$$\psi(\rho,\varphi,z) = R(\rho)F(\varphi)G(z) \quad (2c)$$

after separating the variables, the following set of equations is obtained:

$$R''(\rho) + \rho^{-1}R'(\rho) + (2E_1 - m^2/\rho^2 - \rho^2)R(\rho) = 0, \quad (3)$$

$$F''(\varphi) + m^2F(\varphi) = 0, \quad (4)$$

$$G''(z) + [2E_2 - (z-a)^2]G(z) = 0, \quad (5a)$$

where $E_1$, $E_2$, and $m$ are the separation constants with the requirement that the total energy $E$ be given as

$$E = E_1 + E_2. \quad (5b)$$

The primes in Eqs. (3)–(5) indicate differentiation with respect to the argument of the corresponding function.

Solution of Eq. (4) immediately leads to

$$F(\varphi) = (2\pi)^{-1/2}\exp(im\varphi), \quad (6)$$

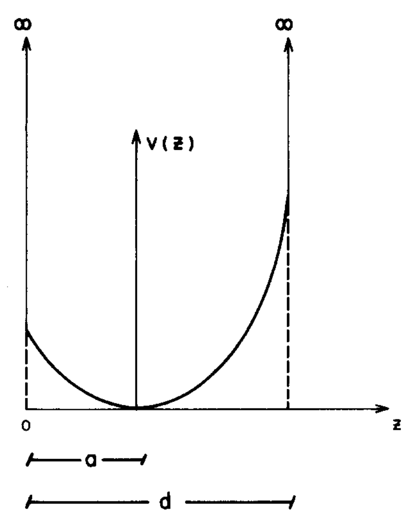


Fig. 1. Potential energy curve for an harmonic oscillator between two infinite potential walls. Only the $z$ dependence is drawn.

  

where the normalization factor has been obtained through the periodicity requirement $F(\varphi) = F(\varphi + 2\pi)$, characteristic of the azimuthal solution. The quantity $m$ in Eq. (6) is recognized as the magnetic quantum number and is restricted to the values $m = 0, \pm 1, \pm 2, \ldots$ .

In order to solve Eq. (3), we first write the radial function as:

$$R(\rho) = w^{-1/2} H(w), \tag{7}$$

where we have defined $w = \rho^2$. After introducing $R(\rho)$ as given by Eq. (7) into Eq. (3), it may be easily shown that $H(w)$ satisfies the equation

$$H''(w) + [-\tfrac{1}{4} + (E_1/2w) + (1 - m^2)/(4w^2)]H(w) = 0 . \tag{8}$$

This is precisely Whittaker's equation, whose solution may be expressed as:[2]

$$H(w) = D \exp(-w/2) w^{\mu + 1/2} M(\mu - \epsilon + \tfrac{1}{2}, 2\mu + 1, w) , \tag{9}$$

where $\epsilon = E_1/2$, $\mu = |m|/2$, and $M(\alpha,\beta,w)$ is the Kummer function[2] with $\alpha = \mu - \epsilon + \frac{1}{2}$, $\beta = 2\mu + 1$, and $D$ is a normalization constant.

To guarantee proper behavior of $H(w)$ as $w \to \infty$, one must have

$$\mu - \epsilon + \tfrac{1}{2} = -n = (|m| - E_1 + 1)/2 \quad (n = 0,1,2,\ldots) , \tag{10}$$

therefore, the energy $E_1$ is given as

$$E_1 = 2n + |m| + 1. \tag{11}$$

Substituting Eqs. (10)–(11) into Eq. (9) yields the following relation:

$$H(w) = D\,[n!/|m'|!(|m| + n)!] \exp(-w/2) \times w^{(|m|+1)/2} L_n^{|m|}(w) , \tag{12}$$

where $L_n^{|m|}(w)$ corresponds to an associated Laguerre polynomial. Returning to the original variable $\rho$, the normalized radial wavefunction results as

$$R_{nm}(\rho) = [2n!/(|m| + n)!]^{1/2} \times \exp(-\rho^2/2)\rho^{|m|} L_n^{|m|}(\rho^2) . \tag{13}$$

## III. SOLUTION OF THE $z$ EQUATION

Due to the boundary conditions, it is clear that the solution of Eq. (5) will contain the relevant information on the effect of confinement on the energy levels of the system. Let us define the auxiliary variable $y = \sqrt{2}(z - a)$. Equation (5) may then be written as

$$G''(y) - (y^2/4 - E_2)G(y) = 0 . \tag{14}$$

This equation is satisfied by the parabolic cylinder functions[2]: $U(-E_2, y)$ and $U(-E_2, -y)$. Therefore, the most general solution will be

$$G(y) = AU(-E_2, y) + BU(-E_2, -y) , \tag{15}$$

with $A$ and $B$ two constants to be determined by imposing the boundary conditions at $z = 0$ ($y = -a\sqrt{2}$) and $z = d$ [$y = \sqrt{2}(d - a)$],

$$G(-a\sqrt{2}) = G[\sqrt{2}(d - a)] = 0 , \tag{16a}$$

plus the normalization condition

$$\int_0^d G^2(z)dz = \frac{1}{\sqrt{2}} \int_{-a\sqrt{2}}^{\sqrt{2}(d-a)} G^2(y)dy = 1 . \tag{16b}$$

Using Eqs. (15) and (16), we obtain the following set of equations:

$$AU(-E_2, -a\sqrt{2}) + BU(-E_2, a\sqrt{2}) = 0, \tag{17}$$

$$AU[-E_2, \sqrt{2}(d - a)] + BU[-E_2, \sqrt{2}(a - d)] = 0. \tag{18}$$

A nontrivial solution to Eqs. (17) and (18) exists only if the secular determinant is zero, i.e.,

$$U(-E_2, -a\sqrt{2})U[-E_2, \sqrt{2}(a - d)] - U(-E_2, a\sqrt{2})U[-E_2, \sqrt{2}(d - a)] = 0 . \tag{19}$$

This last equation furnishes the quantization condition that allows us to find $E_2$ as a function of the distance $d$ between the walls and the position $a$ of the oscillator center relative to one of the walls.

Denoting by $E_2^{(s)}(a,d)$ the $s$th root of Eq. (19), with $E_2^{(1)} < E_2^{(2)} < E_2^{(3)} \cdots$, the total energy of the system then becomes

$$E_{nms} = 2n + |m| + E_2^{(s)}(a,d) + 1 , \tag{20}$$

where $n = 0,1,2,\ldots$; $m = 0, \pm 1, \pm 2, \ldots$, and $s = 1,2,3,\ldots$ .

Note that, just as in the case of the free-oscillator, an accidental degeneracy is observed. For a given value of $s$, we have manifold of values for $n$ and $m$, yielding the same result for $2n + |m| + 1$. For instance, $n = 1$, $|m| = 0$ ($s$ state), and $n = 0$, $|m| = 2$ ($d$ state) give the same energy for fixed $s$. Also, as expected, the ground state is nondegenerate.

Before analyzing the results of the calculations indicated above, it is interesting to evaluate the force exerted by the walls on the oscillator. This may be done through use the Hellmann–Feynman theorem,[3]

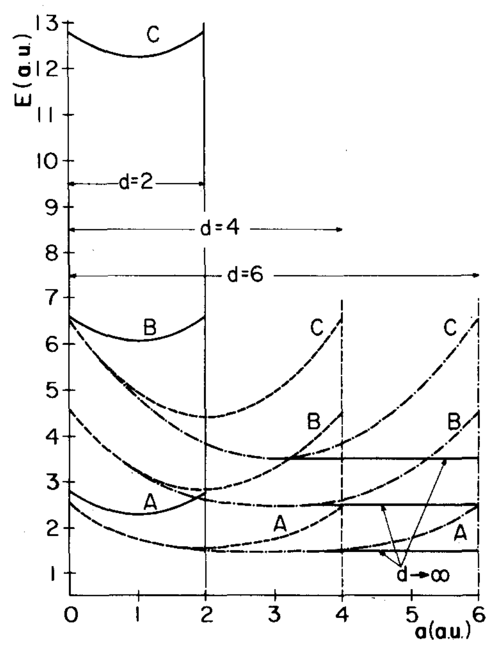


Fig. 2. Ground state ($A$), and first two excited states ($B$) and ($C$) for different wall separations ($d$) as a function of relative position ($a$) of the oscillator center from one of walls (see text).

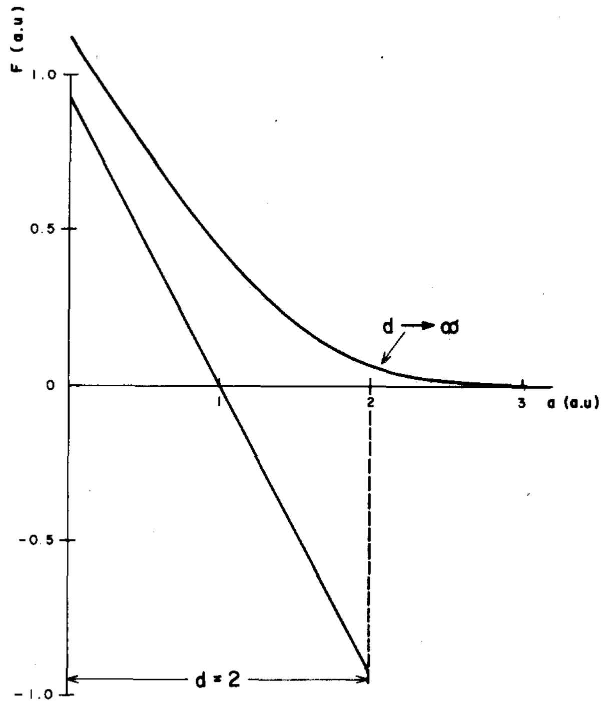


Fig. 3. Force exerted by the walls on the oscillator calculated according to Eq. (21) as a function of parameter ($a$) for $d = 2$ and $d = \infty$.

$$F_e = \frac{-\partial E_{gr}}{\partial a} = \frac{-\partial E_{001}}{\partial a} = \left\langle \psi \left| \frac{\partial V}{\partial a} \right| \psi \right\rangle$$
$$= \int_0^\infty \int_0^{2\pi} \int_0^d (z-a) G^2(z) R^2(\rho) F^2(\varphi) \rho \, d\rho \, d\varphi \, dz$$
$$= \frac{1}{2} \int_{-a\sqrt{2}}^{\sqrt{2}(d-a)} y G^2(y) dy, \qquad (21)$$

with $G(y)$ as defined by Eq. (15).

## IV. RESULTS AND DISCUSSION

The roots of Eq. (19) have been found numerically for different values of the parameters $a$ and $d$ with a precision of $10^{-6}$. Figure 2 shows the values of $E_{nms}$ for the ground state ($E_{001}$) and the first two excited states ($E_{002}$, $E_{003}$), as a function of $a$ and for $d = 2,4$, and 6, respectively. For clarity of presentation, we have labeled the curves for each value of $d$ by $A$, $B$, and $C$, indicating $E_{001}$, $E_{002}$, and $E_{003}$, respectively.

We first note the symmetry shown by the energy curves around $a = d/2$ for all the states. This is not surprising, due to the symmetry of the problem. Note also the shift of the energy levels toward higher values as the distance between the walls is reduced. This energy shift is larger for the excited states, showing a slower tendency to the unperturbed situation as one of the walls is taken to infinity. In fact, in the latter case, the problem is reduced to that of a three-dimensional oscillator in front of a wall. As $a \to 0$ and $d \to \infty$, $U(-E,y)$ approaches the Hermite polynomial $H_s(y)$ and $E_s \to s + 1/2 (s = 1,3,5,...)$. Hence, according to Eq. (20), $E_{nms} \to 2n + |m| + s + 3/2$; i.e., only the odd states will satisfy the bundary condition. This behavior appears due to the lack of nodes of the even $y$ functions at $y = a = 0$. Conversely, if $a,d \to \infty$, we recover the energy spectrum of the free-oscillator, as expected.

With regard to the force on the oscillator, Fig. 3 shows the corresponding values obtained through Eq. (21). We observe that the force is zero for $a = d/2$, which means that the two walls are exerting equal and opposite forces at the center. The oscillator will bounce back and forth between the walls, driven by a restoring force proportional to its displacement relative to the central region of confinement. This is just what we would expect classically, too. When one of the walls is brought to infinity, we see that for distances to the wall $a > 3$, the oscillator is practically unperturbed. Examination of Fig. 2 supports this observation.

We hope that, for the undergraduate and graduate student, the solution to this problem will shed some light on the properties of confined quantum systems. We have shown that Schrödinger's equation is exactly solvable for a three-dimensional harmonic oscillator confined within two infinite potential walls. As in the case of the free-oscillator, the basis set spanned by the wavefunctions found in this article [Eqs. (6), (13), and (15)] could help us to treat more complicated systems under the same confinement conditions.

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[1]See, for instance, M. Moshinsky, *The Harmonic Oscillator in Modern Physics: From Atoms to Quarks* (Gordon and Breach, New York, 1969) and references therein.

[2]M. Abramowitz and I. A. Stegun, *Handbook of Mathematical Functions* (Dover, New York, 1972).

[3]I. N. Levine, *Quantum Chemistry* (Allyn and Bacon, Boston, 1974), 2nd ed.