

Harmonic oscillator wave functions and probability density plots using spreadsheets



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Abstract

Students who are studying quantum physics often find the graphing of wave functions and probability density curves difficult and time consuming. The common spreadsheet of Microsoft ExcelTM is an excellent tool for the teaching of physics. It makes it easy to construct illustrative examples, to manipulate variables, and to plot results in graphical form. In this article efforts have been made to generate spreadsheet for wave functions and probability density curves of quantum harmonic oscillator. A dynamic spreadsheet presentation can help students better appreciate how the graphs are produced from the relationship between the variables.

Keywords: Spreadsheets, Physics Education, Harmonic oscillator, Correspondance principle, Wave functions.

Resumen

Los estudiantes que están estudiando física cuántica a menudo encuentran difícil la graficación de curvas de funciones de onda y de densidad de probabilidad y les lleva tiempo. La hoja de cálculo más comunes de Microsoft ExcelTM es una excelente herramienta para la enseñanza de la física. Esto hace que sea fácil construir ejemplos ilustrativos, para manipular las variables, y para trazar los resultados en forma gráfica. En este artículo se han hecho esfuerzos para generar hojas de cálculo de funciones de onda y de curvas de densidad de probabilidad del oscilador armónico cuántico. Una presentación dinámica de la hoja de cálculo puede ayudar a los estudiantes a apreciar mejor cómo son producidos los gráficos a partir de la relación entre las variables.

Palabras clave: Hojas de cálculo, Educación en Física, Oscilador armónico, Principio de Correspondencia, Funciones de onda.

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I. INTRODUCTION

In the process of teaching and learning of physics mathematical modelling is a central part. The teaching of physical facts and theories should be subsidiary to teaching the principles and techniques of mathematical modeling. Such modelling provides the students a valuable experience that shows how the mathematical concepts are useful for a better understanding of the physical world and focuses on conceptual reconstructions of physical reality [1].

The advantage of using a spreadsheet teaching-learning process is that the programming is streamlined and less time is needed to enter the necessary code. The strong features of spreadsheet are their cell based structure and the simple interface that is easy to use for new users also. The power and simplicity of a spreadsheet is that the data being manipulated are held in front of the user in a very direct and accessible manner. In addition, the spreadsheet program itself provides for screen graphics, charts, easy-data manipulation using large number of functions, on-screen numerical and visual feedback, and fast calculations [2, 3].

Spreadsheets can be used as a specific-purpose software as well as for programming. Due to its structure and tools available in it, the amount of programming needed in a spreadsheet is minimal. It is often done by formula editing and copying. This approach helps students to concentrate on analysis and interpretation of results rather than on time-consuming code debugging [4].

In addition to the features and functions of the MS ExcelTM, it has programming capabilities called Visual Basic for Applications (VBA). This is a very powerful tool and can be used to solve complex physics problems [2, 3]. In Excel we can develop user defined functions using visual basic for application (VBA) in Excel. Users can use these functions and get their desired output directly [5].

A spreadsheet program can be used to solve linear and non-linear differential equations and to obtain their visual solutions [6, 7]. It may be also used for numerical integration techniques like Trapezoidal rule, Simpsons rule etc. When one solves an equation and analyzes the results, step by step, recording the successive values in the worksheet and plotting the results, Then repeating the calculations with different input parameter values and

comparing and analyzing the results we could take full advantage of various spreadsheet features [8]. This method is also sufficiently accurate for a large number of practical applications, since Excel stores numbers and performs calculations using 15 digits of precision. The accuracy of the results may be increased by reducing the step size of the integration. Reduction of the integration step size may lead to an increase in the number of iterations, which makes this method slow in simulating large control systems [9]. However, the spreadsheet could act as a good pedagogical tool.

Spreadsheets can be used to obtain solutions of differential equations of simple harmonic motion, simple pendulum, boundary value problems in electrostatics, wave motion, heat equations and their visual graphical representations. Using spreadsheets the data can be manipulated and visual effects can be observed [8, 10, 11, 12]. Using spreadsheets animations and simulations can be developed. The spreadsheets can be used to visualize potential surfaces of charges as well as surface plots [13].

This paper presented spreadsheet implementation for wave functions of quantum harmonic oscillator and comparing with classical probability density. The harmonic oscillator is a fundamental topic in both classical and quantum physics. Classically, the harmonic oscillator is applicable to numerous physical systems such as spring-mass system, electrical circuits etc. In quantum theory, the harmonic oscillator holds a unique importance in quantum mechanics, as it is both one of the few problems that can really be solved exactly, and is a very generally useful solution, both in approximations and in exact solutions of various problems. The harmonic oscillator is extremely useful in chemistry as a model for the vibrational motion in a diatomic molecule like HCl, HBr, etc. [14].

Being exactly solvable in both the domains, the harmonic oscillator thus provides us with an opportunity to study the differences between the properties maintained by the classical and quantum theories. Here, we use spreadsheet to find the wave functions and probability densities of harmonic oscillators. The probability densities in classical and quantum systems are compared. This used in the classroom will produce intuitive feeling in the students mind.

II. CLASSICAL HARMONIC OSCILLATOR

In linear simple harmonic motion, the restoring force F is proportional to the displacement of a particle from the mean position and directed towards the mean position, so that

$$F = -kx, \tag{1}$$

or

$$\frac{d^2x}{dt^2} + \omega^2x = 0,$$

where $\omega^2 = k/m$ or $k = m\omega^2$.

The solution of above equation is

$$x = a \sin(\omega t + \phi), \tag{2}$$

where a is amplitude of oscillation.

The potential energy is

$$V(x) = \frac{1}{2} kx^2. \tag{3}$$

Thus, particle oscillates between $+a$ and $-a$ with frequency

$$v = \frac{1}{2\pi} \sqrt{\frac{k}{m}}.$$

The total energy of the oscillator is

$$E = \frac{1}{2} ka^2. \tag{4}$$

We can say that the particle must be moving around in the classically allowed region: $|x| < a = (2E/k)^{1/2}$. All subdivisions within the classically allowed region are not equally probable, as the particle is whizzing through equilibrium, while spending more time in the parts through which its slowly moving. The time (dt) a particle spends in a little region dx depends on its speed $v = dx/dt$. The probability (dP) of finding the particle in dx is then proportional to the time it spends there is $dP = 2dt/T$, where T is the period of oscillation.

$$\therefore dP = \frac{2 dt}{T},$$

$$= \frac{2}{T} \left(\frac{1}{v} \right) dx.$$

$\therefore v = \omega^2 \sqrt{a^2 - x^2}$ and $T = 2\pi/\omega$, we get

$$dP = \frac{1}{\pi \sqrt{a^2 - x^2}} dx = P(x) dx,$$

where $P(x)$ is called probability density and given as:

$$P(x) = \frac{1}{\pi \sqrt{a^2 - x^2}}. \tag{5}$$

Classically, there is zero chance for a particle to have a potential energy V greater than its total energy E , and so the motion is strictly confined to the range $-a \leq x \leq +a$.

III. QUANTUM HARMONIC OSCILLATOR

The simple harmonic oscillator has potential energy is $V = \frac{1}{2} kx^2$. This potential energy value for a harmonic oscillator is the classical value and is used in the time independent Schrödinger equation to find the corresponding quantum mechanical value.

The Schrödinger equation for harmonic oscillator is

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} \left(E - \frac{1}{2} kx^2 \right) \psi = 0. \quad (6)$$

It is convenient to simplify Eq. (6) by introducing the dimensionless quantities. Let us introduce dimensionless variable:

$$\xi = \alpha x, \quad (7)$$

where α is constant having dimensions of inverse of length.

Therefore, Eq. (6), will take the form:

$$\frac{d^2\Psi}{d\xi^2} + (\varepsilon - \xi^2)\Psi = 0, \quad (8)$$

where

$$\alpha = \left(\frac{m\omega}{\hbar} \right)^{1/2}; \quad (9)$$

and

$$\varepsilon = \frac{2E}{\hbar\omega}. \quad (10)$$

The Eq. (8) has accepted solutions when $\varepsilon = (2n + 1)$, where $n = 0, 1, 2, 3, \dots$

This gives energy eigen values as:

$$E_n = (2n + 1) \frac{\hbar\omega}{2};$$

or

$$E_n = \left(n + \frac{1}{2} \right) \hbar\omega. \quad (11)$$

The harmonic oscillator energy levels are equally-spaced, by $\hbar\omega$.

The normalized wave functions in terms of dimensional less parameter ξ are given as :

$$\psi_n(\xi) = \left(\frac{1}{\sqrt{\pi} 2^n n!} \right)^{1/2} H_n(\xi) e^{-\xi^2/2}, \quad (12)$$

where $H_n(\xi)$ are Hermite polynomials of order n .

For $n = 0$, the wave function $\psi_0(\xi)$ is called *ground state wave function*. The first few Hermite Polynomials are listed in Table I.

The recurrence relation for Hermite Polynomials is

$$H_n(\xi) = 2\xi H_{n-1}(\xi) - 2(n-1) H_{n-2}(\xi). \quad (13)$$

TABLE I. First few Hermite Polynomials.

n	$H_n(\xi)$
0	$H_0(\xi) = 1$
1	$H_1(\xi) = 2\xi$
2	$H_2(\xi) = 4\xi^2 - 2$
3	$H_3(\xi) = 8\xi^3 - 12\xi$
4	$H_4(\xi) = 16\xi^4 - 48\xi^2 + 12$

The classical turning points are

$$x_0 = \pm \sqrt{\frac{2E}{k}} \text{ or } x_0 = \pm \sqrt{\frac{(2n+1)\hbar}{m\omega}}. \quad (14)$$

The classical turning points in terms of dimensionless variable ξ are

$$\xi_0 = \pm \sqrt{2n+1}. \quad (15)$$

The classical probability density in terms of dimensionless variable ξ is

$$P(\xi) = \frac{1}{\pi\sqrt{\xi_0^2 - \xi^2}}. \quad (16)$$

With the knowledge of our two systems to compare we can now proceed to investigate in detail the harmonic oscillator using spreadsheet.

IV. ORGANIZATION OF SPREADSHEET

The spreadsheet is prepared using MS Excel® 2007. Excel is a highly programmable product, and it is easily the best choice for developing spreadsheet-based applications. Excel uses the VBA language, which is now in widespread use. This language allows the user to create structured programs directly in Excel. On the other hand, with Excel it's easy to access to controls such as scrollbars because their implementation requires little or no macro programming [12].

To prepare spreadsheet the diatomic molecule HCl is used. Its reduced mass is 1.62661×10^{-27} kg and angular frequency 5.63212×10^{14} rad/s.

The order n is selected by using scroll bar. The energy, α , x_0 , and ξ_0 are calculated using above equations. To plot the graph the range of x is selected from $-2x_0$ to $+2x_0$.

The dataset in the spreadsheet is organized in the following way:

A10:A410 is a column that contains the values for $x = -2x_0$ to $x = 2x_0$ by increment of dx . The increment is obtained dividing total length ($4x_0$) by number of intervals (400 in this case).

B10:B410 is a column that contains the values of ξ obtained using $\xi = \alpha x$.

C10:DC10 is a column that contains the Hermite polynomials of order n which obtained by using recurrence relation. For this purpose Visual Basic Editor macro is used.

D10:D410 is a column that contains the values of $e^{-\xi^2/2}$ obtained by using excel function = EXP(-(B10^2)/2) in cell D10 and copying up to D410.

E10:E410 is a column that contains $\psi(\xi)$ obtained using equation (5).

F10:F410 is a column that contains $|\psi(\xi)|^2$.

G10:G210 is a column that contains classical probability density $P(\xi)$ obtained using equation (10).

The VBA macro for Hermite polynomials is given below.

```
Function Hermite()
    Dim H(50) As Double
    Dim j As Integer
    For i = 10 To 410
        Xi = Cells(i, 2) . Value
        H(0) = 1
        H(1) = 2 * Xi
        For j = 2 To n
            H(j) = (2 * Xi * H(j - 1)) - (2 * (j - 1) * H(j - 2))
        Next j
        Cells(i, 3) . Value = H(n)
    Next i
End Function
```

To choose value of n the scroll bar is used. The macro for scroll bar is given below.

```
Private Sub ScrollBar1_scroll()
    ' value of n
    Cells(4, 2) = ScrollBar1.Value
End Sub
Private Sub ScrollBar1_Change()
    ' value of n
    Cells(4, 2) = ScrollBar1.Value
    Hermite 'updates the hermite function
End Sub
```

The cell B4 is named as n .

The screenshot of Excel spreadsheet is shown in Fig. 1.

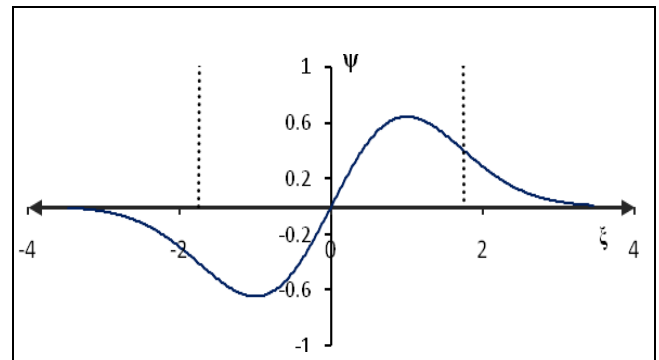
	A	B	C	D	E	F	G
1							
2	Wave Function and Probability Density Curves of Harmonic Oscillator						
3							
4	\hbar	515.9733	Scroll bar	\hbar	1.05E-34		
5	n	9		m	1.63E-27		
6	ω	5.63E+14	$2x_0$	dx	α	x_0	
7	ξ_0	4.358899	9.35E-11	4.6763E-13	9.321E+10	4.68E-11	
8							
9	x	ξ	$H_n(x)$	$\exp(-\xi^2/2)$	Ψ	$ \Psi ^2$	$P(\xi)$
10	-9.3526E-11	-8.7178	-1.2E+11	3.13913E-17	-2.01E-10	4.03E-20	
11	-9.30583E-11	-8.67421	-1.1E+11	4.58595E-17	-2.8E-10	7.81E-20	
12	-9.25907E-11	-8.63062	-1.1E+11	6.68687E-17	-3.88E-10	1.51E-19	
13	-9.21231E-11	-8.58703	-1E+11	9.73178E-17	-5.39E-10	2.9E-19	
14	-9.16554E-11	-8.54344	-9.6E+10	1.41363E-16	-7.45E-10	5.56E-19	
15	-9.11878E-11	-8.49985	-9.1E+10	2.04953E-16	-1.03E-09	1.06E-18	
16	-9.07202E-11	-8.45626	-8.7E+10	2.96584E-16	-1.42E-09	2.01E-18	

FIGURE 1. Screenshot of Excel Spreadsheet. It shows columns for x , ξ , $H_n(\xi)$, Ψ , $|\Psi|^2$, $P(\xi)$. It also shows values of k , m , ω , α for HCl molecule. Scroll bar is used to change value of n .

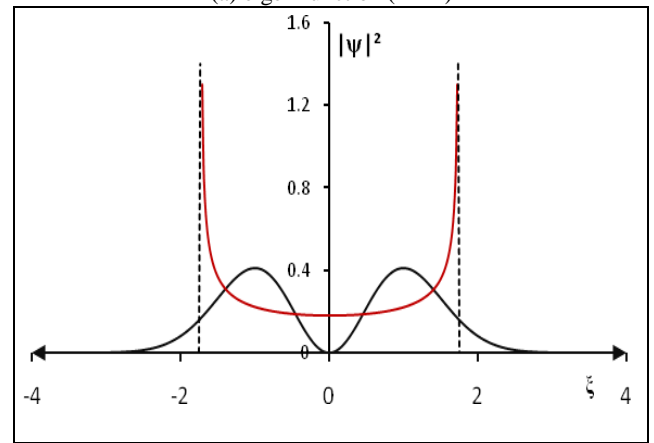
V. WAVE FUNCTIONS AND PROBABILITY DENSITY PLOTS

It is interesting to compare the classical probability distribution (proportional to the inverse of the oscillator's velocity) with $|\Psi|^2$. The wave functions and probability

density curves for different values of n are shown in the following figures.

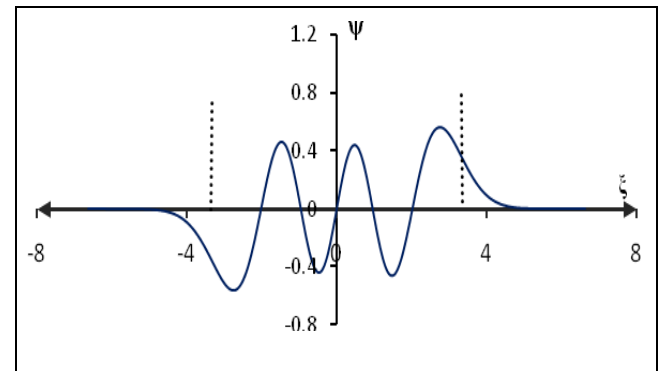


(a) eigen function (n = 1)



(b) probability density (n=1)

FIGURE 2. Wave function and probability density curves for $n = 1$. Vertical dotted lines show the classical limits. The red line curve shows classical probability densities.



(a) eigen function (n = 5)

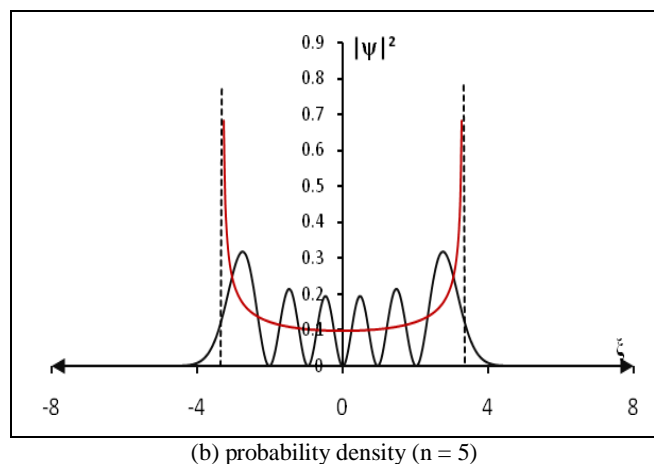


FIGURE 3. Wave function and probability density curves for $n = 5$. Vertical dotted lines show the classical limits. The red line curve shows classical probability densities.

The spreadsheet also calculates $\int_{-2\xi_0}^{+2\xi_0} |\psi(\xi)|^2 d\xi$ over the region $-2\xi_0 \leq \xi \leq +2\xi_0$ and it comes out to be 1. This proves the normalization condition. The total probability inside the classical region is calculated by using $\int_{-\xi_0}^{+\xi_0} |\psi(\xi)|^2 d\xi$ in the region $-\xi_0 \leq \xi \leq +\xi_0$. The total probability outside the classical region is calculated by using $\int_{-2\xi_0}^{-\xi_0} |\psi(\xi)|^2 d\xi$ and $\int_{\xi_0}^{2\xi_0} |\psi(\xi)|^2 d\xi$.

VI. CORRESPONDENCE PRINCIPLE

Correspondance principle may be easily explained using spreadsheet results. If you examine the ground state and first excited state of the *harmonic oscillator*, the classical and quantum predictions for the most probable location are in total contradiction. For the first few quantum energy levels, one can see little resemblance between the quantum and classical probabilities, but when you reach the value $n = 10$ there begins to be some similarity. For example see the probability density curve for $n = 20$ as shown in Fig. 4.

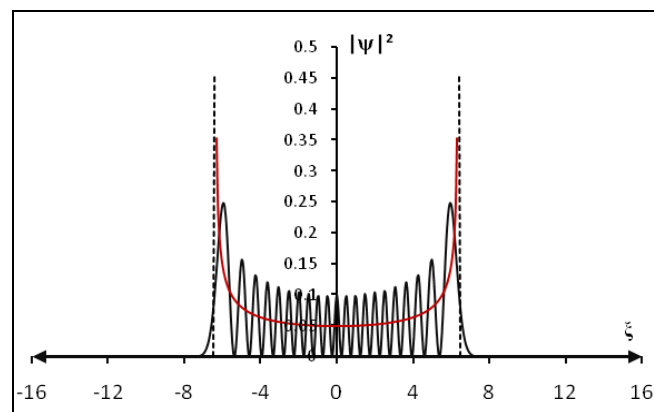


FIGURE 4. The probability density curves for $n = 20$.

As we go to higher and higher states of the quantum oscillator by increasing n , the most probable location shifts towards the classical turning points. The two plots don't look the same, but they do agree that the probability is greatest near the classical turning points. When we proceed to very high n values, the overall trend of the quantum probability begins to look more like the classical probability shown by red line. The fact that the overall picture of probability of finding the oscillator at a given value of x converges for the quantum and classical pictures is called the *correspondence principle* [15]. It is observed that the higher is the quantum number, the smaller the distance between peaks. At high enough n , the uncertainty principle prevents us from resolving the gaps without altering the physical state of the oscillator. The exponential tails into the classically forbidden region decrease with increasing n , so the quantum oscillator looks more and more like the classical one.

It is possible to find out the total probability outside the classical region and inside the classical region. As n increases, the probability inside the classically allowed region increases and outside it decreases. Percentages of the probabilities inside the classically allowed region and outside it obtained using spreadsheet are shown in the Table II.

TABLE II. Percentage of probabilities outside and inside the classically allowed regions.

n	$P_{in}(\%)$	$P_{out}(\%)$
0	83.80	16.20
1	89.13	10.17
5	93.04	6.96
10	94.53	5.47
15	95.31	4.69
20	95.83	4.17
25	96.20	3.8
30	96.50	3.5
35	96.74	3.26
40	96.94	3.06

Table II shows that the probability outside the classical region goes on decreasing as n increases. This allows us to state that the the total probability due to quantum and classical oscillators are within the classical region ad n tends to be very high.

VII. CONCLUSIONS

The example discussed in this article show a little of what can be achieved by using spreadsheets to find visual representations of wave functions and probability densities that are commonly used in quantum physics. The MS Excel spreadsheet is an easy to use and versatile pedagogical tool. With a variety of built-in mathematical functions and

excellent graphics capabilities, the spreadsheet is a powerful instrument for teaching and learning in many areas of the physics. Students can easily learn to use spreadsheets in physics, and this is good career training outside physics also. When students do physics with a spreadsheet, they benefit in two ways: they enhance their ability of using mathematical experiences to study the several phenomena of physics and gain a dynamic perspective and analytical power of this software tool [12].

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