

Visualizing superposition principle in Infinite Square well potential



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Abstract

The quantum physics is difficult for students to understand due to its abstract nature. Students can easily understand the quantum mechanics concepts when visual representations are used. In this article author has developed computer simulation using Microsoft Excel 2007® to graphically illustrate to the students the superposition principle of wave functions in one dimensional infinite square well potential. The expectation values of x and x^2 from the resultant wave functions can be obtained by using the simulation. The Spreadsheet also simulates the momentum representation of resultant wave function. From momentum representations, the expectation values of p and p^2 are obtained. Using the expectation values of position and momentum the uncertainty principle verified. This will make the concept, which so far is left to the abstract imagination come alive for the student, and initiate a deeper understanding of quantum physics.

Keywords: Infinite Square well potential, Superposition principle, Spreadsheets, Uncertainty principle.

Resumen

La Física cuántica es difícil de entender para los estudiantes debido a su naturaleza abstracta. Los estudiantes pueden entender fácilmente los conceptos de la mecánica cuántica cuando las representaciones visuales son usadas. En este artículo los autores han desarrollado una simulación por computadora usando Microsoft Excel 2007® para ilustrar gráficamente a los estudiantes el principio de superposición de funciones de onda en una dimensión infinita cuadrada y potencial. Los valores esperados de x y x^2 de las funciones de onda resultantes que pueden ser obtenidas mediante la simulación. La hoja de cálculo también simula la representación del momento de la función de onda resultante. Desde las representaciones del momento, los valores esperados de p y p^2 se obtienen. Usando los valores esperados de posición y momento el principio de incertidumbre verificado. Esto hará el concepto, el cual hasta ahora se deja a la imaginación abstracta que cobra vida para el estudiante, e iniciar un entendimiento más profundo de la física cuántica.

Palabras clave: Infinito cuadrado y potencial, Principio de superposición, Hojas de cálculo, Principio de incertidumbre.

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I. INTRODUCTION

Quantum mechanics is technically difficult to learn because it is mathematically challenging and abstract in nature. It is difficult for students to interpret and draw qualitative inferences from mathematics representations [1]. The particle in a one-dimensional infinite square well is one of the most elementary problems in quantum mechanics, and insights into the dynamics exhibited in this problem can be used in a wide range of physical systems [2, 3, 4].

Fast and realistic based computer visualization tools can play key role in teaching and learning physics [5, 6, 7]. A spreadsheet is a powerful calculation tool. The programming in MS Excel® is streamlined and less time is needed to enter the necessary code. Microsoft Excel® has features that make using it for instruction and solving physics problems very attractive. With a variety of built-in mathematical functions and excellent graphics capabilities,

the spreadsheet becomes a powerful instrument for modeling problems in quantum physics as well as in many areas of the physics. In a spreadsheet, the data manipulations 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, and easy-data manipulation using large number of functions, on-screen numerical and visual feedback, and fast calculations [8, 9, 10]. A spreadsheet provides instant data storage of any type of data in the form of an extendable two-dimensional array of cells. This data can be used by a simple mechanism of referencing in terms of rows and columns. It is possible to apply algebraic and mathematical operations to the elements of the spreadsheet, and these operations can be repeated, either interactively or by creating macros [11]. A spreadsheet program can be used to solve linear and non-linear differential equations in physics numerically and to obtain their visual graphical

representations [12, 13, 14, 15]. 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 [16]. Using spreadsheets animations and simulations in physics can be developed. Simulations developed using spreadsheets can be a powerful pedagogical tool in physics teaching-learning.

This paper presented spreadsheet implementation for particle in Infinite Square well potential and plotting of wave functions in position-space and their representations in momentum space. Analytical solutions are used to plot the superposition of wave functions. Using Fourier transform, the functions are obtained in momentum space. From these wave functions uncertainties in position and wave number are calculated. Scrollbars and naming facility to the cells and range are used to make the spreadsheet interactive.

II. INFINITE DEEP POTENTIAL WELL

The one-dimensional infinite square-well potential confines a particle to a box of width a and is described by

$$V = \begin{cases} 0 & |x| < a/2, \\ \infty & |x| \geq a/2 \end{cases}$$

A particle of mass M is placed in this potential. The energy eigenvalues and eigenstates are found by solving the time independent Schrödinger Eq. [4, 17].

$$u_n(x) = \begin{cases} \sqrt{\frac{2}{a}} \cos\left(\frac{n\pi}{a}x\right) & n = 1, 3, 5, \dots \\ \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right) & n = 2, 4, 6, \dots \end{cases} \quad (1)$$

The energy eigenstates are states of definite parity, as they must be for any system with symmetric potential $V(x)$.

The discrete energy eigenvalues are

$$E_n = \frac{\hbar^2 \pi^2}{2Ma^2} n^2.$$

The expectation values of x and x^2 are

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$$\langle m | x | n \rangle = \begin{cases} 0 & u_m \text{ and } u_n \text{ same parity or } m = n \\ \frac{8mna(-1)^{(m+n+1)/2}}{\pi^2(m^2 - n^2)} & u_m \text{ and } u_n \text{ opposite parity} \end{cases},$$

$$\langle m | x^2 | n \rangle = \begin{cases} a^2 \left(\frac{1}{12} - \frac{1}{2m^2\pi^2} \right) & \text{when } n = m \\ 0 & u_m \text{ and } u_n \text{ of parity} \\ \frac{8mna^2(-1)^{(m\pm n)/2}}{\pi^2(m^2 - n^2)^2} & u_m \text{ and } u_n \text{ same parity} \end{cases}$$

Let us consider the superposition of two Eigen functions

$$\Psi(x) = c_n u_n(x) + c_m u_m(x), \quad (2)$$

$$|\Psi(x)|^2 = |c_n u_n(x)|^2 + |c_m u_m(x)|^2 + c_n^* u_n(x) c_m u_m(x) + c_n u_n(x) c_m^* u_m(x)^* \quad (3)$$

It is normalized as $\int_{-a/2}^{a/2} |\Psi(x)|^2 dx = 1$, which gives

$$|c_n|^2 + |c_m|^2 = 1.$$

The expectation values are

$$\langle x \rangle = \int_{-a/2}^{a/2} x |\Psi(x)|^2 dx,$$

$$\langle x^2 \rangle = \int_{-a/2}^{a/2} x^2 |\Psi(x)|^2 dx,$$

When u_m and u_n are of the same parity, we have

$$\langle x \rangle = 0,$$

$$\langle x^2 \rangle = |c_m|^2 \langle m | x^2 | m \rangle + |c_n|^2 \langle n | x^2 | n \rangle + 2c_m c_n^* \langle m | x^2 | n \rangle,$$

And when u_m and u_n are of the opposite parity, we have

$$\langle x \rangle = 2 \langle m | x | n \rangle c_n c_m^*,$$

$$\langle x^2 \rangle = |c_m|^2 \langle m | x^2 | m \rangle + |c_n|^2 \langle n | x^2 | n \rangle,$$

The uncertainty in position is

$$\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2}. \quad (4)$$

The momentum representation of wave function is given as [17]:

$$\Phi(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-a/2}^{a/2} \psi(x) e^{-ipx/\hbar} dx,$$

Since $p = \hbar k$, we write above equation in k -space as

$$\Phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-a/2}^{a/2} \psi(x) e^{-ikx} dx,$$

The function $\Phi(k)$ also satisfies the normalization equation,

$$i.e. \int_{-\infty}^{\infty} |\Phi(k)|^2 dk = 1.$$

The expectation values are

$$\langle k \rangle = \int_{-\infty}^{\infty} \Phi(k)^* k \Phi(k) dk;$$

$$\langle k^2 \rangle = \int_{-\infty}^{\infty} \Phi(k)^* k^2 \Phi(k) dk.$$

The uncertainty of wave number k is

$$\Delta k = \sqrt{\langle k^2 \rangle - \langle k \rangle^2}. \tag{5}$$

The expected value in the given situation is

$$(\Delta k)^2 = |c_n|^2 \frac{n^2 \pi^2}{a^2} + |c_m|^2 \frac{m^2 \pi^2}{a^2}. \tag{6}$$

The product of uncertainties has value as

$$\Delta x \Delta k \geq \frac{1}{2}, \text{ or } \Delta x \Delta p \geq \frac{\hbar}{2}.$$

The graphical representations are obtained using MS Excel 2007.

III. ORGANIZATION OF SPREADSHEET

Using spreadsheet the wave functions are obtained from $-a/2$ to $+a/2$. The probability density is plotted. The uncertainty in the position is obtained. The values of k are set from $-3m\pi/a$ to $+3m\pi/a$. The Fourier transform is obtained. The real part and imaginary parts of Fourier transform are

$$R(k) = \frac{1}{\sqrt{2\pi}} \sum_{-a/2}^{a/2} \psi(x) \cos(kx) dx;$$

$$I(k) = \frac{1}{\sqrt{2\pi}} \sum_{-a/2}^{a/2} \psi(x) \sin(kx) dx.$$

- C3: Cell named as 'n' and it contains value of n which can be varied using scroll bar.
 - G3: Cell named as 'm' which contains value of m which can be varied using scroll bar.
 - C4: Cell named as 'a' and it contains value of width a of infinite square well.
 - C5: Cell named as 'dx' and it contains value of dx obtained by formula = a/400.
 - C6: Cell named as 'dk' and it contains value of dk obtained by formula = 4*m*pi/(400*a).
 - B27: B427: Range named as 'x' contain values of x by increment of dx .
 - C27: C427: Range named as 'y' contain values of $u_n(x)$ which is obtained by formula " =If(MOD(n,2)=0, SQRT(2/a)*sin(n*x*pi()/a), SQRT(2/a)*cos(n*x*pi()/a))" in cell c27 and pasting up to C427.
 - E27: E427: Contain values of 'k' by the interval of dk .
 - L27: L427: Range named as 'um' contains value of $u_m(x)$
 - Q27: Q427 : Range named as 'Ps' which contains value of $\psi(x)$
 - R27: R427: Range named as 'Pr' contains value of $|\psi(x)|^2$
- The real part of Fourier transform is obtained in F27:F427. In cell F27 the formula used is " = SUMPRODUCT(Ps, cos(E27*x)*dx)/SQRT(2*pi())"
- The real part of Fourier transform is obtained in F27:F427. In cell F27 the formula used is " = SUMPRODUCT(Ps, cos(E27*x)*dx)/SQRT(2*pi())"
- The formula gives the value of $R(k)$ for k value in cell E27. The formula is copied up to F427.
- The imaginary part of Fourier transform is obtained in G27:G427. In cell G27 the formula used is " = SUMPRODUCT(Ps, sin(E27*x)*dx)/SQRT(2*pi())"
- The formula gives the value of $I(k)$ for k value in cell E27. The formula is copied up to G427.
- H27:H427 contain value of $|\phi(k)|^2$ and the range is named as Pk.

To obtain uncertainty product values the formulas used are listed in Table I.

TABLE I. List of formulas used in different cells of worksheet.

Cell	Value	Formula in cell
F4	$\langle x \rangle$	= SUMPRODUCT(x,Pr*dx)
F5	$\langle x^2 \rangle$	= SUMPRODUCT(x^2,Pr*dx)
F6	Δx	= SQRT(F5 - F4^2)
H4	$\langle k \rangle$	= SUMPRODUCT(k,Pk*dk)
H5	$\langle k^2 \rangle$	= SUMPRODUCT(k^2,Pk*dk)
H6	Δk	= SQRT(H5 - H4^2)
H8	$\Delta x \Delta k$	= F6*H6

$$C7 \quad \sum |\psi(x)|^2 dx = \text{SUMPRODUCT}(Pr*dx)$$

$$E7 \quad \sum |\Phi(k)|^2 dk = \text{SUMPRODUCT}(Pk*dk)$$

The screenshot of spreadsheet used for superposition of eigen functions is shown in Fig. 1.

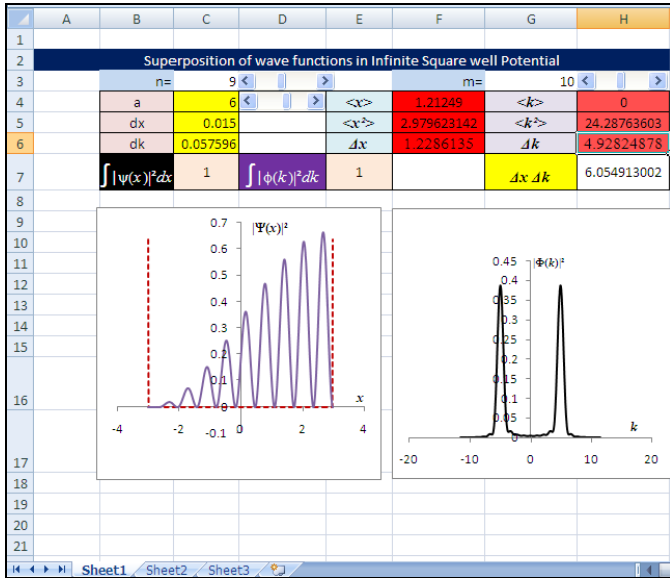
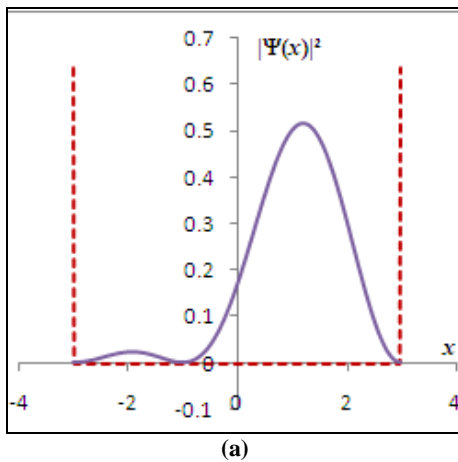


FIGURE 1. Screenshot of the worksheet.

IV. RESULTS AND DISCUSSION

The probability distributions in position space and momentum space are shown in Fig. 2 and Fig. 3 for superposition of different states.



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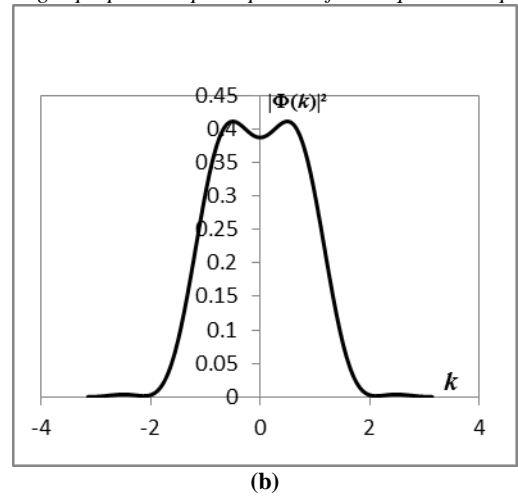


FIGURE 2. (a) Probability distribution in position space with a=3 atomic units and n=1, m=2 (b) The spread of P(k) in momentum space.

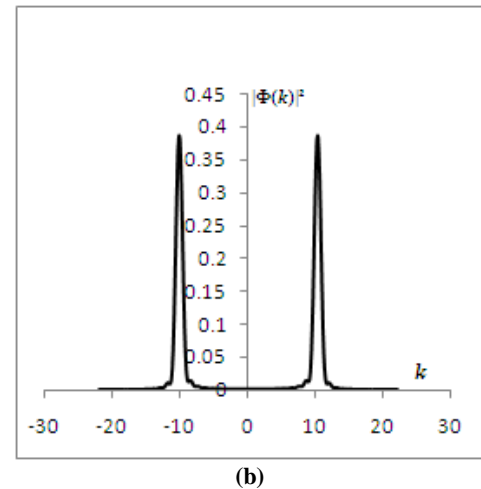
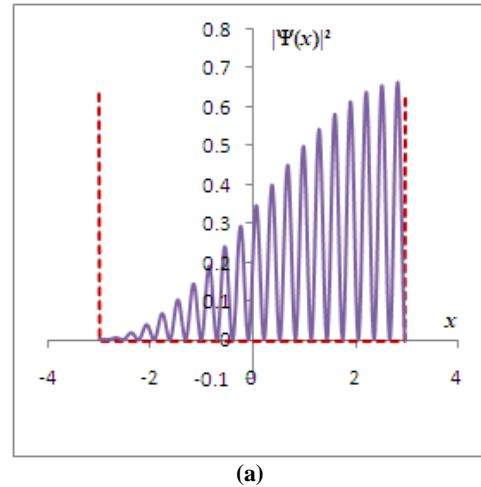


FIGURE 3. (a) Probability distribution in position space with a=3 atomic units and n=10, m=20, (b) The spread of P(k) in momentum space.

If $|\psi(x)|^2$ is proportional to the probability density of a measurement of the particle's position yielding the value x then it stands to reason that $|\phi(k)|^2$ is proportional to the probability density of a measurement of the particle's wave number yielding the value k . It is possible to verify Parseval's theorem that if the function is normalized to 1 its Fourier transform also normalized to 1 [18]. In our example it is found that $\sum |\psi(x)|^2 dx = 1$ and $\sum |\Phi(k)|^2 dk = 1$.

The momentum representation has several interesting aspects. First, $|\phi(k)|^2$ is a symmetric distribution with respect to k . Consequently, the expectation value of the $\langle k \rangle$ is zero, since positive and negative wave vectors (momenta) compensate each other. Second, the momentum representation has two maxima, which are about $p_0 = \pm \sqrt{(|c_n|^2 n^2 + |c_m|^2 m^2)} \pi \hbar / a$. The two maxima are increasingly pronounced with increasing number of nodes of the wave function. The uncertainty in momentum is governed not by the intrinsic width of the individual peaks, but rather by the 'distance' between the two sharp and well-isolated momentum peaks at approximately $\pm p_0$ which gives $\Delta p \approx + p_0$.

The following Table II shows the uncertainties for different states with $n > m$ and $c_n = c_m = 1/\sqrt{2}$.

TABLE II. Uncertainties for superposition of different states.

n	m	$\langle x \rangle$	$\langle x^2 \rangle$	$\langle k \rangle$	$\langle k^2 \rangle$	$\Delta x \Delta k$
1	2	1.08076	1.86014	0	0.63619	0.66355
1	3	0	0.61895	0	1.33863	0.91025
2	4	0	1.09390	0	2.71437	1.72315
8	9	-1.21165	2.97449	0	19.41709	5.40831
18	19	-1.21497	2.99466	0	92.79377	11.87047

The spreadsheet simulation show that when u_n and u_m are of same parity $\langle x \rangle = 0$ and $\langle x \rangle$ is non-zero when u_n and u_m are of opposite parity. When u_n is odd parity and u_m is even parity such that $m > n$, the $\langle x \rangle$ is negative. If u_n is even parity and u_m is odd parity function, the $\langle x \rangle$ is positive.

V. CONCLUSION

In the examples discussed so far, the superposition of two eigen functions is obtained using Spreadsheet program. The momentum wave function is found by a numerical Fourier transform of the analytical form of the resultant wave function. In this article superposition principle of eigen functions is presented for an infinite square well problem and its momentum representation is obtained by Fourier transformation. The proposed approach makes it possible to represent wave functions and their Fourier transforms with remarkable simplicity, and it provides valuable insight into the origin of the uncertainty principle. It can be stated that the preference for the position or momentum formulation of

quantum mechanics is guided by the uncertainty principle [19].

The example used here demonstrates that spreadsheet programs have proven to be an important pedagogical tool for a variety of problems in quantum physics education. The proposed method provides a useful link between the mathematical representations in quantum physics and their graphical representations. The spreadsheet programs like MS Excel are very flexible, familiar, and relatively easy to use. With variety of built in functions and excellent graphics capability Spreadsheets can be used to model complex quantum physics problems such as perturbation theory and thus provide graphical representations to equations [20, 21]. These features are difficult to obtain by using a structured programming language such as C/C++. Use of this program in undergraduate classroom has resulted in favorable comments by the students. Due to its cell base structure and easy to use mathematical functions, Excel is very good pedagogical tool. When students do physics with a spreadsheet, they benefit in two ways: (i) they enhance their learning ability by drawing connections between the language of mathematics and context of applications in physics; and (ii) gain a dynamic perspective and analytical power of this software tool to solve problems, develop understanding, and explore concepts [14, 22].

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