



Spreadsheet Implementation for Momentum Representation of Gaussian Wave Packet and Uncertainty Principle

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(Received 11.09.2011 Accepted 03.11.2011)

Abstract

The objective of this article is to graphically illustrate to the students the Gaussian wave packet and its momentum representation using spreadsheets. Gaussian wave packet with different standard deviations is obtained using interactive spreadsheet. Using Fourier transform the momentum representation is obtained. Using Gaussian wave function and its momentum representation the uncertainties in position and wave number are obtained and the uncertainty relation is 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 problems.

Keywords: Quantum mechanics, wave packet, spreadsheets, uncertainty principle.

Introduction

Quantum mechanics is one of the most widely taught topics on the college and university level as it has fundamental role in physics and chemistry. Quantum mechanics is technically difficult to learn because it is mathematically challenging and abstract in nature. Students constantly struggle to master the basic concepts. It is difficult for students to interpret and draw qualitative inferences from mathematics representations (Singh, 2001). Fast and realistic based computer visualization tools can play key role in teaching and learning of quantum mechanics (Singh, 2008; Singh et. al., 2006).

Simulation developed with using spreadsheets can be a powerful pedagogical tool in during teaching and learning physics. The advantage of using a spreadsheet in teaching-learning process is that the programming is streamlined and less time is needed to enter the necessary code. From data analysis and graphing to animation and simulations, Microsoft Excel® is a very versatile program for the teachers and students. The strong features of spreadsheet are their cell based structure and the simple interface that is easy to use for new users also. 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 (Cooke, 1997; Wagner, 2007; Yamani and Kharab, 2001). 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 (Tabor, 2004). A spreadsheet program can be used to solve linear and non-linear differential equations in physics numerically and to obtain their visual graphical representations (Benacka, 2009; Lingard, 2003; Oliveira and Napoles, 2010; Webb, 1993). 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 (El-Hajj, Karaki, and Al-Husseini, 2004). Using spreadsheets animations and simulations in physics can be developed.

This paper presented spreadsheet implementation for plotting of Gaussian wave functions in position-space and their representations in momentum space. Analytical solutions are used to plot the Gaussian 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.

The Gaussian Wave Packet

The Gaussian wave packet is a more rewarding problem both in pedagogical and physical points of view (Liboff, 2006). Let us consider a one-dimensional Gaussian wave function at $t = 0$ given by

$$\psi(x) = \frac{1}{(2\pi a^2)^{1/4}} e^{-x^2/4a^2} \quad (1)$$

where a is the initial width of the associated wave packet which is peaked at $x = 0$.

The position probability density is given by

$$\rho(x) = |\psi(x)|^2 = \frac{1}{(2\pi a^2)^{1/2}} e^{-x^2/2a^2} \quad (2)$$

It is normalized as $\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1$.



The expectation values are

$$\langle x \rangle = \int_{-\infty}^{\infty} x |\psi(x)|^2 dx$$

$$\langle x^2 \rangle = \int_{-\infty}^{\infty} x^2 |\psi(x)|^2 dx$$

The uncertainty in position is

$$\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} = a \quad (3)$$

The momentum representation of wave function is given as (Liboff, 2006) :

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

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

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

Inserting the wave function, given by equation (1), into the Fourier integral yields the result

$$\Phi(k) = \frac{1}{(2\pi/4a^2)^{1/4}} e^{-k^2 a^2} \quad (4)$$

or

$$\Phi(k) = \frac{1}{(2\pi\sigma_k^2)^{1/4}} e^{-k^2/4\sigma_k^2}$$

where σ_k is standard deviation of the k-space distribution. It is also a Gaussian distribution. Thus, the Fourier transform of a Gaussian function is also a Gaussian function. The function

$\Phi(k)$ also satisfies the normalization equation, i.e. $\int_{-\infty}^{\infty} |\Phi(k)|^2 dk = 1$

The expectation values are

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

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



The uncertainty of wave number k is

$$\Delta k = \sqrt{\langle k^2 \rangle - \langle k \rangle^2} \quad (5)$$

The product of uncertainties has its minimum value in a Gaussian wave packet and its value is

$$\Delta x \Delta k = \frac{1}{2} \quad \text{or} \quad \Delta x \Delta p = \frac{\hbar}{2}$$

Using Microsoft Excel 2007® this result is verified.

Implementation of Spreadsheet

Using spreadsheet the Gaussian wave functions are obtained from $-7a$ to $+7a$. The probability density is plotted. The uncertainty in the position is obtained. The values of k are set from $-7/a$ to $+7/a$. The Fourier transform is obtained. The real part of Fourier transform is

$$R(k) = \frac{1}{\sqrt{2\pi}} \sum_{-7a}^{7a} \psi(x) \cos(kx) dx$$

The imaginary part is

$$I(k) = \frac{1}{\sqrt{2\pi}} \sum_{-7a}^{7a} \psi(x) \sin(kx) dx$$

The spreadsheet developed as

C4: cell named as 'a' and it contains value of standard deviation.

C5: cell named as 'dx' and it contains value of dx obtained by formula = 14*a/400

C6: cell named as 'dk' and it contains value of dk obtained by formula = 14/(a*400)

B27:B427: Range named as 'x' contains values of x by increment of dx

C27:C427: Range named as 'y' contain values of $\psi(x)$ which is obtained by the following formula,

“= SQRT(1/(SQRT(2*pi()*a))*exp(-(x/a)^2/4)” in cell c27 and pasting up to C427.

D27:D427: contain values of $|\psi(x)|^2$

E27:E427: contain values of 'k' by the interval of dk.

The real part of Fourier transform is obtained in F27:F427. In cell F27 the formula used is
= SUMPRODUCT(y, 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

$$= \text{SUMPRODUCT}(y, \sin(E27*x)*dx)/\text{SQRT}(2*\pi())$$

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 $|\phi(k)|$. To obtain uncertainty product values the formulas used are listed in table 1.

Table 1: List of formulas used in different cells of worksheet

cell	Value	Formula in cell
F4	$\langle x \rangle$	$= \text{SUMPRODUCT}(x,y^2*dx)$
F5	$\langle x^2 \rangle$	$= \text{SUMPRODUCT}(x^2,y^2*dx)$
F6	Δx	$=\text{SQRT}(F5 - F4^2)$
G4	$\langle k \rangle$	$= \text{SUMPRODUCT}(k,D*dk)$
G5	$\langle k^2 \rangle$	$= \text{SUMPRODUCT}(k^2,D*dk)$
G6	Δk	$=\text{SQRT}(G5 - G4^2)$
E8	$\Delta x \Delta k$	$=F6*G6$
C7	$\sum \psi(x) ^2 dx$	$=\text{SUMPRODUCT}(P*dx)$
E7	$\sum \Phi(k) ^2 dk$	$=\text{SUMPRODUCT}(D*dk)$

The screenshot of spreadsheet used for Gaussian wave packet is shown in figure 1.

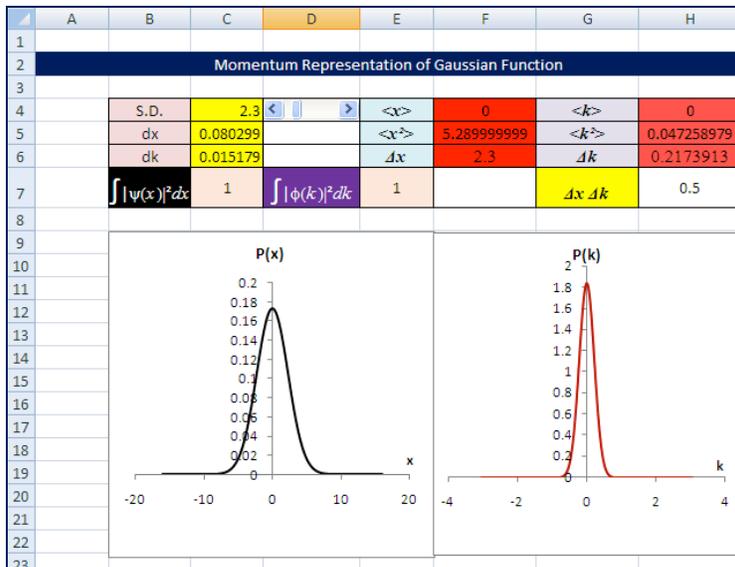


Fig. 1 Screenshot of the worksheet



Results and Discussion

The distributions in position space and momentum space are shown in figures 2 and 3 for different standard deviations.

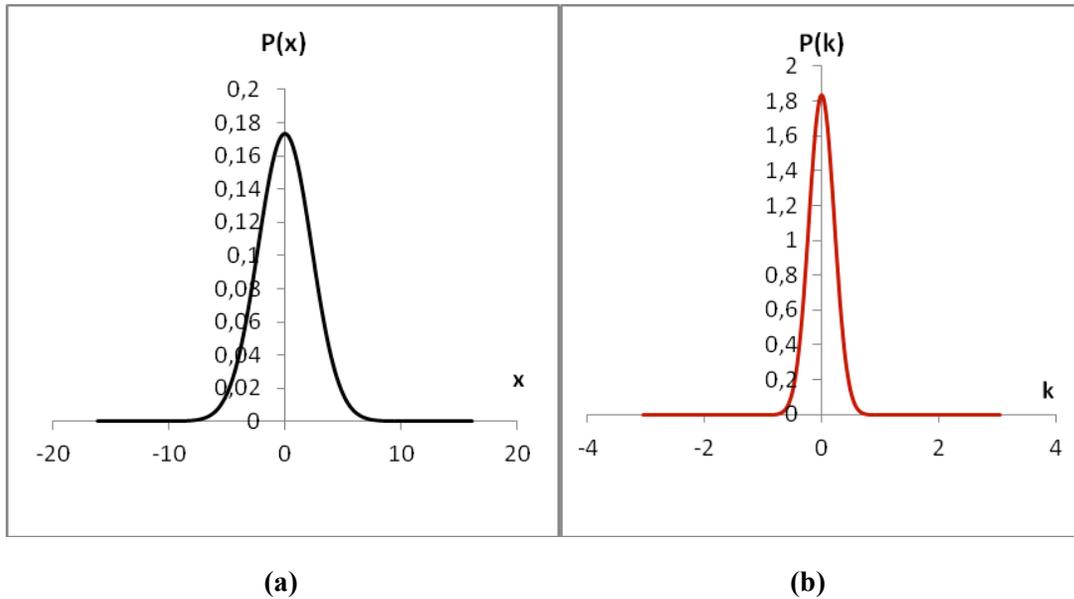


Fig.2 (a)Gaussian distribution with $a = 2.3$ units (Δx). (b) The spread of $P(k)$ is $\Delta k = 0.217391$ units

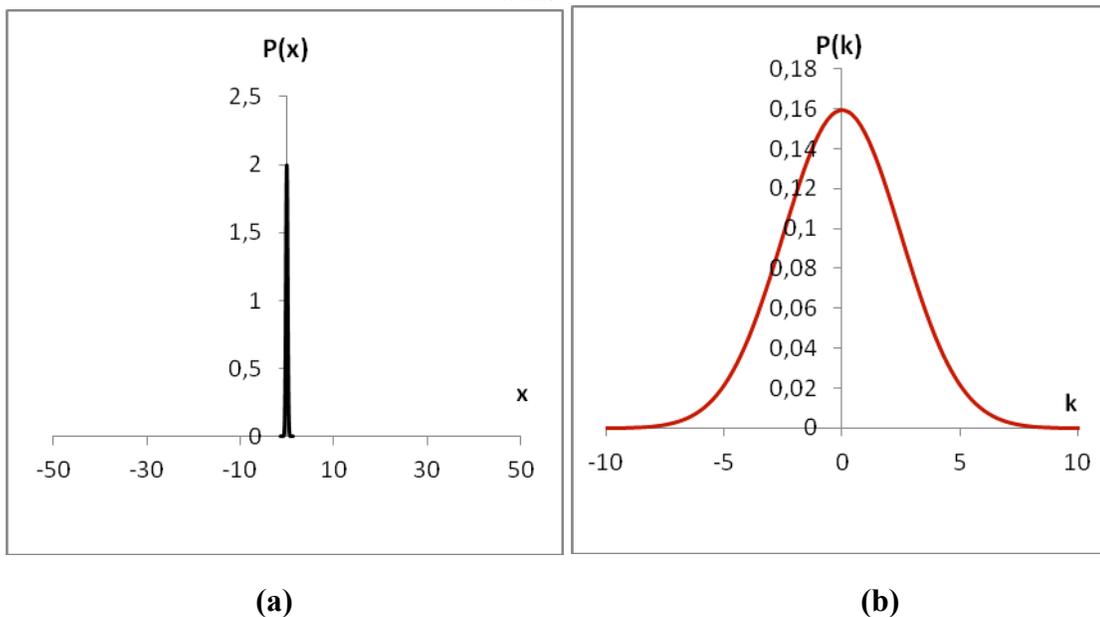


Fig. 3 (a)The wave packet localized in x -space ($\Delta x = 0.04$ units); (b) The resulting packet is extended in k ($\Delta k = 6.25$ units).



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 Parsavel's theorem that if the function is normalized to 1 its Fourier transform also normalized to 1 (Gasiorowicz, 2003). In our example it is found that $\sum |\psi(x)|^2 dx = 1$ and $\sum |\Phi(k)|^2 dk = 1$.

In our special example the $|\psi(x)|^2$ is peaked about $x = 0$ with width of packet 'a'. The $|\phi(k)|^2$ is peaked about $k = 0$ with width 'a/2'. There is reciprocity here: a function strongly localized in x is broad in k . The spreadsheet result shows that the Gaussian packet presents the ultimate case when the product $\Delta x \Delta k$ has the lowest possible value ($1/2$) for any value of standard deviation a . This is minimum value of uncertainty relation. This is general property of functions that are Fourier transforms of each other. It is possible to verify a small uncertainty of one variable implies a large uncertainty of other variable of pair of variables x and k .

If a packet which is much localized in x -space (*i.e.*, if Δx is small) then we need to combine plane waves with a very wide range of different k -values (*i.e.*, Δk will be large). Conversely, if plane waves whose wave numbers differ by a small amount (*i.e.*, if Δk is small) combine then the resulting wave packet will be much extended in x -space (*i.e.*, Δx will be large). These results are shown in Fig. 2 and Fig. 3.

Conclusions

In the examples discussed so far, the momentum wave function is found by a numerical Fourier transform of the analytical form of the position wave function. In this article a Gaussian wave packet problem is presented that relies on a simple Fourier transformation. Besides its simplicity, the proposed method provides a useful link between the materials that students typically learn in a course on mathematical physics and applications to physical problem. The proposed approach makes it possible to represent eigenfunctions 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 (Rioux, 1997).

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. These programs are very flexible, familiar, and relatively easy to use. Spreadsheets can be used to model physical situations involving motion of particle, and thus provide graphical representations to equations. These features are difficult to obtain by using a structured programming language such as C/C++. Use of this program in undergraduate classroom and laboratory has resulted in favorable comments by the students. Due to its cell base structure and easy to use mathematical functions, naming facility to cells and ranges, the students can easily use Excel. 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 (Oliveira and Napoles, 2010 ; Shafii-Mousavi and Kochanowski, 2010).

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