Momentum Representation of Wave Function in Quantum Harmonic Oscillator Using Spreadsheets

Popat S. Tambade

Department of Physics
Prof. Ramkrishna More Arts, Commerce and Science College, Akurdi
Pune 411044, India.
Savitribai Phule Pune University, Pune
Email: pstam3@rediffmail.com

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Abstract

In this article author have developed computer simulation using Microsoft Excel 2007® to graphically illustrate the wave functions and their momentum representations. Using this simulations wave functions in different states can be plotted. The expectation values of x and x^2 can be obtained by using the simulation. Using momentum representation <p> and $<p^2>$ are obtained. Using the expectation values of position and momentum the uncertainty principle verified. The momentum representation is seldom used in quantum mechanics courses hence students find it difficult to understand.

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 [1]. Fast and realistic based computer visualization tools can play key role in teaching and learning of quantum mechanics [2].
From data analysis and graphing to animation and simulations, Microsoft Excel® is a very versatile program for the researchers, 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[3, 4, 5].
In quantum mechanics, the position ($\hat{x}$), and the linear momentum ($\hat{p}$) operators play very symmetrical roles as it must be obvious from the fundamental commutation relation $[\hat{x}, \hat{p}] = i\hbar$. However, this fundamental symmetry may not be apparent to many students of quantum mechanics since more emphasis is given on the coordinate representation in lectures and in textbooks. In this

study, the author has discussed an example of one-dimensional harmonic oscillator in quantum mechanics from the point of view of momentum space [6]. For this purpose, spreadsheet based simulation was developed and graphical representation of momentum space counterpart $\varphi(p)$ of coordinate space wave function $\psi(x)$ is obtained using Fourier transform. From the $\psi(x)$ and $\varphi(p)$ representations uncertainties in the position and momentum are obtained. These values found to be in agreement with the desired results. From these wave functions uncertainties in position and momentum are calculated.

1. Harmonic Oscillator

The potential energy for harmonic oscillator is

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

The Hamiltonian is given as

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}kx^2$$

The Schrodinger's steady state equation for harmonic oscillator is given as

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

The energy eigen values of harmonic oscillator are

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

The unperturbed eigen functions are

$$\psi_n(x) = \left(\frac{1}{2^n n!\sqrt{\pi}}\right) H_n(\alpha x) e^{-\alpha^2 x^2/2} \qquad \ldots(2)$$

where n=0, 1, 2, …….

The classical limit is given as

$$x_0 = \sqrt{\frac{2E_n}{m\omega^2}} \qquad \ldots(3)$$

It is convenient to simplify Eq. (1) by introducing the dimensionless quantities. Let us introduce dimensionless variable $\xi = \alpha x$, we get

$$\frac{d^2\psi}{d\xi^2} + \left(2\varepsilon - \xi^2\right)\psi = 0 \qquad \ldots(4)$$

where $\alpha = \left(\frac{m\omega}{\hbar}\right)^{1/2}$ and $\varepsilon = \frac{E}{\hbar\omega}$.

The eigen functions are

$$\psi_n(\xi) = \left(\frac{1}{2^n n!\sqrt{\pi}}\right)^{1/2} H_n(\xi) e^{-\xi^2/2} \qquad \ldots(5)$$

where $H_n(\xi)$ are Hermite polynomials of order n. The Hermite polynomials satisfy the following recurrence relation,

$$H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x) \qquad \ldots(6)$$

The classical limit in terms of dimensionless variable is $\xi_0 = \sqrt{2n+1}$

The energy parameter is defined as

$$\varepsilon_n = \frac{E_n}{\hbar\omega}$$

Therefore,

$$\varepsilon_n = \left(n + \frac{1}{2}\right) \qquad \ldots(7)$$

The uncertainty is ξ is

$$\Delta\xi = \sqrt{n + \frac{1}{2}}$$

We generate the momentum wave function by Fourier transform of the coordinate-space wave function and given as [7]:

$$\Phi_n(p) = \frac{1}{\sqrt{2\pi\,\hbar}} \int_{-\infty}^{\infty} \psi_n(x)\, e^{-ipx/\hbar} dx \qquad \ldots(8)$$

This Fourier transform illustrates that each point in p-space is intertwined with every point in x-space, and vice versa.

Let $\eta = p/\sqrt{m\omega\hbar}$ with classical limit $\eta_0 = \sqrt{2n+1}$, we write above equation in η-space as

$$\Phi_n(\eta) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi_n(\xi)\, e^{-i\eta\xi} d\xi \qquad \ldots(9)$$

The function $\Phi(\eta)$ also satisfies the normalization equation, i.e. $\int_{-\infty}^{\infty} |\Phi_n(\eta)|^2 \, d\eta = 1$

The expectation values are

$$<\eta> = \int_{-\infty}^{\infty} \eta\, |\Phi_n(\eta)|^2 \, d\eta$$

$$<\eta^2> = \int_{-\infty}^{\infty} \eta^2\, |\Phi_n(\eta)|^2 \, d\eta$$

The uncertainty of wave number *k* is

$$\Delta\eta = \sqrt{<\eta^2> - <\eta>^2}$$

We get $(\Delta\eta)^2 = \left(n+\frac{1}{2}\right)$

The product of uncertainties has value as

$$\Delta\xi\ \Delta\eta = \left(n+\frac{1}{2}\right) \text{ or } \Delta x\ \Delta p = \left(n+\frac{1}{2}\right)\hbar$$

Because of its symmetry, the harmonic oscillator is as easy to solve in momentum space as it is in position space. It gives the same results as the wave function in the position basis.

Using Microsoft excel 2007 this result is verified..

2. Organization of Spreadsheet

Using spreadsheet the wave functions are obtained from $-3\xi_0$ to $+3\xi_0$. The probability density is plotted. The uncertainty in the position is obtained. The values of ηare set from $-3\eta_0$ to $+3\eta_0$. The Fourier transform is obtained. The real part of Fourier transform is

$$R(\eta) = \frac{1}{\sqrt{2\pi}} \sum_{-3\xi_0}^{3\xi_0} \psi(\xi)\cos(\eta\xi)d\xi$$

The imaginary part is

$$I(\eta) = \frac{1}{\sqrt{2\pi}} \sum_{-3\xi_0}^{3\xi_0} \psi(\xi)\sin(\eta\xi)d\xi$$

The spreadsheet developed as

B5: cell named as ‘n’ and it contains value of n.
B7:cell named as ‘a’ and it contains value of ξ_0.
D8: cell named as ‘dx’ and it contains value of dx obtained by formula = $3\xi_0/400$
F7: cell named as ‘dk’ and it contains value of dη obtained by formula = $3\eta_0/400$
B28:B828: Range named as ‘x’ contain values of ξ by increment of dξ
C28:C828: Range named as ‘y’ contain values of ψ(ξ) which is obtained by formula

“=SQRT(1/(fact(n)*2^n*sqrt(pi()))*Her(n,x)*exp(-x^2/2)” …(5)

E28:E828: Range named as ‘k’ and contain values of ‘η’ by the interval of dη.

The real part of Fourier transform is obtained in F28:F828. In cell F28 the formula used is

= SUMPRODUCT(y, os(E27*x)) *dx /SQRT(2*pi())

The formula gives the value of R(η) for η value in cell E28. The formula is copied up to F828.

The imaginary part of Fourier transform is obtained in G28:G828. The formula used in the range is

= SUMPRODUCT(y, sin(E27*x)) *dx /SQRT(2*pi())

The formula gives the value of I(η) for η value in cell E28. The formula is copied up to G828.

H28:H828 contain value of $|\phi(\eta)|^2$ and the range is named as D.

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
H6	$<\xi>$	= SUMPRODUCT(x,y^2*dx)
H7	$<\xi^2>$	= SUMPRODUCT(x^2,y^2*dx)
H8	$\Delta\xi$	=SQRT(H7 – H6^2)
J6	$<\eta>$	= SUMPRODUCT(k,D*dk)
J7	$<\eta^2>$	= SUMPRODUCT(k^2,D*dk)
J8	$\Delta\eta$	=SQRT(J7 – J6^2)
J9	$\Delta\eta\ \Delta\xi$	=H8*J8
D9	$\sum \lvert\psi(\xi)\rvert^2\ d\xi$	=SUMPRODUCT(y^2*dx)

F9	$\sum \lvert \Phi(\eta) \rvert^2 \, d\eta$	=SUMPRODUCT(D*dk)

To find value of Hermite polynomials an User Define function Her(n,x) was built up using VBA and recurrence relation given in Eq. (6) is used to find values of higher order polynomials.

The screenshot of spreadsheet used for Harmonic oscillator is shown in Fig. 1.

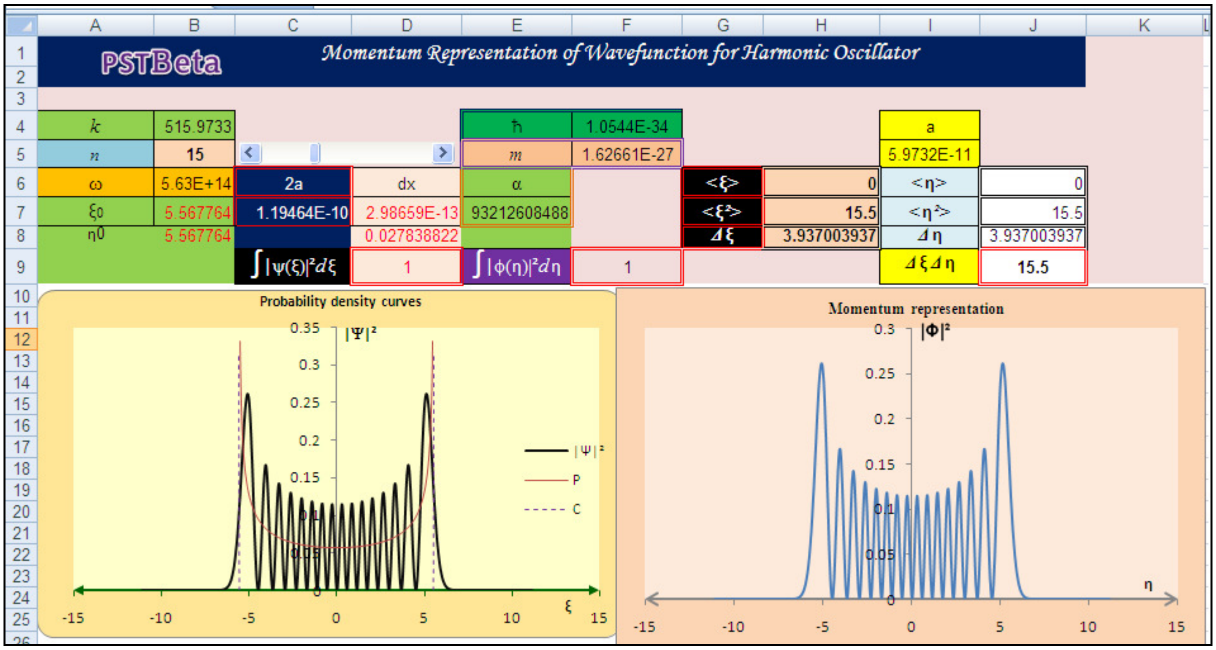


FIG. 1: Screenshot of spreadsheet worksheet developed for wave function and its momentum representation.

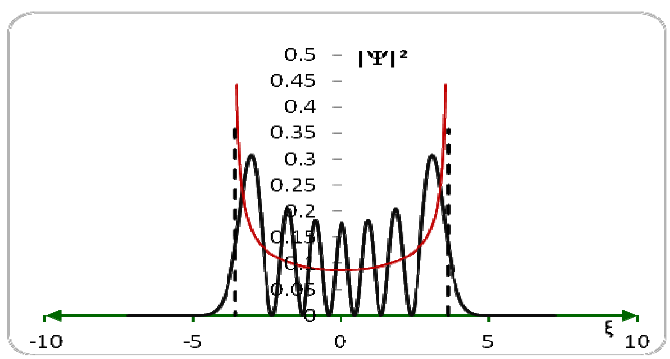
The above development of spreadsheet simulation shows that it is very easy to develop simulations using spreadsheets.

Representation of wave function in position and momentum space representation for different values of n is shown in following figures.

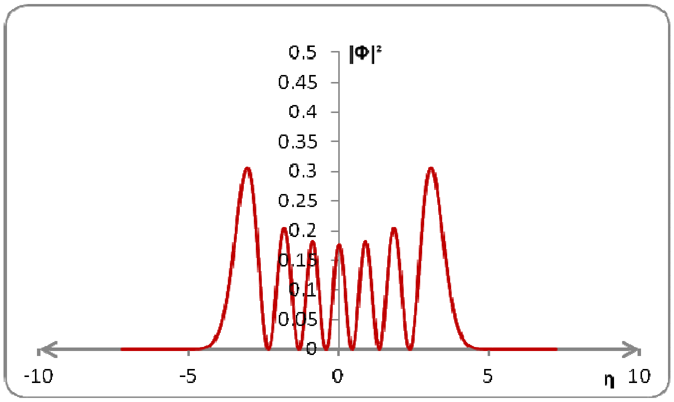
3. Results and Discussion

For numerical calculations of wave functions and its momentum space counterpart the limits of integration in any state were taken from three times classical limit from negative values to positive values. These values also give appreciably good accuracy because of rapidly decreasing wave functions outside the classical regions.

The distributions in position space and momentum space are shown in Fig. 2 and Fig. 3 for different values of n. In position representation classical limits are show by vertical dotted lines and classical probabilities are shown by red line curve.

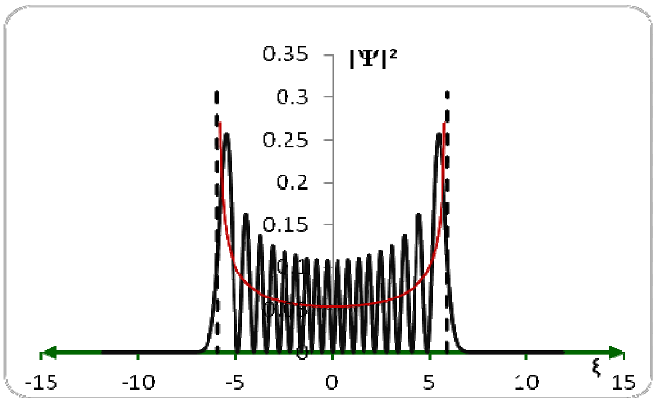


(a)Position representation



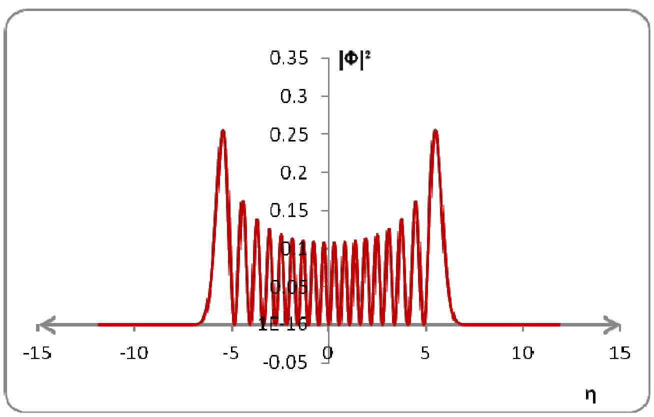
(b) momentum representation

FIG. 2: Graphical representation of probability distributions for n= 6.



(a) Position representation

(b)



(b)Momentum representation

FIG. 3: Graphical representation of probability distribution for n= 17.

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 $|\phi(p)|^2$ is proportional to the probability density of a measurement of the particle's momentum yielding the value p. It is possible to verify Parsavel's theorem that if the function is normalized to 1 its Fourier transform also normalized to 1 [8]. Using simulation developed in this study it is found that $\sum|\psi(x)|^2\, dx = 1$ and $\sum|\Phi(p)|^2\, dp = 1$. The momentum representation has several interesting aspects. First, $|\phi(p)|^2$ is a symmetric distribution with respect to p, Consequently, the expectation value of the $<p>$ is zero, since positive and negative momenta compensate each other.

Conclusion

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. The proposed approach makes it possible to represent eigen functions and their Fourier transforms with remarkable simplicity, and it provides valuable insight into the origin of the uncertainty principle [9].

Author expect to contribute with this approach to the development of physical insight for problems posed in the momentum representation and, furthermore, to help students to understand the different features of operators in quantum physics. The spreadsheet simulation developed in this study can easily be used to represent momentum representation of other problems in quantum mechanics. The understanding of momentum representation of wave functions is important for the students because some complex problems in quantum mechanics are easy to study in momentum representation. Such problems are scattering process, dispersion relations and the study of resonant states as solutions of a Lippmann-Schwinger equation.

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