

Quantum Harmonic Oscillator, a computational approach

Sarmistha Sahu,

Maharani Lakshmi Ammanni College for Women, Bangalore

Abstract:

Why should the wavefunction have a **Gaussian Function** for a Harmonic Oscillator?

What is the lowest energy?

What does the “Zero point energy” signify?

When is a wavefunction oscillatory?

Does the wavefunction have any bearing with the turning points?

What is parity? When is parity even or odd?

Many such questions can be answered by the computational method. The **computational methods** used for solving the second degree differential equation (Schroedinger's time independent equation) is by **Runge-Kutta fourth order method** using Microsoft-Excel.

For harmonic oscillator, the accuracy of the results is good. An initial guess of the wavefunction at a point can give the value at successive points using a small step size.

Keywords: Zero point energy, oscillations, turning point, Gaussian function.

I. Introduction

Obtaining the eigen value and eigen functions by solving the Schrodinger equation is pretty involved. Solving a second degree differential equation by computational method using Runge Kutta 4th order is another easy way.

The animated wavefunction speaks volume about the characteristics of eigenfunctions. It also explains the discrete eigenvalues. Concept of parity becomes obvious and, comparison with the classical oscillator, pictorially, is satisfying. The correspondence principle for large quantum number becomes visual. [View the spread sheet](#)

II. Methodology

The potential of a harmonic oscillator is $V = \frac{1}{2}kx^2$ The parabolic potential of a harmonic oscillator is shown in Fig 1.

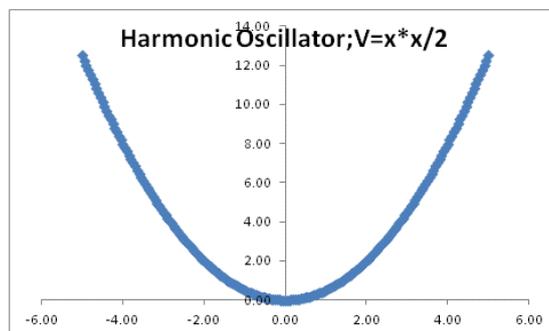


Fig 1. Parabolic potential

Eigenvalue Problem

The time independent Schroedinger equation for a non-relativistic quantum system, in one dimension, and in atomic units ($m = 1, \hbar = 1$), can be written as

$$\frac{\partial^2 \psi}{\partial x^2} = -2(E - V(x))\psi$$

For a harmonic oscillator

$$V = \frac{1}{2}x^2 \quad \dots 1$$

With $k = 1$, the equation is

$$\frac{\partial^2 \psi}{\partial x^2} = -2(E - \frac{1}{2}x^2)\psi$$

Guess solution with a Gaussian function gives

$$\psi(x) = Ce^{-ax^2/2} \quad \dots 2$$

The Gaussian function satisfies the requirement of the wavefunction at $x \rightarrow \infty$ or $x \rightarrow -\infty$. But, C is to be determined!

Boundary conditions are essential in determining the solution. Since the energy of the oscillator should be equal to or larger than the potential, the turning points at x_1 and x_2 gives [1]

$$E = V(x_1) = V(x_2) \quad \dots 3$$

The turning points are symmetrically placed from the origin. We can write $x_1 = -x_0$ and $x_2 = x_0$, then

$$x_0(E) = \pm \sqrt{\frac{2E}{k}}, \quad \text{where } E = \frac{kx_0^2}{2} \quad \dots 4$$

For a **bound state**, the energy eigenvalues are discrete and each of the eigen solution corresponding to the eigen value describes some physical **stationary state**.

The simplest numerical method is to start with a trial energy and keep on changing the value till it satisfies the boundary condition

$$\psi_n \rightarrow 0 \text{ for } |x| \rightarrow \infty \quad \dots 5$$

With ψ as the wavefunction, ψ' and ψ'' the first derivative and second derivative respectively., the fourth order

$$k_1 = \psi'$$

$$m_1 = \psi''(x, \psi) = -2(E - \frac{1}{2}x^2)\psi$$

$$k_2 = \psi' + \frac{1}{2}m_1h$$

$$m_2 = \psi''(x + \frac{h}{2}, \psi + \frac{1}{2}k_1h) \\ = -2(E - \frac{1}{2}(x + \frac{h}{2})^2)(\psi + \frac{1}{2}k_1h)$$

Runge-Kutta coefficients [2] are $k_3 = \psi' + \frac{1}{2}m_2h$ 6

$$m_3 = \psi''(x + \frac{h}{2}, \psi + \frac{1}{2}k_2h) \\ = -2(E - \frac{1}{2}(x + \frac{h}{2})^2)(\psi + \frac{1}{2}k_2h)$$

$$k_4 = \psi' + m_3h$$

$$m_4 = \psi''(x + h, \psi + k_3h) \\ = -2(E - \frac{1}{2}(x + h)^2)(\psi + k_3h)$$

Hence, the wavefunction and its derivative at $(x+h)$ is

$$\psi(x + h) = \psi(x) + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)h$$

$$\psi'(x + h) = \psi'(x) + \frac{1}{6}(m_1 + 2m_2 + 2m_3 + m_4)h$$

Computation using Microsoft excel gives the following.

The eigenfunction obtained with $E = 2.5$ and the corresponding graphs is shown in Fig. 2

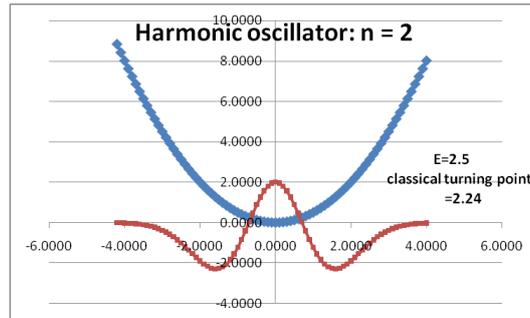


Fig. 2 Wavefunction of harmonic oscillator with $E = 2.5$

The continuity of the derivative of the eigenfunction is shown in Fig. 3

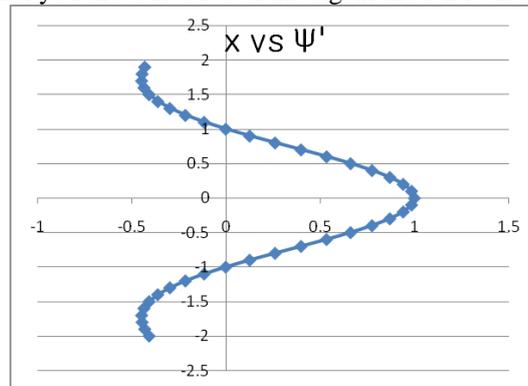


Fig. 3 The derivative of the eigenfunction is also continuous.

III. Results of harmonic oscillator

- The eigen values are discrete, $E = 0.5, 1.5, 2.5, \dots$ energy units only satisfy the boundary condition $\psi \rightarrow 0$ for $x \rightarrow \infty$ and $x \rightarrow -\infty$
- For eg., $E = 0.5$ satisfies the boundary condition $\psi \rightarrow 0$ for $x \rightarrow \infty$ and $x \rightarrow -\infty$ as shown in Fig. 5 (a) But, for E greater than 0.500 the wavefunction tends to minus infinity (as shown in Fig. 5 (c)) while for E lesser than 0.500 , the wavefunction tends to plus infinity (as shown in Fig. 5 (b)). These wavefunctions are not physically acceptable.
- All acceptable eigenfunctions have eigen values that are **half integers**. Thus, $E_n = (n + \frac{1}{2})$ units where $n = 0, 1, 2, \dots$
- n refers to the nodes of the oscillatory function within the potential well. For example, at $E = 2.5$ units, there are only two nodes.
- Odd n wavefunctions are **as**symmetrical, hence refer to odd parity while for even n the wavefunction are symmetrical, thus have even parity (Fig 4 & 5(a) respectively)

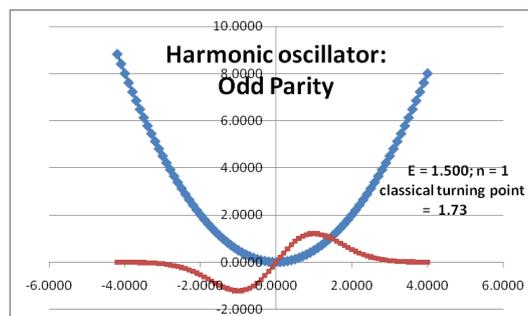


Fig 4. Odd parity for odd n

- $\psi = 0$ at $x = 0$ for odd n
- $\psi = \pm 1$ at $x = 0$ for even n

- For even n
- Let $n = 2m$ where $m = 0, 1, 2, \dots$
- When m is even
- $\psi = +1$
- and when m is odd
- $\psi = -1$

- $\psi' = \pm 1$ at $x = 0$ for odd n
- $\psi' = 0$ at $x = 0$ for even n

- For odd n
- let $n = 2m + 1$ where $m = 0, 1, 2, \dots$
- When m is even
- $\psi' = +1$
- and when m is odd
- $\psi' = -1$
- Accuracy of the eigenvalue depends on the step-size h . Uncertainty decreases with decreasing step-size.
- Refer to (Fig 5(a) & 6 (a)).
-

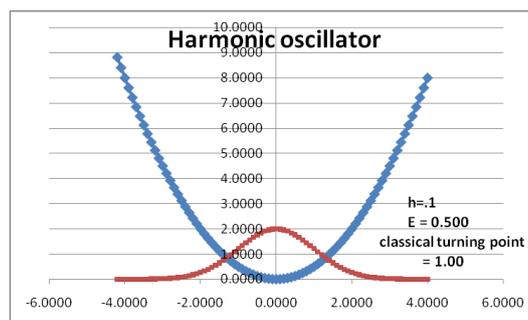


Fig 5(a) Wavefunction tends to zero at $\pm\infty$ and has even parity for even n .

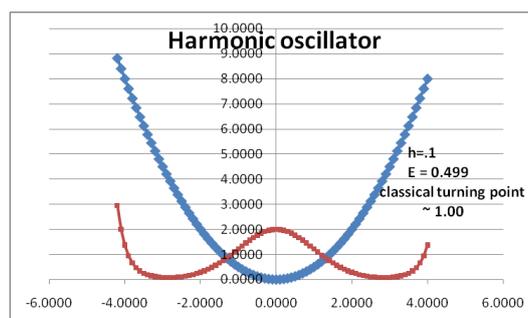


Fig 5(b) Not a meaningful wavefunction.

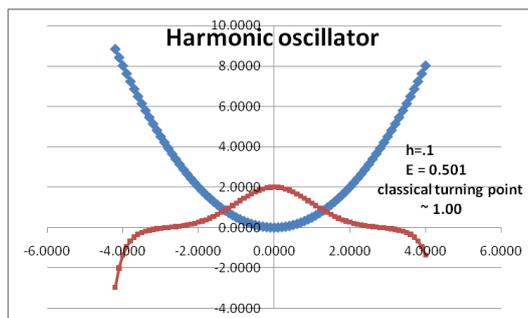


Fig 5(c) Not a meaningful wavefunction

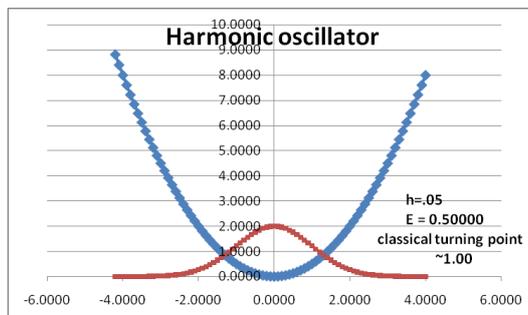


Fig. 6(a) Meaningful wavefunction with Energy 0.50000

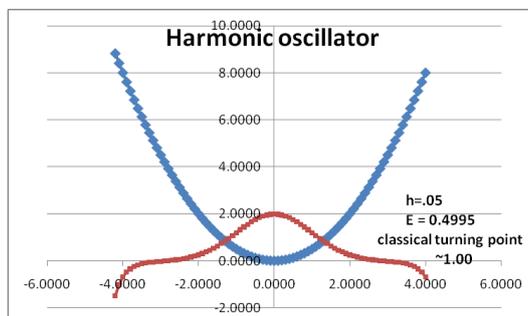


Fig 6 (b) Not a meaningful wavefunction, h=0.05.

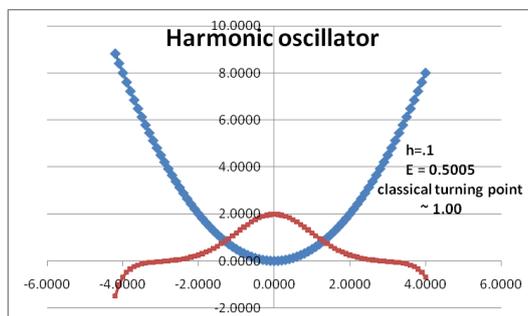


Fig 6 (c) Not a meaningful wavefunction h=0.05

Eg., $E = 1.500 \pm 0.001$ for $h = 0.1$ as shown in Fig 5 (a),(b),(c) and $E = 1.5000 \pm .0005$ for $h = 0.05$ as shown in Fig 6 (a),(b),(c).

○ The normalization constant increases the amplitude/intensity of the wave function, but does not affect otherwise.

○ Like in Classical theory, for large n ($\cong 100$) the probability of obtaining the particle at the turning points is more as shown in the Fig. 7. This is the **Bohr's correspondence principle**. [3]

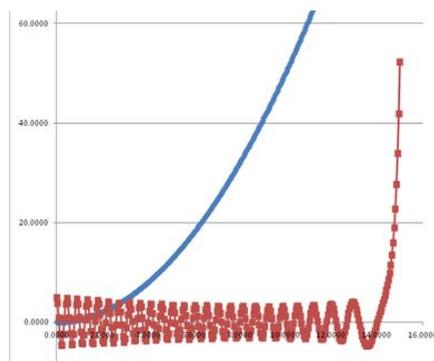


Fig 7. Bohr's correspondence principle for $n = 100$

Thus, the animated wavefunction answers all the questions and is a novel method to explain difficult topics to young students of Physics in the classroom.

For watching the animation, go to the link [View the spread sheet](#) and use the excel sheet. Change the eigenvalue E quickly and watch the modifications in the wavefunction in the graph. The wavefunction explains it all.

Acknowledgement

I am grateful to my students who have prompted me to delve deep into a topic for writing good books.

References

- [1]. Eyvind Wichman, "Quantum Physics", Berkeley Physics Course, Vol 4 McGraw Hill Companies Inc.(2011)
- [2]. RC Verma, PK Ahluwalia, KC Sharma, "Computational Physics An introduction", New Age International Publishers pp (1999)
- [3]. Sarmistha Sahu, "Concise Physics", Vol 5 Statistical Physics and Quantum Mechanics, Subhas Stores (2013)
- [4]. C N Banwell "Fundamentals of Molecular Spectroscopy" Tata McGraw-Hill Publishing Company Limited , 3rd ed (1983)