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Derivative Analysis of Schrodinger Wave Equation based on Theory of Particle in a Box

[1]K. Udaya Kumari
[1]*Assistant Professor, Department of Humanities & Sciences,*
Dr. K. V. Subba Reddy College of Engineering for Women, Kurnool, Andhra Pradesh
[1]*k.meryudaya125@gmail.com*
[2]B.Sridevi
[2]*Associate Professor, Department of Humanities & Sciences,*
Dr. K. V. Subba Reddy College of Engineering for Women, Kurnool, Andhra Pradesh
[2]*sridevi.rcew@gmail.com*

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Abstract
Schrodinger wave equation is basically a partial differential equation applicable to linear systems, which more specifically describes about the wave function of quantum mechanical related systems. In this paper, much focus is emphasized on explaining about a particle which is inside a 1-dimensional box is considered to be as a fundamental and quantum mechanical related approximation usually describing about the translatory motion of a single-particle which is confined inside a deep well from which it cannot be escaped further respectively.

Keywords: *Schrodinger wave equation, quantum mechanical, translatory motion, wave function.*

I. INTRODUCTION

The particle in a box problem is considered to be as one of the common applications of a quantum mechanical based models and has to be converted as a simplified system which consisting of a particle moving in horizontal direction. The solutions to the problem will basically give the possible resultant values of E and ψ respectively, in which the particle can have inherently. E generally represents the value of allowed energy levels and $\psi(x)$ is a type of wave function, which when further squared results in giving the probability of locating a particular particle at a certain position within the box at that energy level [1].

The equation is employed in physics domain and most of chemistry related problems basically deals with the atomic structure of matter [2]. It is considered to be a powerful mathematical tool and the complete basis of wave mechanics. Schrodinger's equation shows the entire wave such as properties of matter.

The Schrodinger equation essentially consists of two forms: one is time-dependent and other is time-independent form. One usually solves any of the two forms in order to get the probability distribution of an electron which depends up on its three quantum numbers. Solving the time-dependent form shall also give us the time evolution of the wave function in particular.

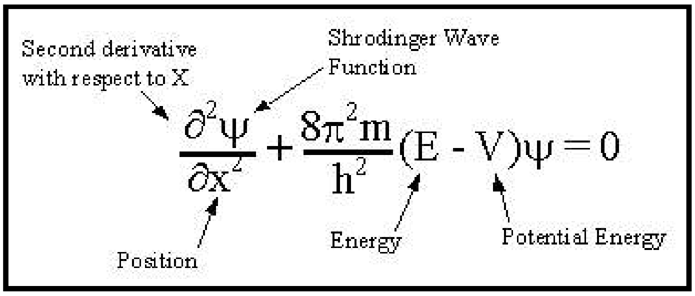

Fig: 1 description of Schrodinger equation

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The solution to the above mentioned equation is a wave which more specifically describes about the quantum aspects of a system. Furthermore, the physical interpretation of the wave is one of the crucial philosophical issues related to quantum mechanics field.

II. Analysis of particle in a box

Mathematically, in order to solve the problem of a particle in a 1-dimensional box respectively one should basically follow the following steps mentioned below:

1. Defining the Potential Energy function (V)
2. Solving the Schrodinger wave Equation
3. Defining the wave related function
4. Defining the allowed various energy levels.

Step1: Defining the potential function (V):

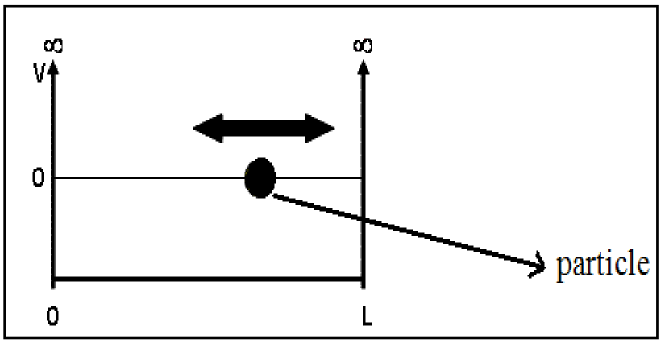

Fig: 2 A particle in a well of 'L' dimension

The potential energy is assumed to be as '0' inside the box in particular i.e., V=0 for 0<x<L and reaches to infinity at the walls of the box with V=∞ for x<0 or x>L.

Step2: Solving the Schrodinger equation:

$$-\frac{h^2}{2m}\frac{d^2\varphi(x)}{dx^2}+V(x)\varphi(x)=E\varphi(x) \text{ ------------ (1)}$$

The above equation can be further modified for a particle of mass *'m'* which is free to move parallel towards the x-axis with zero potential energy i.e., V = 0 everywhere in the box further resulting in the quantum mechanical related description of the free motion of particle in one-dimensional analysis.

$$-\frac{h^2}{2m}\frac{d^2\varphi(x)}{dx^2}=E\varphi(x) \text{ (for V=0) ---------- (2)}$$

The equation (2) represents a general solution of,

$\varphi(x)=P\sin(kx)+Q\cos(kx)$ ------- (3), where P, Q, and k are termed as constants.

Step3: Defining the wave function:

For defining the wave function, we need to apply the boundary conditions in order to obtain the solution to a particular system. According to the boundary conditions specified, the probability of finding a particle at x=0 or x=L is considered to be as 'zero'.

When x=0, sin (0) = 0, and cos(0) =1; thus, Q must be equal to 0 in order to fulfill the boundary condition giving further relation,

$$\varphi(x)=P\sin(kx) \text{ ---------- (3)}$$

Now, differentiating the above wave function with respect to x, we get,

$$\frac{d\varphi}{dx}=kP\cos(kx) \text{ ------ (4)}$$

Again differentiating equation (4), we obtain,

$$\frac{d^2\varphi}{dx^2}=-k^2P\sin(kx) \text{ ------- (5)}$$

Further one can express equation (5) as,

$$\frac{d^2\varphi}{dx^2}=-k^2\varphi \text{ ------ (6) (based on equation (3))}$$

We can further obtain the value of k based o Schrodinger equation as,

$$k=\sqrt{\left(\frac{8\pi^2mE}{h^2}\right)} \text{ ---------- (6)}$$

Step4: Determining the various energy levels:

We can find the value of E_n as follows:

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$$E_n = \frac{n^2h^2}{8mL^2} \text{ --------- (7)}$$

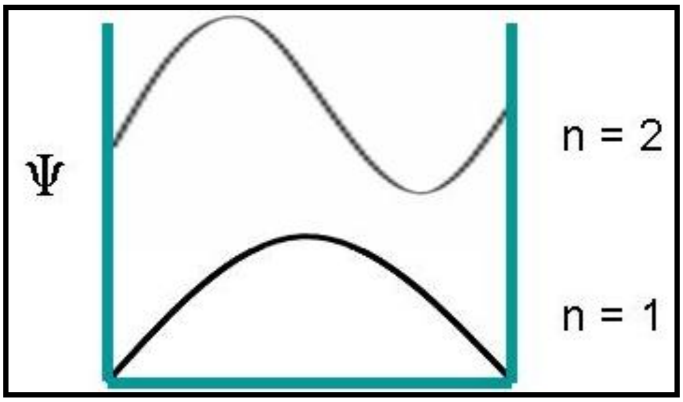

Fig. 3 Wave function changing with ‘n’

III. INFERENCES

The above result explains us about:

1. The energy of a particle is said to be quantized.

2. The lowest possible energy of a particle is NOT considered to be as zero. This is called the ‘zero point energy’. This means that, the particle can never be at rest because it possesses little kinetic energy in it. This is also considered to be in consistent with ‘Heisenberg Uncertainty Principle’.

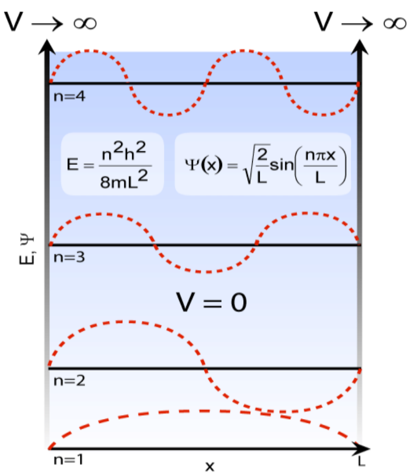

Fig. 4 Wave function analysis varies with ‘n’ value

IV. CONCLUSION

This paper illustrates about the derivation of finding the values of k and En related to Schrodinger wave equation, based on the particle in a box of a 1-dimensional system. In this paper, one can identify the importance of the Schrodinger wave equation in terms of finding the various energy levels. A step by step analysis has been illustrated to understand the method of obtaining the parameters of Schrodinger equation. Clearly, it has been illustrated that, with the change in the parameter of n, there will be considerable variation in the wave function.

V. REFERENCES

[1] Raymond, Chang, “Physical Chemistry for the Biosciences”, Sansalito, CA University Science, 2005.

[2] Schrodinger, Erwin, "An Undulatory Theory of the Mechanics of Atoms and Molecules", Physics, Rev-28 (6), 1049–1070, December 1926.

[3] Erwin Schrodinger, "The Present situation in Quantum Mechanics", page no. 9-22, 1983.

[4] K. Algeilani, “Derivation of Klein Gordon equation from Maxwell’s electric wave equation”, International Journal of Physical Sciences, USA, 2014.

[5] Taylor JR, “Classical Mechanics”, University Science Books, 2005.