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Analyzing the Time Evolution of a Particle by Decomposes the Initial State Confinement in 1D Well into the Lowest Eigenstates Energy

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ABSTRACT

In this work, we obtained the time evolution of the wave function of a limited quantum system (1D Box), hence getting a mathematical model to describe the system. By using programming computes, it performs a time evolution that decomposes the initial state into the 2,10, and 20 lowest energy eigenstates. Finally, by comparing numerical de-composition coefficients for the wave function to the analytical values, it found the number of knots increases directly versus the energy of the particle's quantum state. As a result, the mean bending given by the second derivative which is proportional to the kinetic energy operator should increase. We found there is a negligible mean and standard deviation of the energy in units of the ground state energy.

Keywords- Schrodinger-equation, Particle-in-Box, Confinement, Time-evolution.

I. INTRODUCTION

In the usual quantum mechanics, for the general stationary-state problems, the wave function should vanish at infinity as a constraint imposed on it [1,2,3]. However, in some special systems, it is recommended to be desirable to presumption a bounded or enclosed system by requiring that the same vanishes on nodes or surfaces of a finite region of space [4]. The first was attempted in 1937 by confinement mode in a quantum system to simulate the effects of pressure on the energy of a hydrogen atom, depolarization, and ionization potential within an impenetrable spherical cavity [5]. Then, followed by [6]. The molecule or a multi-electron atom has different properties of a confined quantum system that are fundamentally different from their free or unbounded [7].

In the last ten years, models of spatially confined quantum particles by external potentials had great interest from various fields of physics and chemistry [8]. All practical applications which include atoms and molecules confined within cavities, charges in semiconductor wells and neutral, Excitons in quantum dots and Synthetic atoms, etc., are used as important models for the impurities or luminescence in solids, vibrational spectra of point defects, magnetic properties in semiconductor nanostructures [9,10], thermodynamic of nonideal gases, ionized plasmas, etc. [11]. It also holds promise for potential applications in nano and molecular-sized circuit devices including quantum computers [12].

The form was studied by many researchers employing a variety of techniques such as WKB and perturbation theory [13,14,15,16]. The effect of finite boundaries on energy levels was reported by [17], while the quantum confinement in 1D box systems was demonstrated by [18,19].

This work focuses on analytical and numerical solutions, using the exact known method. We are going to present an algorithm to solve the time-independent

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equation efficiently of a particle in a box with different states, while that program will expand the initial wave function onto the basis formed from the eigenstates of the Hamiltonian to get the time evolution.

In this work, we are going to calculate the evolution time and lowest eigenstates for the electron whose confinement in the well by Solving the box model which is used to describe a trapped particle in a 1D well.

II. THEORY

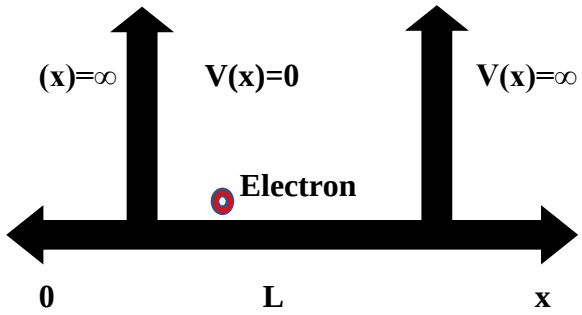
The simplest application of the Schrödinger equation is the particle in the box model system, but it leads to the clarification of many basic concepts in quantum mechanics, especially the movement of electrons within metals [20,21,22]. For a particle moving in one dimension in the direction of the x-axis, the equation of the Schrödinger equation is [23]:

$$-(\hbar/2m)\,\psi''(x) + V(x)\psi(x) = E\psi(x) \quad \ldots(1)$$

This is a way of making sure that the electron is confined to the region of the central box which acts as a bound box. In this case, the potential (V = 0) is inside the box and the walls of the box cannot be penetrated [24]. We can place the origin of our x coordinate system anywhere we choose for convenience, see Scheme 1.

Here we assume that the particle's motion is free between the two ends x=0 and x=L, which represents the limits of a box and cannot penetrate past either end. These limits are equivalent to potential energy which depends on the position x [25].

$$V(x) = \begin{cases} 0 & 0 \le x \le L \\ \infty & x < 0 \text{ and } x > L \end{cases} \quad \ldots(2)$$



Scheme 1. The box barriers have a very high large potential, but the potential inside the box is zero [26].

In this case, the particle is bound inside the potential well between x=0 or x=L, and by the requirement of the wave function to be continuous, this means:

$$\psi(x) = 0 \text{ for } x < 0 \text{ and } x > L \quad \ldots(3)$$
$$\psi(0) = 0 \text{ and } \psi(L) = 0 \quad \ldots(4)$$

Schrodinger equation reduces to the free particle form:

$$-\hbar^2/2m\,\psi''(x) = E\,\psi(x) \quad \ldots(5)$$

Which have a solution as:

$$\psi''(x) + k^2\psi(x) = 0 \quad \ldots(6)$$
$$k^2 = \frac{2mE^1}{\hbar^2} \quad \ldots(7)$$
$$\psi(x) = A\sin kx + B\cos kx \quad \ldots(8)$$
$$\psi(0) = A\sin 0 + B\cos 0 = B = 0 \quad \ldots(9)$$
$$\psi(a) = A\sin kL = 0 \quad \ldots(10)$$
$$kL = n\,\pi \quad \ldots(11)$$

Where A and B are constant. From the above equations we can get:

$$E_n = \frac{\hbar^2\pi^2}{2mL^2}n^2 = \frac{h^2}{8mL^2}n^2 \quad \ldots(12)$$

Where: $n = 1,2,,3$ ...n called quantum number. When n=1 we can get the first energy level of the particle in the box.

$$E_1 = \frac{h^2}{8mL^2} \quad \ldots(13)$$

The eigenfunction of the particle in the box is given by:

$$\psi_n(x) = A\sin(n\pi x/L) \quad \ldots(14)$$
$$\int_0^a |\psi_n(x)|^2 dx = 1 \quad \ldots(15)$$

By normalized condition, we can get A constant:

$$A^2\int_0^L \sin^2(n\pi x/L)dx = A^2(L/\pi n)\int_0^{n\pi}\sin^2\theta\,d\theta$$
$$= A^2(L/2) = 1 \quad \ldots(16)$$

So that:

$$A = \sqrt{\frac{2}{L}} \quad \ldots(17)$$

So, we get normalized eigenfunctions for the particle inside the box which are dependent on the quantum number n and length of the box.

$$\psi_n(x) = \sqrt{L/2}\sin(n\pi x/L) \quad \ldots(18)$$

By using this equation there are several solutions can be obtained for different values of n.

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The time evolution of the wave function with the time-dependent Schrodinger equation is given as:

$$\Psi(x,t) = \psi(x)e^{-iEt/\hbar} \quad \ldots (19)$$

Wave function becomes:

$$\psi_n(x) = \sqrt{L/2}\sin(n\pi x/L)\, e^{-iEt/\hbar} \quad \ldots (20)$$

In this case, the phase part in equation (20) can be expanded into two parts real and imaginary part, so that the wave function becomes as:

$$\Psi(x,t) = \underbrace{\left(\sqrt{L/2}\sin(n\pi x/L)\right)(\cos E_n t/\hbar)}_{\text{real part}} - \underbrace{i\left(\sqrt{L/2}\sin(n\pi x/L)\right)(\sin E_n t/\hbar)}_{\text{imaginary part}} \quad \ldots (21)$$

Which can rewrite slightly to:

$$\Psi(x,t) = \underbrace{\left(\sqrt{L/2}\sin(n\pi x/L)\right)(\cos E_n t/\hbar)}_{\text{real part}} - \underbrace{i\left(\sqrt{L/2}\sin(n\pi x/L)\right)\left(\cos(E_n t/\hbar) - \frac{\pi}{2}\right)}_{\text{imaginary part}} \quad \ldots (22)$$

The complex part of the equation (22) oscillates out of phase by $\frac{\pi}{2}$, and represents the time evolution behavior of the lowest eigenstates [27].

III. RESULTS AND DISCUSSION

One of the most important features of the quantum states (wave functions of lowest energy) of particles trapped in the box is the phenomenon of knots [28]. At these knots, the wave functions disappear. There is a completely zero probability of finding the particle. Three probability densities have been identified at which the particle can be located, at the 20 lowest energies It seems from general mathematics logic that the number of knots increases directly versus the energy of the particle's quantum state, which can be justified by a symmetry between the increase in the number of nodes and the number of vibrations in the wave function and its steepness. According to that symmetry, the mean bending given by the second derivative which is proportional to the kinetic energy should increase. So, proportionally the higher number of nodes, the power is higher. This conclusion is profound evidence that is invaluable in more complex quantum systems.

Fig. 1. A comparison between the analytical and 5 numerical values of the wave function for the lowest energy of the eigenstates of a particle confined inside the box. The evolution of the states of the function is clear from the lowest energy to the highest energy. The yellow line represents the highest energy of the eigenstates considered part of the separated values of the lowest eigenstate's energy. It is clear that eigenstates reduce to respective unbounded values inside the potential enclosure but not near the walls. They become wave box eigenstates when the separation of points is large compared to the box size**.**

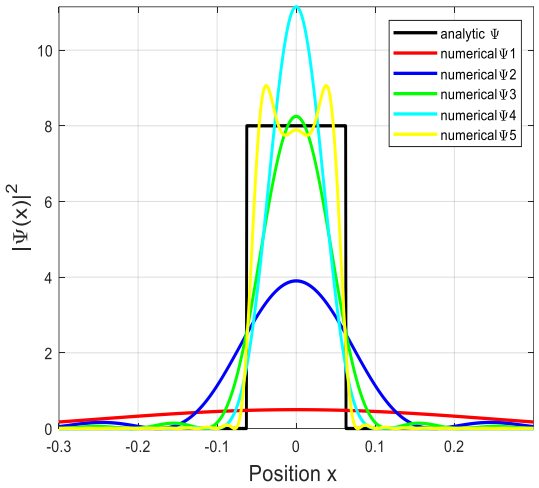

Fig. 1. Approximation of the Initial State wave function for N(2-20) Lowest Particle in Box Energy Eigenstates.

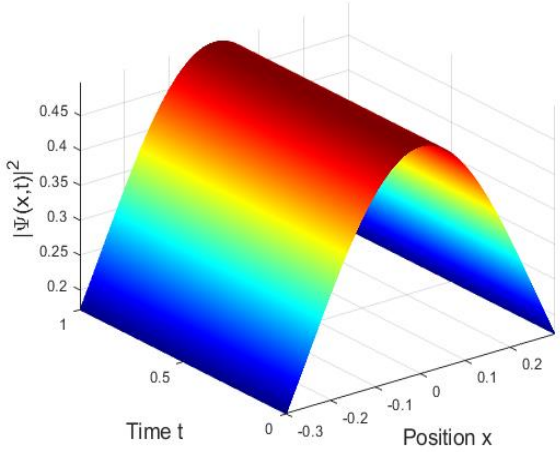

Fig. 2. Numerical Time Evolution at two Lowest Particle in Box Energy Eigenstates, probability density in length unit = 0.2246.

In fig. 2. The time evolution of the wave function inside the box at the lowest energy of the eigenstates 2 per unit length, at the value of the probability density 0.2246. Fig. 3 and 4 are generated in three dimensions by solving equation (22) of the ground state of the well on a 1D box basis. The time evolution wave function is then simply the superposition of the box basis states with appropriate time-dependent phase factors and using the probability density as a function of the time to show the wave function at the 10 and 20 lowest energies. Probability density in length unit = 0.8512 and 0.9629 respectively.

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As shown in table 1. the probability density is fixed at the 2 lowest eigenstates energy, while the variation begins to occur at the higher 10 and 20 lowest eigenstates energy.

Table 1. Probability Density Function at 2,10 and 20 lowest energy eigenstates per length units.

Probability Density Function		
2 lowest energies	**10 lowest energies**	**20 lowest energies**
0.2246	0.8512	0.9629
0.2246	0.4636	0.4815
0.2246	0.7874	0.8906
0.2246	0.4636	0.4815
0.2246	0.8512	0.9629

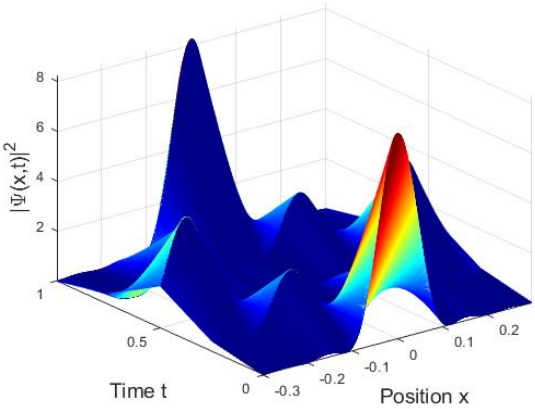

Fig. 3. Numerical Time Evolution at ten Lowest Particle in Box Energy Eigenstates, probability density in length unit = 0.8512.

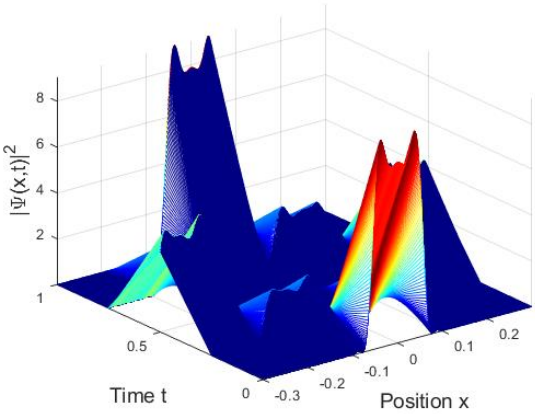

Fig. 4. Numerical Time Evolution at twenty Lowest Particle in Box Energy Eigenstates, probability density in length unit = 0.9629.

IV. CONCLUSION

A solution of the Schrodinger equation analytically and numerically methods have been employed to the problem of a particle confined in a 1D box and time evolution for the lowest eigenstates energy of the particle. the lowest eigenstates energy was chosen between 2 to 20 of the wave function and comparing the analytical with the numerical results using a computer program.

The eigenstates reduce to respective unbounded values inside the box potential enclosure but not near the barriers. The eigenstates of the wave function are formed when the separation of nodes is large compared to the box size. also, a negligible standard deviation of energy values was obtained about (177.652305378225) in units of the ground state energy.

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