Significant Analogies of Classical Mechanics and Quantum Mechanics

Sandar Myint Oo*

Abstract

This paper is illustrated about the behavior of quantum mechanics looked like the that of classical mechanics when the principle quantum number approaches large values. This phenomenon was explained based on the energy quantization and probability density. When the energy levels of Bohr hydrogen atom for large quantum states are determined, these energy values are continuous values. It has been stated that the one- dimensional particle in a box wave function and probability density by changing the quantum numbers. The probabilities of finding the particle in a box for two sections are calculated with the aid of computer programming. It is found that the calculated probability density results depend not only on the quantum number but also on particle's location.

1. Introduction

All branches of physics which were developed before the year 1900 are known as classical physics or the classical theory of physics. Newtonian mechanics and Maxwell's electromagnetic theory were the two main branches of classical physics. The classical physics works perfectly well within the realm of the macroscopic world. Attempts were made to explain the microscopic systems by introducing the new concepts contrary to the classical ideas. Quantum mechanics is the theory of microscopic systems. It must yield accurate results not only on the microscopic scale, but also the classical limit as well. For microscopic systems, the size of action variables is of the order of h; for instance, the angular momentum of the hydrogen atom is $\ell = n\hbar$, where n is infinite. Since λ =h/p the classical domain can be specified by the limit $\lambda \to 0$. This means that, for a system whose de Broglie wavelength is too small compared to its size, this system can be described accurately by means of classical physics. The classical limit can be described by the limit $h \to 0$ or, equivalently, by $\lambda \to 0$. In these limits the results of quantum mechanics should be similar to those of classical physics. Bohr formulated the correspondence principle in 1923 to serve as a guide in the development of quantum theory. It states that the quantum theory should agree with classical physics in the limit in which quantum effects become insignificant. The classical limit is attained when the quantized variables are much larger than their minimum quantum size. The correspondence principle inspired most of Bohr's work and has played an important role in the initial development of quantum theory. Quantum mechanics cannot predict the occurrence of an event with certainty. The quantum mechanics determines only probability of an event. Therefore, the probability plays a fundamental role in quantum mechanics. The wave function Ψ which represents the wave nature of the particle can be regarded as a measure of the presence of the particle. The probability ranges from zero to one. A probability of one means certainty where as a probability of zero means non-occurrence. The probability of finding the particle in a finite region of space defined by $x_1 < x < x_2$ is given by the integral. The probability of finding the particle under consideration move between $x = -\infty$ and $x = \infty$ is described by

$$\int_{x_1}^{x_2} P(x)dx = \int_{-\infty}^{\infty} \Psi^*(x)\Psi(x)dx = 1 \qquad (1.1)$$

* Lecturer, Dr, Department of Physics, Yadanabon University

2. Energy of the Electron in the nth Bohr Orbit

For the electron moving in an orbit the electrostatic attractive force acting on it provides the centripetal force. Therefore,

$$\frac{mv^2}{r}=\frac{e^2}{r^2} \tag{2.1}$$

where m, e, v and r are the mass, the charge, the tangential velocity and the radius of the electron in the orbit. The total energy E_n of the electron is the sum of the kinetic and potential energies:

$$E_n=\frac{1}{2}mv_n^2-\frac{e^2}{r_n}=-\frac{e^2}{2r_n} \tag{2.2}$$

From Bohr's quantum condition

$$r_n=\frac{n^2h^2}{4\pi^2me^2} \tag{2.3}$$

The energy of the electron in the nth orbit equation may be expressed as

$$E_n=-\frac{2\pi^2me^4}{n^2h^2} \tag{2.4}$$

Substituting the values of m, e and h constants

$$E_n=-\frac{13.6}{n^2}\text{eV} \ , \qquad n = 1, 2, 3, \dots \tag{2.5}$$

This shows that the energy of the ground state of hydrogen is −13.6 eV.

3. The Probabilities in Classical Mechanics and Quantum Mechanics

The classical Mechanics predicts that the probability of finding the particle in a box (PIB) is uniform throughout the box. Classically, the probability is one inside the box of length L. The particle passes back and forth between the walls and it has an equal probability of being found anywhere between x=0 and x=20Å. The classical probability is constant as follow;

$$\text{Classical P(x)} = \frac{1}{L}=0.05 \tag{3.1}$$

Thus the particle is equally likely to be found at any point in the box. In classically, the probability of finding the particle between x=a and x=b is,

$$\text{Classical Probability (a,b)} = \int_a^b \text{Classical P(x) dx} \tag{3.2}$$

The probability of finding the particle in the left-half (or) right-half of the box (between 0 to 10 Å) is 0.5. Consider for the section between a=L/4(5 Å) and b=2L/4(10 Å) with box length 20 Å, the probability of finding the particle is

$$\text{Classical Probability (a,b)} = \int_{L/4}^{2L/4} \text{Classical P(x) dx} = 0.25 \tag{3.3}$$

Therefore, for any quarter of the box (between 0 to 5 Å) is 0.25. The section from L/4 to 2L/4 spans one-fourth of the box, and CM says the probability of finding the particle there is 0.25, which is one-fourth. For another section between a=0.2293L and b=0.6817L, the probability of finding the particle is

$$\int_{0.2293L}^{0.6817L} \text{Classical P(x) dx} = 0.4524 \tag{3.4}$$

In Quantum Mechanics (QM), the wave function of the particle in a box is

$$\Psi_n(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right) \qquad \text{where } (n = 1,2,3,\ldots) \qquad (3.5)$$

In this paper, the wave functions with the box length L is 20Å and quantum number n is the lowest five states(n=1,2,3,4,5) are determined against the x-coordinate by using following excel formula.

= (SQRT (2/20))*(SIN (N*A2*3.141592653589/20)) (3.6)

The probability density in quantum mechanics is denoted by P(x);

$$P(x) = \Psi_n^*(x)\Psi(x) = |\Psi(x)|^2 \qquad (3.7)$$

and it is real. The lowest five probability distribution functions are determined against the x-coordinate by using excel formula as follow;

= ((SQRT (2/20))*(SIN (N*A2*3.141592653589/20))) ^2 (3.8)

Then the probability of finding the particle in each region for the ground state wave function inside the box length 20 Å is determined by the following;

$$P(x)dx = \frac{2}{L}\int_0^{L/4}\sin^2\frac{\pi x}{L}dx = 0.0909 \qquad (3.9)$$

$$P(x)dx = \frac{2}{L}\int_{L/4}^{2L/4}\sin^2\frac{\pi x}{L}dx = 0.4092 \qquad (3.10)$$

$$P(x)dx = \frac{2}{L}\int_{2L/4}^{3L/4}\sin^2\frac{\pi x}{L}dx = 0.4092 \qquad (3.11)$$

$$P(x)dx = \frac{2}{L}\int_{3L/4}^{L}\sin^2\frac{\pi x}{L}dx = 0.0909 \qquad (3.12)$$

Now, examine the probability of finding the particle in a specific section of the box for the various quantum numbers. The probability of finding the particle from x=a to x=b, in quantum state n is;

$$\text{Quantum Probability (n,a,b)} = \int_a^b \text{Quantum}\, P(x)\, dx \qquad (3.13)$$

$$P\,dx = \int_a^b \Psi_n^*(x)\Psi_n(x)dx = \int_a^b\left(\sqrt{\frac{2}{L}}\sin\frac{n\pi x}{L}\right)^*\sqrt{\frac{2}{L}}\sin\frac{n\pi x}{L}dx \qquad (3.14)$$

$$P\,dx = \frac{1}{L}\left[(b-a) - \frac{L}{2n\pi}\left(\sin\frac{2n\pi}{L}b - \sin\frac{2n\pi}{L}a\right)\right] \qquad (3.15)$$

The above equation is solved with FORTRAN programming. In this paper consider for two sections, start to do first is used a= L/4 and b = 2L/4. Then another section a = 0.2293L and b = 0.6817L is calculated.

4. Results and Discussion

According to energy of hydrogen atom, the calculated energy values of hydrogen atom from n= 1 to n=100 levels are shown in Figure (4.1). The energy values of hydrogen atom for large values of n are so close together and they become indistinguishable. Since the energy of a Bohr orbit is proportional to $1/n^2$, it can be seen the energy values of hydrogen atom are continuous values in limit quantum number $n \to 100$. The continuous value of energy is one of the concepts of classical physics. The quantum theory must approach classical theory in the limit $n \to \infty$, where n is a quantum number. This phenomenon is the Bohr's correspondence principle. Then the particle in a box system is proved the wave functions and probability densities change as the quantum number increase. The graph of the lowest five state wave functions against the x-coordinate is shown in Figure (4.2(a)). By changing the n=1, 2, 3, 4, 5 the plots change as n increases. If the description is denoted by 'node', a node is a location where Ψ changes sign. The five wave functions graph shows that the number of nodes increases as n increases. For the graph of the lowest five probability densities for n=1, 2, 3, 4, 5 against the x-coordinate is shown in Figure (4.2(b)). It can be seen that the peaks are closer when the quantum number n becomes larger. This means that the probability of finding the particle at any point inside the box is nearly. Thus, the results of quantum mechanics reduce to those of classical physics when the quantum number n becomes very large.

Next, the corresponding principle by using particle in a box in terms of probability density of finding a particle is attempted to explain. The classical probability function is constant with a value of 1/L. This is, the probability density is the same at any point in the box. When the classical probability distribution of ground state (n=1) wave function PIB is performed inside the box length L=20Å, it is 0.05 at any point. In quantum mechanics, the quantum functions show peaks of magnitude 2/L and some points of the box where the probability is very small. The CM and QM are not the same in the probability density for ground state wave function against the x-coordinate at any point illustrated by Figure (4.3). Then the probability of finding the particle between within the each quarter region for ground state of PIB is calculated in Table (4.1). It is found that there are difference between CM and QM. Therefore, the probabilities of finding the particle in a specific section of the box are continued to determine by increasing the values of n (n = 2, 3, 4, …, 100). The first section from a=L/4 (5Å) to b=2L/4 (10Å) and second section from a=0.2293L (4.586Å) to b=0.6817L (13.634Å) for the value of n =1 to 100 are determined. The calculated results for each section are shown in Figures (4.4) and (4.5) respectively. If the particle is in various quantum state n=1 to 100, for two sections of the CM and QM probabilities of finding the particle are nearly equal. It can be seen that the probability of finding a particle of QM is not constant values for small quantum states and large quantum states give the same values in both sections. Second section of probability values are more differ than the first section. Significance difference in the behavior is observed at small values of n. It is found that more agreement at large values of quantum number. Therefore, the probability density function depends not only on the particle location in the box but also on the quantum state.

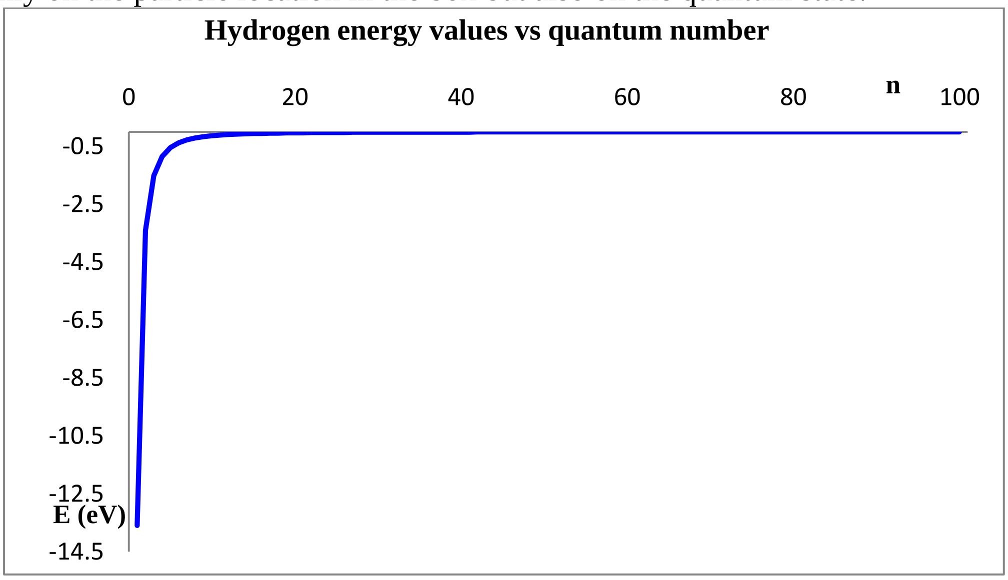
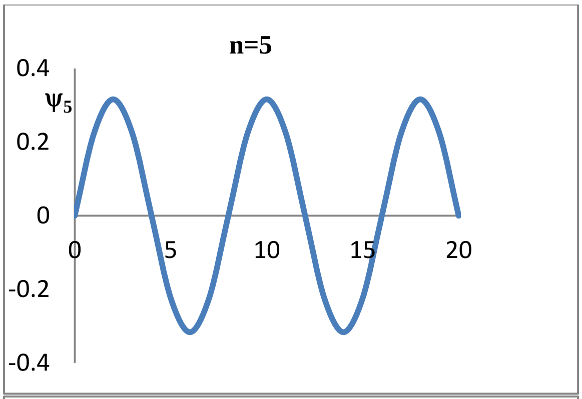


Figure (4.1) The energy values of hydrogen electron Vs quantum number n.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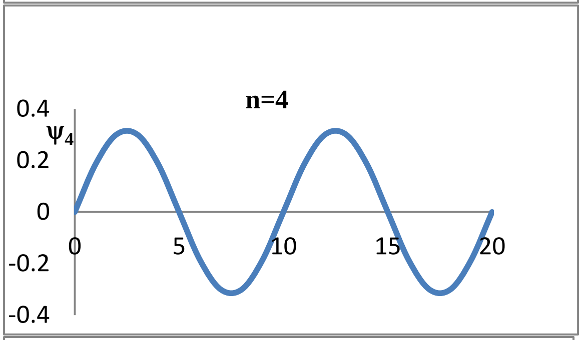
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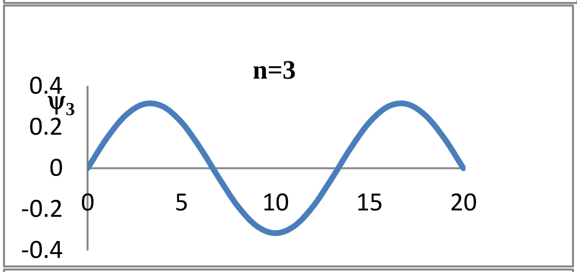
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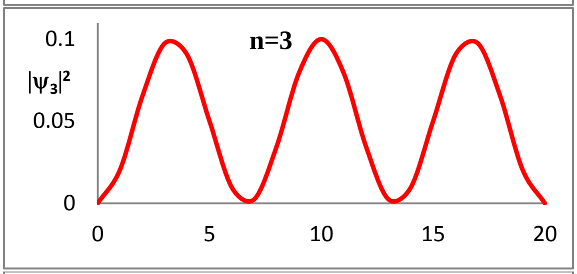
0 5 10 15 20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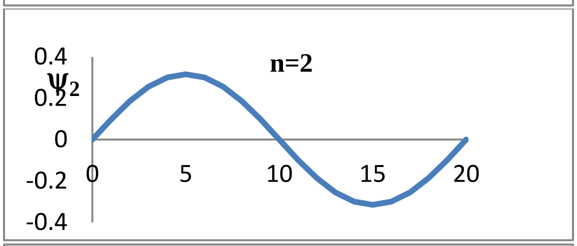
0.05
0
0 5 10 15 20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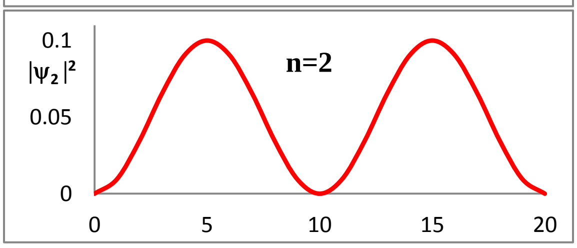
0.2
0
-0.2
-0.4
0 5 10 15 20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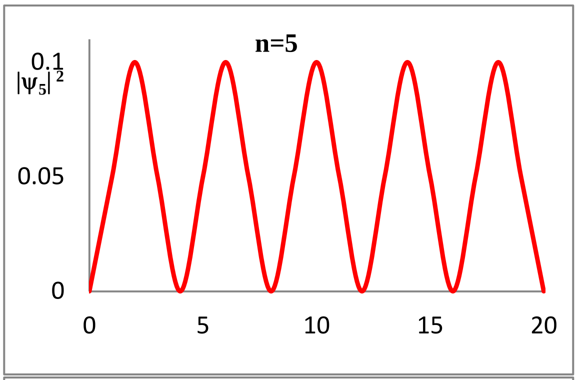
0.05
0
0 5 10 15 20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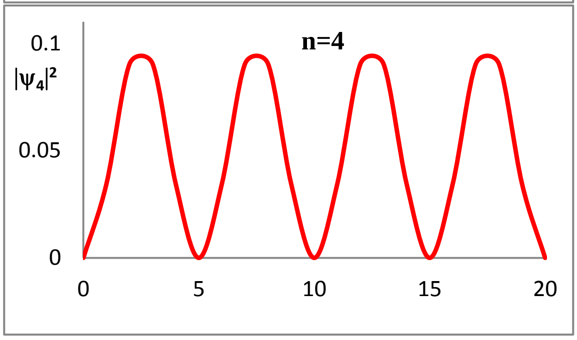
0
0 5 10 15 20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0.05
0
0 5 10 15 20

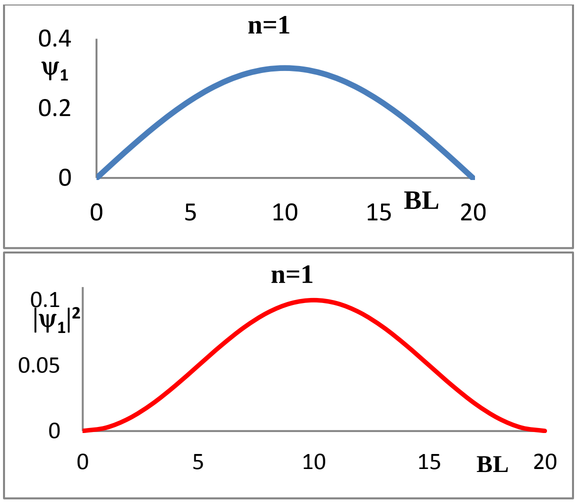

Figure (4.2) (a) The PIB wave functions and (b) The probability densities PIB against the x-coordinate. (n=1 to 5) respectively.

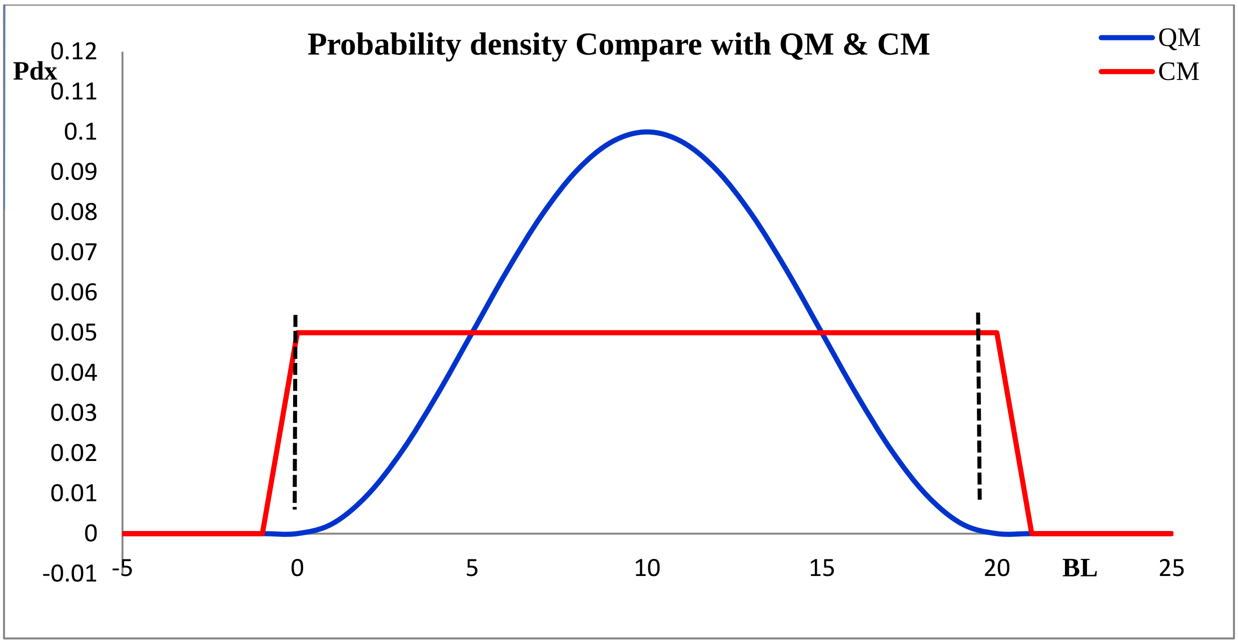

Figure (4.3) The probability density of PIB for ground state compare with QM & CM.

Table(4.1) The calculated values of probability of finding a particle within the quarter region in ground state.

within the region	CM probability density	QM probability density
0 to $\frac{L}{4}$ (0 to 5 A°)	0.25	0.0909
$\frac{L}{4}$ to $\frac{2L}{4}$ (5 to 10 A°)	0.25	0.4092
$\frac{2L}{4}$ to $\frac{3L}{4}$ (10 to 15 A°)	0.25	0.4092
$\frac{3L}{4}$ to L (15 to 20 A°)	0.25	0.0909

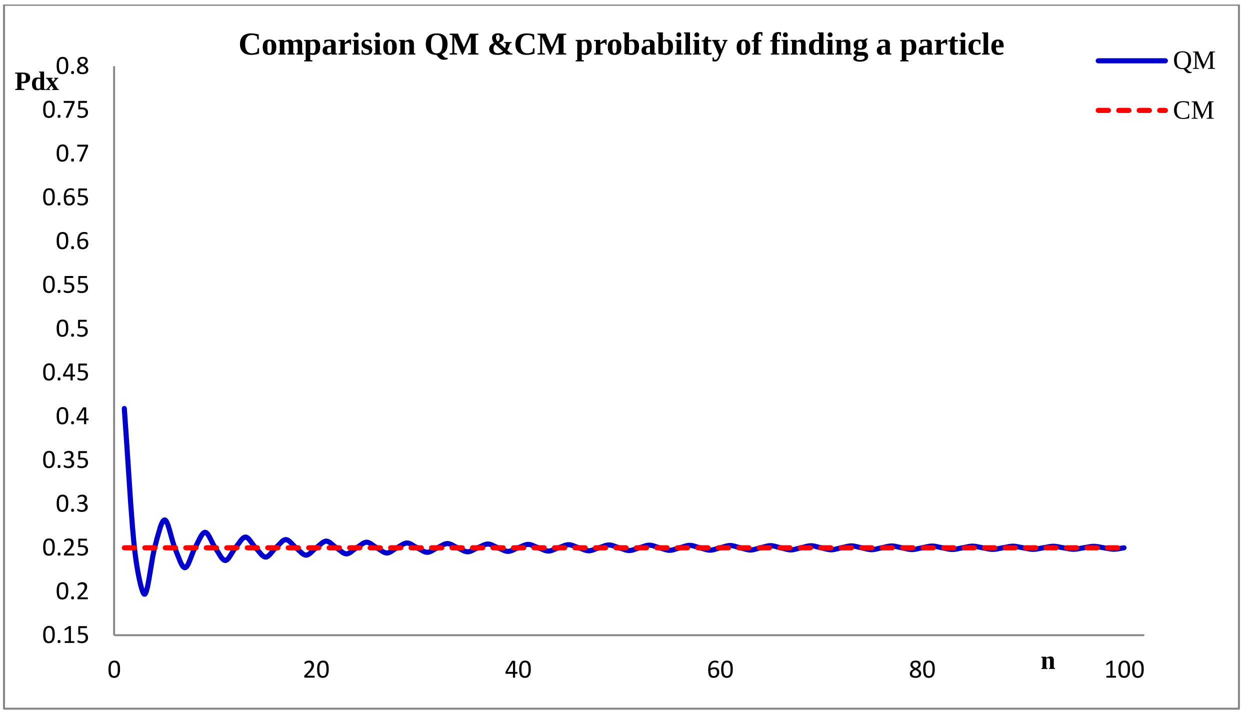

Figure (4.4) The probability of finding the particle for first section from a=L/4 to b=2L/4.

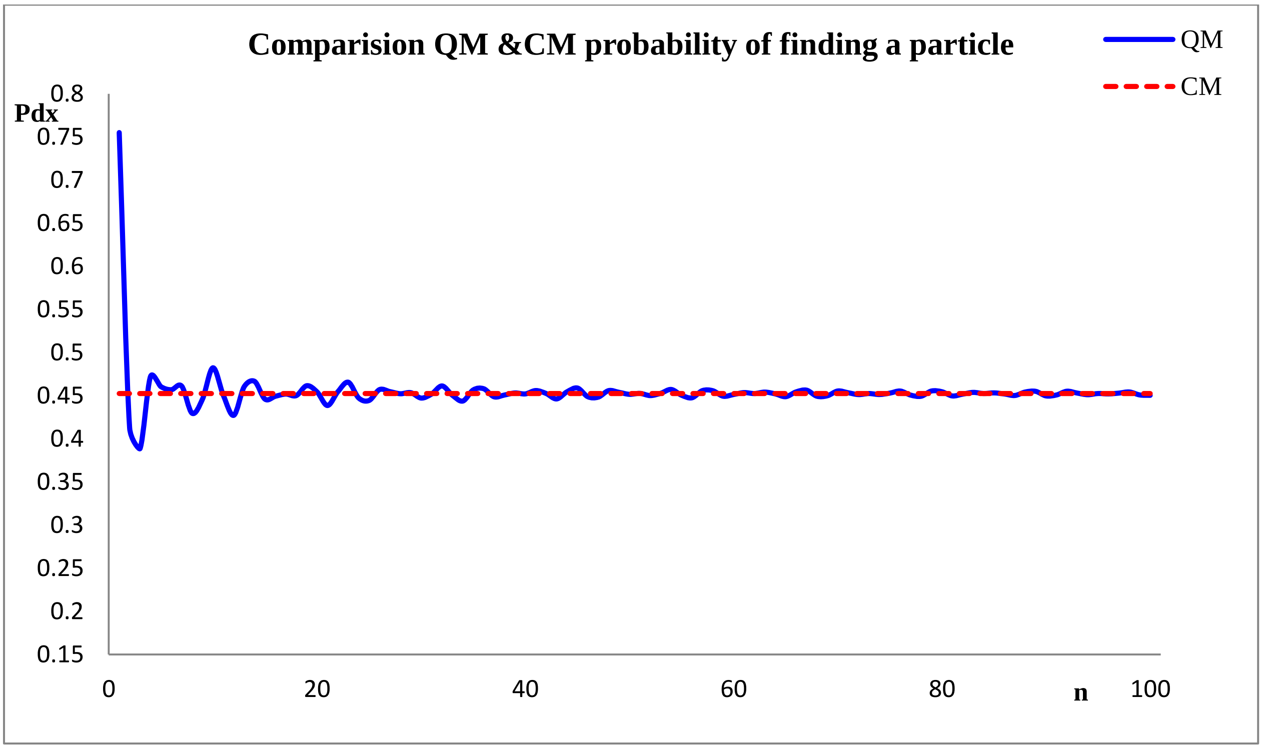

Figure (4.5) The probability of finding the particle for second section from a=0.2293L to b=0.68172L.

Acknowledgements

I would like to express my gratitude to Dr Mg Mg Naing, Rector of Yadanabon University for his encouragement. I am also grateful to Prof. Dr Yi Yi Myint, Head of Physics Department, Yadanabon University, for her valuable comments and suggestions in this research.

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