

CALCULATION OF ENERGY LEVELS AND WAVE FUNCTIONS FOR A QUANTUM DOT

Cho Cho Win*

Abstract

Quantum dot is a nano-scale particle that is confined to the semiconductor as an exciton. The behavior of an exciton in quantum dot has the similar manner as a particle in a box (PIB). It is an individual quantum system which can be analyzed by Schroedinger equation. In this paper, Numerov technique is also used to solve the Schroedinger equation and the results are compared with analytical solutions.

Keywords:Exciton, Quantum dot, Numerov technique

Introduction

Infinite Square Well Potential and Quantum Confinement

Basic quantum mechanical problems such as an infinite and a finite square well may provide insight into the quantum confinement effect for the study of the nanostructured systems.

The quantum confinement means that critical dimensions of the material are on the order of the de Broglie wavelength of an electron. The degree of confinement can be controlled by the width and depth of the confining potential well as shown in Figure (1).

In quantum well, electrons are confined only in one dimension. The quantum wires confine electrons in two dimensions. The electron is not confined along the wire. An electron, in a quantum dot, is confined in three dimensions.

As the confining dimension decreases and reaches a certain limit, typically in nanoscale, their energy levels become discrete and their electronic and optical properties deviate substantially from those of bulk materials [Buhro, W. E., and V. L. Colvin,(2003)]. The use of low dimensional structures has significantly improved the performance of optoelectronic devices [Bimberg, D., et al.,(2001) and Alferov, Z. I.,(2001)].

Quantum Dot

Applying some energies to a semiconductor results in the excitation of the electron from the valence band to the conduction band leaving a hole behind. It corresponds to the excited electron in the conduction band. The excitation gives rise to an electron-hole pair called exciton pairs. The portions of a semiconductor that contains these pairs are called Quantum Dots as shown in Figure(2)[[http://en.Wikipedia.org/wiki/Quantum dot](http://en.Wikipedia.org/wiki/Quantum_dot)]. Quantum dots are nano-scale semiconductor that emit light depending on the size of the dot. The fluorescence of the quantum dots is due to the excitation and recombination of the exciton pairs. Quantum dots are confined to a semiconductor in the similar manner as particle in a box thus we use this as a model to study different quantum properties of a dot. The quantum dots were discovered at the beginning of the 1980s by Alexei Ekimov in a glass matrix and by Louis E. Brus in colloidal solutions. The term "Quantum Dot" was coined by Mark Reed [Reed, M. A., et al.,(1988)].

* Dr, Lecturer, Department of Physics, University of Mandalay

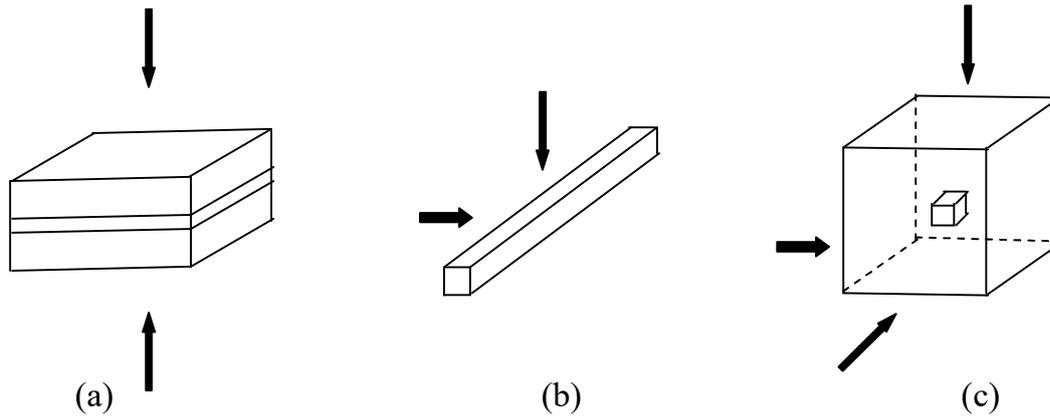


Figure 1(a) Confinement along 1 dimension. It is analogous to a quantum well.
 (b) Confinement along 2 dimensions. It is analogous to a quantum wire.
 (c) Confinement along 3 dimensions. It is analogous to a quantum dot.

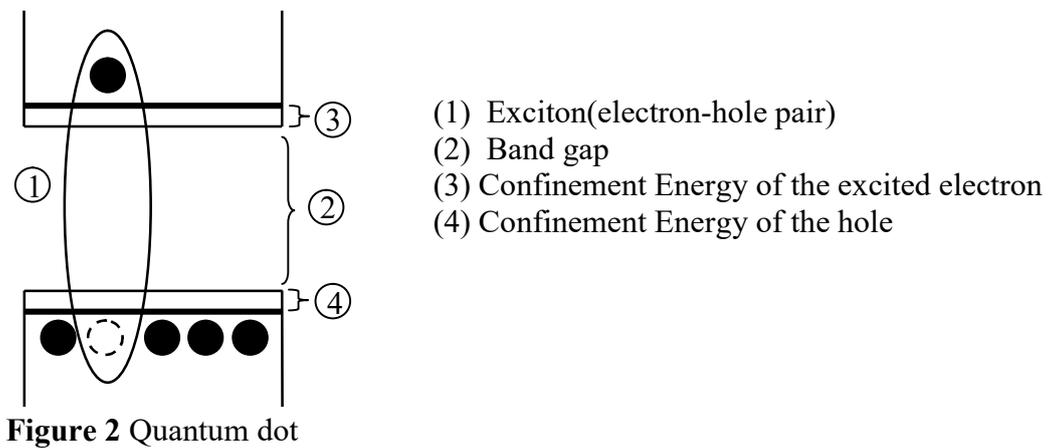


Figure 2 Quantum dot

Calculation of Energies and Wave Functions for Quantum Dot

Analytical Solution of Radial Equation

The Schrodinger equation is used to describe the quantum states of quantum dot. The Schrodinger equation for three dimensions is simply given as follows:

$$-\frac{\hbar^2}{2m} \frac{1}{r^2 \sin \theta} \left[\sin \theta \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin \theta} \frac{\partial^2}{\partial \phi^2} \right] \psi(r, \theta, \phi) + V(r) \psi(r, \theta, \phi) = E \psi(r, \theta, \phi) \tag{1}$$

If the potential energy and boundary condition are spherically symmetric then the spherical Schrodinger equation can be written as a product of a radial and angular portion as:

$$\psi(r, \theta, \phi) = R_{nl}(r) Y_{lm}(\theta, \phi) \tag{2}$$

The angular part of the wave function $Y_{lm}(\theta, \phi)$ is the same for all spherically symmetric potentials. After some manipulation, the equations for the factors become:

$$\frac{d^2\Phi(\phi)}{d\phi^2} = -m^2\Phi(\phi), \tag{3}$$

$$\sin\theta \frac{d}{d\theta} \left(\sin\theta \frac{d\Theta(\theta)}{d\theta} \right) + \ell(\ell+1)\sin^2\theta \Theta(\theta) = m^2\Theta(\theta), \tag{4}$$

and
$$\frac{d}{dr} \left(r^2 \frac{dR(r)}{dr} \right) - \frac{2mr^2}{\hbar^2} [V(r) - E] R(r) = \ell(\ell+1)R(r), \tag{5}$$

where, m^2 and $\ell(\ell+1)$ are constants of separation.

The solutions to the angular equations with spherically symmetric boundary conditions are: $\Phi_m = (2\pi)^{-1/2} e^{im\phi}$ and $\Theta_\ell^m = C_{\ell m} P_\ell^m(\cos\theta)$, where m is restricted to the range $-\ell, \dots, \ell$, $P_\ell^m(x) \equiv (1-x^2)^{|m|/2} \left(\frac{d}{dx}\right)^{|m|} P_\ell(x)$ is the 'associated Legendre function', and $P_\ell(x)$ is the ℓ^{th} Legendre polynomial.

The product of Θ and Φ occurs so frequently in quantum mechanics that it is known as a spherical harmonic: $Y_\ell^m(\theta, \phi) = \left[\frac{(2\ell+1)(\ell-|m|)!}{4\pi(\ell+|m|)!} \right]^{1/2} e^{im\phi} P_\ell^m(\cos\theta)$, where $\epsilon = (-1)^m$ for $m \geq 0$ and $\epsilon = 1$ for $m \leq 0$, and the spherical harmonics are orthonormal:

$$\int_0^\pi d\theta \sin\theta \int_0^{2\pi} d\phi [Y_\ell^m(\theta, \phi)]^* [Y_{\ell'}^{m'}(\theta, \phi)] = \delta_{\ell\ell'} \delta_{mm'}. \tag{6}$$

While the angular part of the wavefunction is $Y_\ell^m(\theta, \phi)$ for all spherically symmetric situations, the radial part varies. The equation for R can be simplified in form by substituting $u(r) = rR(r)$:

$$-\frac{\hbar^2}{2m} \frac{d^2u}{dr^2} + \left[V + \frac{\hbar^2}{2m} \frac{\ell(\ell+1)}{r^2} \right] u = Eu, \tag{7}$$

with normalization $\int dr |u|^2 = 1$.

This is now referred to as the radial wave equation, and would be identical to the one-dimensional Schrodinger equation were it not for the term αr^{-2} added to V , which pushes the particle away from the origin and is therefore often called 'the centrifugal potential.'

For infinite spherical well,

$$V(r) = \begin{cases} 0, & r < a \\ \infty, & r > a. \end{cases} \tag{8}$$

The wavefunction = 0 for $r > a$; for $r < a$, the differential equation is $\frac{d^2u}{dr^2} = \left[\frac{\ell(\ell+1)}{r^2} - k^2 \right] u$,

where
$$k \equiv \frac{\sqrt{2mE}}{\hbar}. \tag{9}$$

The allowed energies for $\ell = 0$ are given as

$$E_{n0} = \frac{n^2 \pi^2 \hbar^2}{2 m a^2} \tag{10}$$

The first three ψ_{n00} can be given as shown in figure (3).

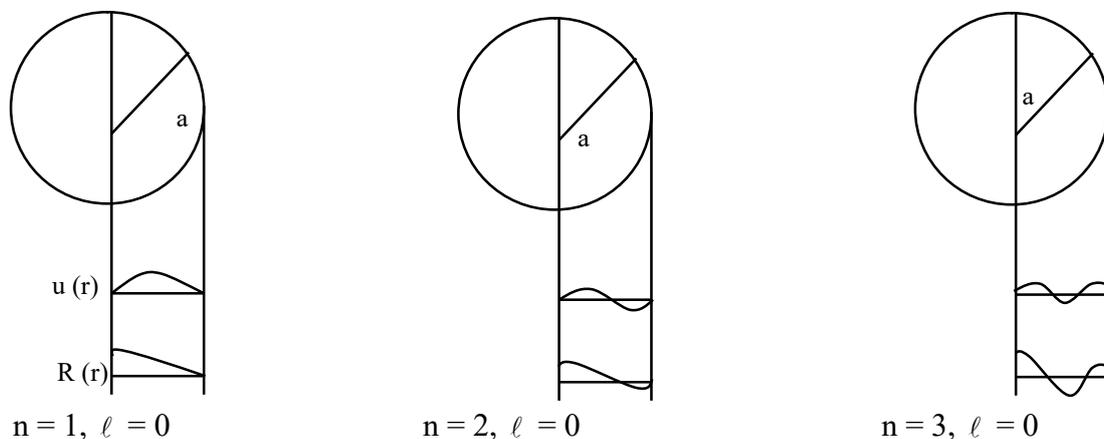


Figure 3 The first three wave functions

The 'stationary' eigenfunctions of this potential are all bound states, confined to the region $r < a$. The solutions to this equation are Bessel functions, specifically the spherical Bessel and spherical Neumann functions of order ℓ :

$$u(r) = Ar j_\ell(kr) + Br n_\ell(kr), \tag{11}$$

Where
$$j_\ell(x) \equiv (-x)^\ell \left(\frac{1}{x} \frac{d}{dx} \right)^\ell \frac{\sin x}{x}, \tag{12}$$

and
$$n_\ell(x) \equiv -(-x)^\ell \left(\frac{1}{x} \frac{d}{dx} \right)^\ell \frac{\cos x}{x}. \tag{13}$$

The requirement that the wavefunctions be 'regular' at the origin eliminates the Neumann function from any region including the origin. The Bessel function is similarly eliminated from any region including ∞ .

For small values of x , the functions can be given as:

$$j_0(x) = \frac{\sin x}{x}$$

$$j_1(x) = \frac{\sin x}{x^2} - \frac{\cos x}{x}$$

$$j_2(x) = \left(\frac{3}{x^2} - 1 \right) \frac{\sin x}{x} - \frac{3 \cos x}{x^2}$$

$$j_3(x) = \left(\frac{15}{x^3} - \frac{6}{x} \right) \frac{\sin x}{x} - \left(\frac{15}{x^2} - 1 \right) \frac{\cos x}{x},$$

and

$$n_0(x) = -j_{-1}(x) = -\frac{\cos x}{x}$$

$$n_1(x) = j_{-2}(x) = -\frac{\cos x}{x^2} - \frac{\sin x}{x}$$

$$n_2(x) = -j_{-3}(x) = \left(-\frac{3}{x^2} + 1\right) \frac{\cos x}{x} - \frac{3\sin x}{x^2}$$

$$n_3(x) = j_{-4}(x) = \left(-\frac{15}{x^3} + \frac{6}{x}\right) \frac{\cos x}{x} - \left(\frac{15}{x^2} - 1\right) \frac{\sin x}{x}$$

The first four Bessel functions are shown in figure (4).

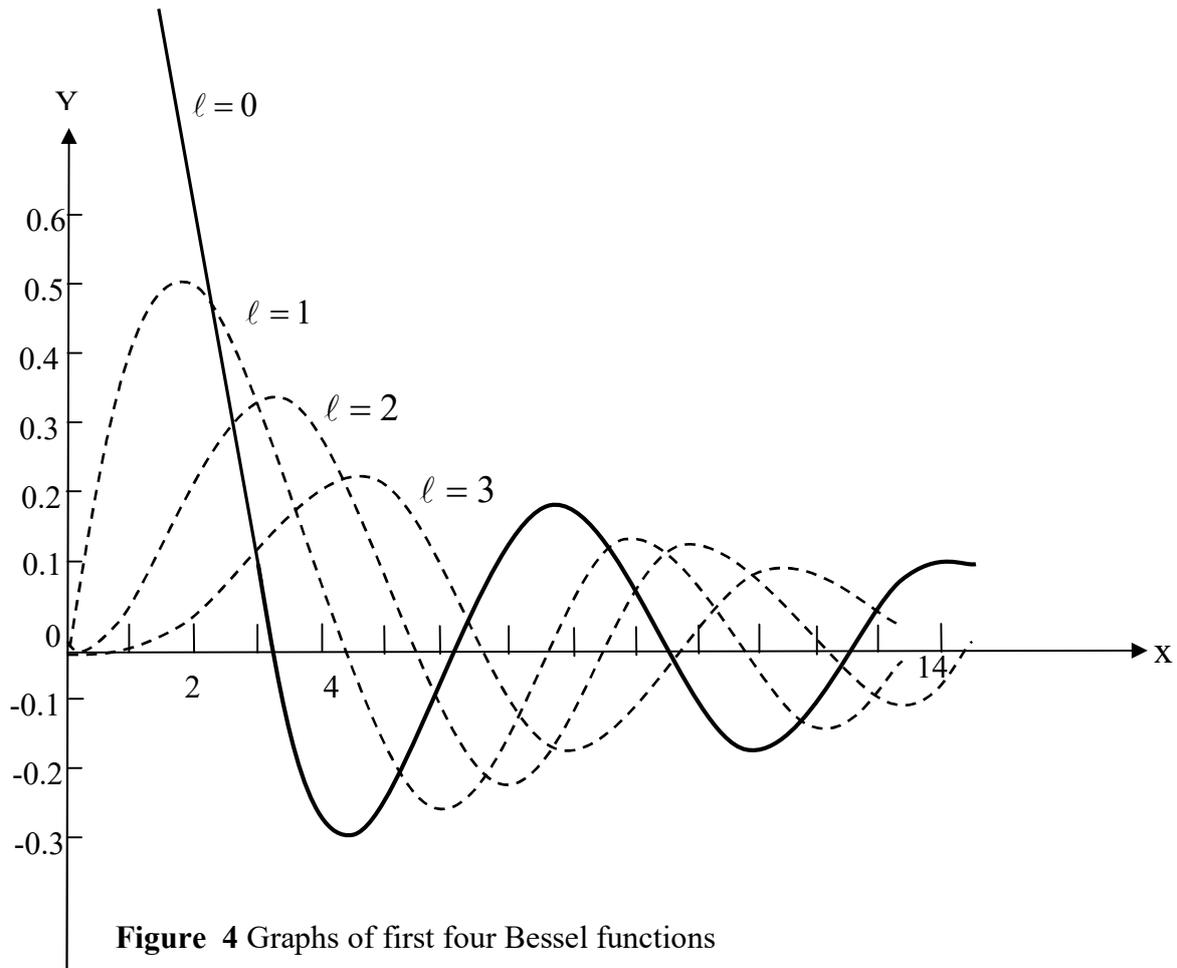


Figure 4 Graphs of first four Bessel functions

The remaining constants, k (substituting for E) and A, are satisfied by requiring that the solution vanishes at $r = a$ and normalizing, respectively: $j_\ell(ka) = 0 \Rightarrow ka = \beta_{n\ell}$, where $\beta_{n\ell}$ is the n^{th} zero of the ℓ^{th} spherical Bessel function.

Adding the angular portion, the complete time-independent wavefunctions are

$$\psi_{n\ell m}(r, \theta, \phi) = A_{n\ell} j_\ell(\beta_{n\ell} r/a) Y_\ell^m(\theta, \phi),$$

where, $E_{n\ell} = \frac{\hbar^2}{2ma^2} \beta_{n\ell}^2$.

The first few values of $\beta_{n\ell}$ are given in Table (1) [Atnafe, N., and P.Ohmann,(2012)].They both increase with increasing n and ℓ .

Numerical Solution of Radial Equation

There are only few cases for which the Schroedinger equation can be solved analytically. In most cases, such equations are solved numerically[Atnafe, N., and P. Ohmann,(2012)].

For $\ell=0$: since the r^2 disappears for this case, the radial equation reduces to ODE that can be solved easily. For numerical simulation, we should be able to convert the equation into other forms. We can write the second order differential equation as a difference of two close points by the two point approximation method. This method allows us to calculate the derivatives with smaller errors.

It can be given as:

$$u''(r) \approx \frac{u(r+h_0) - 2u(r) + u(r-h_0)}{h_0^2} + O(h_0^2)$$

h_0 refers to the discretizing factor that divides the interval into equal spaces. Substituting this in to the radial equation,

$$\frac{d^2u}{dr^2} = -k^2u$$

We can find some of the eigenvalues. This eigenvalues match the analytical ones as shown in Table (2).

For $\ell \neq 0$: In numerical physics the Numerov's method is used to find solutions of the radial Schroedinger Equation for arbitrary potentials.

$$\left[-\frac{\hbar^2}{2m} \left(\frac{1}{r} \frac{d^2}{dr^2} r - \frac{\ell(\ell+1)}{r^2} \right) + V(r) \right] R(r) = ER(r) \quad (14)$$

The above equation can be rewritten in the form

$$\left[\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2} + \frac{2m}{\hbar^2} (E - V(r)) \right] u(r) = 0 \quad (15)$$

with $u(r) = rR(r)$.

Table 1 The first few values of $\beta_{n\ell}$ for n = 1 to 4

	n = 1	n = 2	n = 3	n = 4
$\ell=0$	3.142	6.283	9.425	12.566
$\ell=1$	4.493	7.725	10.904	14.066
$\ell=2$	5.763	9.095	12.323	15.515
$\ell=3$	6.988	10.417	13.698	16.924
$\ell=4$	8.183	11.705	15.040	18.301

Table 2 Analytical and numerical energyvalues for n = 1 to 5

n	Analytical values(eV)	Numerical values(eV)
1	0.3765	0.3667
2	1.5060	1.4665
3	3.3886	3.2989
4	6.0241	5.8633
5	9.4127	9.1585

If we compare this equation with the defining equation of the Numerov method, we see

$$f(r) = \frac{2m}{\hbar^2}(E - V(r)) - \frac{\ell(\ell+1)}{r^2} \tag{16}$$

and thus can numerically solve the radial Schroedinger equation. Starting from the Taylor expansion for $u(r_n)$ we get the two sampling points adjacent to r_n .

$$u_{n+1} = u(r_n + h) = u(r_n) + hu'(r_n) + \frac{h^2}{2!}u''(r_n) + \frac{h^3}{3!}u'''(r_n) + \frac{h^4}{4!}u^{(4)}(r_n) + O(h^5) \tag{17}$$

$$u_{n-1} = u(r_n - h) = u(r_n) - hu'(r_n) + \frac{h^2}{2!}u''(r_n) - \frac{h^3}{3!}u'''(r_n) + \frac{h^4}{4!}u^{(4)}(r_n) - O(h^5) \tag{18}$$

The sum of those two equations gives

$$u_{n-1} + u_{n+1} = 2u_n + h^2u''_n + \frac{h^4}{12}u^{(4)}_n + O(h^6) \tag{19}$$

This equation can be solved for u''_n and replace it by the expression $u''_n = -f_nu_n$ which we get from the defining differential equation.

$$h^2 f_n u_n = 2u_n - u_{n-1} - u_{n+1} + \frac{h^4}{12}u^{(4)}_n + O(h^6) \tag{20}$$

The second derivative of our defining differential equation is taken and we get

$$u^{(4)}(r_n) = -\frac{d^2}{dx^2} [f(r_n)u(r_n)] \tag{21}$$

The second derivative $\frac{d^2}{dx^2}$ is replaced with the second order difference quotient and is inserted into our equation for f_nu_n

$$h^2 f_n u_n = 2u_n - u_{n-1} - u_{n+1} - \frac{h^4}{12} \frac{f_{n-1}u_{n-1} - 2f_nu_n + f_{n+1}u_{n+1}}{h^2} + O(h^6) \tag{22}$$

We solve for u_{n+1} to get

$$u_{n+1} = \frac{(2 - \frac{5h^2}{6}f_n)u_n - (1 + \frac{h^2}{12}f_{n-1})u_{n-1}}{1 + \frac{h^2}{12}f_{n+1}} + O(h^6). \tag{23}$$

This yields Numerov’s method if one ignore the term of order h^6 .

For this case, it can start at one end of our infinite spherical wall with $u(r_0)=0$ and $u(r_0+h)=1$. The wave function $R(r)$ is used instead of $U(r)$. It can be clearly seen that the Numerov’s method can be used to solve the radial equation for any value of ℓ .

Figure (5) is the graph of the analytical solutions for $\ell=0$. The dots each represent points from the Numerov’s formula. We can also use Numerov’s method to solve the radial equation for the $\ell \neq 0$ case. Figures (6) to (8) are the graphs of the analytical and numerical solutions for $\ell=1, 2$ and 3 .

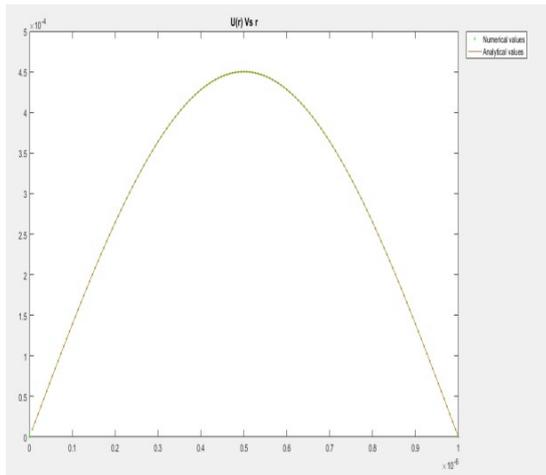


Figure 5 Wave function for $l = 0$

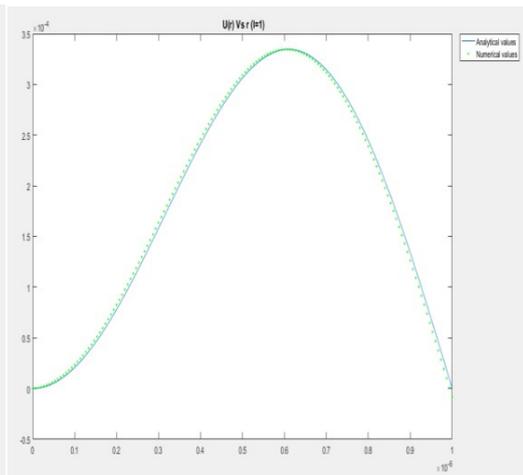


Figure 6 Wave function for $l = 1$

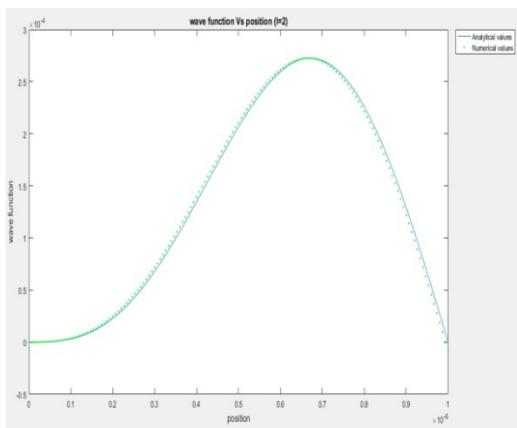


Figure 7 Wave function for $l = 2$

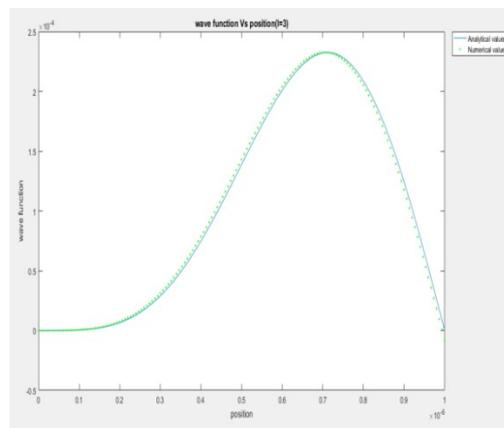


Figure 8 Wave function for $l = 3$

Conclusion

A quantum dot is a semiconductor whose excitons are confined in all three spatial dimensions. Researchers have studied quantum dots in transistors, solar cells, LEDs, and diode lasers. They have also investigated quantum dots as agents for medical imaging and hope to use them as qubits.

From quantum theory, we know that quantum dot has similar manner as particle in a box. We can imagine the walls of the box with infinite large potential energy thus preventing the particle from escaping while the potential inside to be zero. The behavior of electrons in quantum

dots is dominated by quantum mechanical behavior. In particular, this behavior is determined by the electron wave function and its evolution as determined by the Schrodinger equation.

The graphs in the figures (5) to (8) show that the analytical and numerical values of electron wave function with position match for most cases such as $\ell=0, 1, 2,$ and 3. This means that the Numerov's method also shows promising results for solving the radial equation for any value of ℓ .

As future work, we would like to explore the properties of quantum dots such as energy and electronic structures using the particle in a box model.

Acknowledgements

I express my thanks to Rector DrThida Win, University of Mandalay, her permission and encouragement to conduct this research work. I would like to express my gratitude and sincere thanks to Dr Lei Lei Win, Professor, Head of Department of Physics, University of Mandalay, for her kind permission to do this work.

References

- Alferov, Z. I., (2001), *Rev. Mod. Phys.* 73,767.
- Atnafe, N. and P. Ohmann,(2012), "Quantum Dots As Particles in the Infinite Spherical Well", Center for Applied Math 2115 summiave, saint paul, mn 55105.
- Bimberg, D., M. Grundmann, and N. N. Ledentsov,(2001), "Quantum Dot Heterostructures", JohnWiley& Sons.
- Buhro, W. E. and V. L. Colvin, (2003), "Semiconductor nanocrystals: Shape matters", *Nat Mater* 2(3): 138-9.
- http://en.Wikipedia.org/wiki/Quantum_dot.
- Reed, M. A., J. N. Randall, R. J. Aggarwal, R. J. Matyi, T. M. Moore and A. E. Wesel, (1988), "Observation of discrete electronic states in a zero-dimensional semiconductor nanostructure", *Phys. Rev Lett.* 60 (6):535-537.