ASSESSMENT OF ENERGY AND DENSITY OF STATE OF QUANTUM DOTS IN ONE DIMENSION (1D)

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Abstract

Quantum Dots (QDs) also known as artificial atoms or low-dimension structuresare tiny semiconductor particles or semiconductor nanocrystals commonly used as building blocks in nanotechnology.They containtiny droplets of free electrons whose electron wave functions are confined within its volume. The density of state of quantum dotis the possible number of discrete state an excited electron can occupy per unit volume. The density of state depends on the energy at which the electron moves when excited. In this paper, a onedimensional potential well was used to compute the energies and density of states of quantum dots. The results obtained revealed that for the one dimensional quantum dot, the density of states increases exponentially with energies showing that the density of state of higher energy levels is greater than that of lower energy levels. The results obtained are in agreement with theoretical predictions and can be used as guide for experimental researches.The applications of quantum dots include: bioconjugates, solar cells, photovoltaic, photo and electrochromic devices etc.

Keywords: Density of State, Energy of State, Potential Well, Quantum Dot

1.0 Introduction

Quantum dots are semiconductor crystals with very low dimensions and obey quantum mechanical principle of quantum confinement.They are formed from thinsemiconductor

filmsbuckled due to the stressof having latticestructures slightlydifferent in size fromthose of the materialupon which the films aregrown [1]. Quantum dots are mostlyassembled fromatoms from groups II-VI or III-V elements in the periodic Table [1, 2]. They have electronic properties intermediate between those of bulk semiconductors and those of discrete molecules Whencompared to their bulk they have relatively small Exciton Bohr Radius (EBR) that describes theirdefinition. The sizes of quantum dot ranges from 1 – 100 nm [3, 4]. This imposes QuantumConfinement (QC) when special optical and electronic properties are produced. They exhibit energy band gaps used in determining required wavelength of radiation absorption and emission spectra. The absorption spectra and emission corresponding to the energy band gap of the quantum dot is governed by quantum confinement principles in an infinite square quantum well potential. The energy band gap decreases with an increase in the quantum dot size [5].Quantum dot offers an efficient process relative to bulk semiconductor but quantized because of the low-dimension scales involved. Figure 1 describes a behavioral view of the quantum dots relative to bulk semiconductor [2].

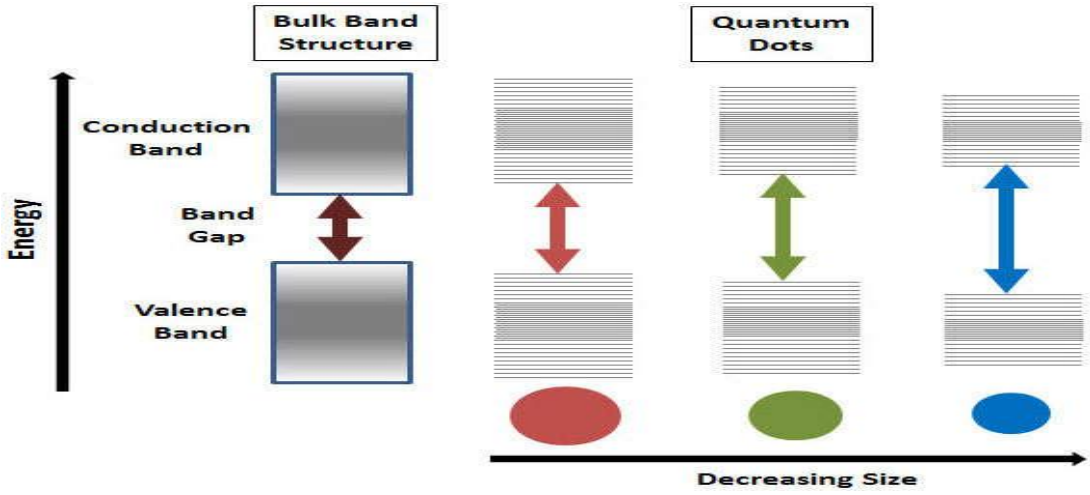

Figure 1: Splitting of energy levels in quantum dots due to the quantum confinement effect

Semiconductors depend on electron excitation from the ground state into some excited energy level. Energy band gap is the space between the excited and ground states. When an electron is excited and moves to the conduction band, a corresponding hole is created at the valence band [6]. The separation between the excited electrons (negative charge) sets up a potential difference. When this happens, a circuit is completed and electron flows begins in the conductive band of the semiconductor. To re-establish the ground state, electrons and holes recombine, emitting photons over a wide and continuous wavelength range. However, this behavior in a bulk semiconductor primarily occurs over a range of energy levels and is limited by dimensions of the absorbing surface and range of incident photon wavelength.A quantum wellis a sandwich of stacked thin slices of semiconductormaterials with different band gaps [1]. In a quantum well, the centrallayer has the smallest band gap, which meansthe larger gaps of the outer layers act like barriers,restricting the electrons in the middle one. Thestructure vertically confines the energy levels of themiddle layer in one dimension.

Quantum Confinement allows quantum dots to be tailored to specific incident energy levels based on particle size. Quantum confined structure is categorized based on the conferment direction into quantum well, quantum wire and quantum dots [7]. In quantum dots, the charge carriers are confined in all three dimensions. In addition, nanoparticles offer superior surface area which enhances increase in the absorption properties per unit volume and/or conductive properties. Varying quantum dot size leads to change in the size of the energy band gap. Large size quantum dots are observed to create decrease in energy band gap andlarge emission of wavelength photons [7]. This effect is demonstrated by quantum dot solutions of different particle sizes emitting different colors when exposed to an ultra violet (UV) light source as seen in Figure 2 [1].

Figure 2: Photoluminescence from CdSe/ZnS (core-shell colloidal) quantum dots of different sizes (~2-6 nm) pumped with the same laser

Due to the surface area effects on quantum dots, the efficiency of energy transfer properties is enhanced. This makes quantum dots to still emit light long after exposure to a UV energy source has seized. Electrons and holes are confined if the conduction and valence band edge of the surroundingmaterials are higher and lower respectively.Color formations vary with the size of the dots that is;the smaller dots exhibit blue color while larger dots exhibit red color as shown in the Figure 2 [1].

The number of states attained by a quantum system is the possible number of available states. It is given mathematically as [1]:

$$\varphi\,(E) = \frac{V\ \text{system}}{V\ single\ -state}\ x\ \boldsymbol{N} \qquad (1)$$

where

φ(E) is number of states, V_{system}isvolume of whole system (sphere, circle, line), V_{single} is volume of single state of that system, and N is the number of atoms in the crystal.

Density of state is the possible number of state an electron when excited can occupy per unit volume. The density of state depends on the energy at which the electron moves when

excited. It is the first derivative of the number of state with respect to the energy. It is given mathematically as [2].

$$g(E) = \frac{d\,\phi(E)}{dE} \qquad (2)$$

where

g(E) is the density of state and ϕ is number of states.

Density of electron states in bulk, 2D, 1D and 0D semiconductor structure is shown in Figure 3 [2]. 0D structures has very well defined and quantized energy levels. The quantum confinement effect corresponding to the size of the nanostructure can be estimated via a simple effective-mass approximation model.

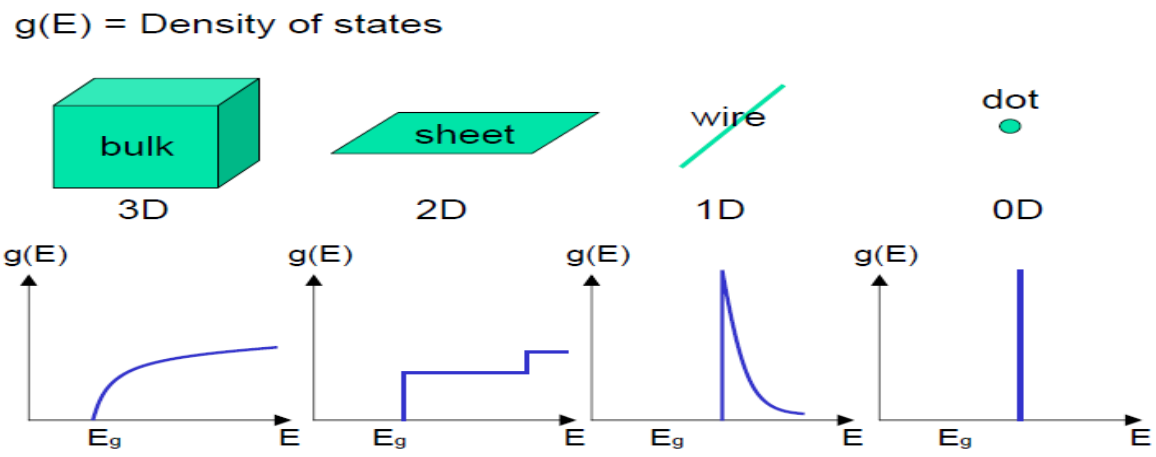

Figure 3: Density of electron states of a semiconductor as a function of dimension

2.0 Research Methodology

Energy and Density of States of 1-Dimensional Quantum Dot

For the case of a 1-dimensional quantum system such as quantum dot, Schrodinger equation is deployed.

$$\nabla^2\Psi\,(x) + \frac{2m\,(E-V)}{\hbar^2}\Psi\,(x) = 0 \qquad (3)$$

For 1- dimension, $\nabla^2 = \frac{\partial^2}{\partial x^2}$, thus

$$\nabla^2\Psi\,(x) = \frac{\partial^2\Psi\,(x)}{\partial x^2} = \frac{d^2\Psi\,(x)}{dx^2} \qquad (4)$$

Substituting equation 4 into equation 3 yields:

$$\frac{d^2\Psi\,(x)}{dx^2} + \frac{2m\,(E-V)}{\hbar^2}\Psi\,(x) = 0 \qquad (5)$$

For V=0, equation 5 becomes:

$$\frac{d^2\Psi\,(x)}{dx^2} + \frac{2mE}{\hbar^2}\Psi\,(x) = 0 \qquad (6)$$

Taking $\frac{2mE}{\hbar^2} = K^2$, then K = $\sqrt{\frac{2mE}{\hbar^2}}$ and substituting into equation 6 yields:

$$\frac{d^2\Psi\,(x)}{dx^2} + K^2\Psi\,(x) = 0 \qquad (7)$$

The solution of the equation 7 is:

$$\Psi\,(x) = A\sin Kx + B\cos Kx$$

At the boundary condition where $\Psi\,(x) = 0, x = 0$

then, $0 = A \sin(0) + B \cos(0)$

For B=0, $\Psi(x) = A \sin Kx$

At the point $\Psi(x) = 0, x = l$

$0 = A \sin Kl$ But $A \neq 0$

Since $Kl = 0$, then $Kl = \sin^{-1}(0) = n\pi$

Therefore, $K = \frac{n\pi}{l}$ $K_x = \frac{n_x \pi}{l}$

So, $\Psi(x) = A \sin \frac{n_x \pi x}{l}$

Normalizing the wave function:

$$\int \Psi(x)\, \Psi(x)^* = \int A^2 sin^2 \frac{n_x \pi}{l} = 1 \quad (8)$$

$A = \sqrt{\frac{2}{l}}$ and $\Psi(x) = \sqrt{\frac{2}{l}} \sin \frac{n_x \pi x}{l}$

Thus, the energy of the system is obtained as:

$$E = \frac{\hbar^2 K^2}{2m^*} \quad (9)$$

where $K_x = \frac{n_x \pi}{l}$

By substitution,

$$E = \frac{\hbar^2}{2m^*} \left(\frac{n_x \pi}{l}\right)^2 = \frac{\hbar^2}{2m^*} \, x \, \frac{{n_x}^2 \pi^2}{l^2} \quad (10)$$

and

$n_x{}^2 = \frac{2m^*lE}{\hbar^2\pi^2}$ = R = length of the line (11)

Thus, since the 1-dimnsional system is likened to a straight line the k-space volume of its single state is V single-state = $\frac{\pi}{a} = \frac{\pi}{V} = \frac{\pi}{l}$

K-space value of the 1-dimensional line = V system (line) =R=$(\frac{2m^*lE}{\hbar^2\pi^2})^{1/2}$ (12)

The number of atoms for a line at position (0) and (½) is = $2\ x\frac{1}{2}$

Therefore,

$\phi(E) = \frac{(\frac{2m^*lE}{\hbar^2\pi^2})^{1/2}}{\frac{\pi}{l}}\ x\ 2\ x\frac{1}{2} = \frac{\sqrt{\frac{2m^*E}{\hbar^2}}\ x\ \frac{l}{\pi}}{\frac{\pi}{l}} = \sqrt{\frac{2m^*l^2}{\hbar^2\pi^2}}\ x\ E^{1/2}$ (13)

$g(E) = \frac{1}{2}\sqrt{\frac{2m^*l^2}{\hbar^2\pi^2}}\ x\ E^{\frac{1}{2}} = \frac{1}{2}\ x(\frac{2m^*}{\hbar^2\pi^2})^{\frac{1}{2}}l^{\frac{2}{2}}E^{\frac{1}{2}-1} = \frac{(2m^*)l(2m^*)^{-\frac{1}{2}}}{2\hbar\pi}E^{-\frac{1}{2}}$ (14)

$g(E) = \frac{m^*l}{\pi}\ x\ \frac{(2m^*E)^{\frac{-1}{2}}}{\pi} = \frac{(2m^*E)^{\frac{-1}{2}}ml}{\hbar\pi}$ (15)

For 1 dimension:

$g(E)_{1D} = \frac{\frac{(2m^*E)^{\frac{-1}{2}}m\cancel{l}}{\hbar\pi}}{\cancel{l}} = \frac{m}{\hbar\pi}\sqrt{\frac{1}{2mE}} = \frac{m}{\hbar\pi\sqrt{(2m^*E)}}$ (16)

$g(E)_{1D} = \frac{m}{\hbar\pi\sqrt{(2m^*E)}}\ x\ \frac{\sqrt{m^*}}{\sqrt{m^*}} = \frac{m\ \sqrt{m^*}}{\hbar\pi\ x\ \sqrt{2E}\ m} = \frac{1}{\hbar\pi}\sqrt{\frac{m}{2E}}$

$g(E)_{1D} = \frac{1}{\hbar\pi}\sqrt{\frac{m}{2E}}$ (17)

Equation 17shows that the density of state for a quantum dot (0D) depends on the energy, E, and is inversely proportional to the square root of the energy.

Data Analysis

The following parameters were used in the calculations of the energy and density of states of quantum dots in one dimension and result tabulated in Table 1.

$\hbar = \frac{h}{2\pi} = 1.054 \times 10^{-34} J.S$

π =22/7 = 3.142

L = dimension of well and line assumed =10 A^0 = 10 x 10^{-10} m

m^* = mass of the electron = 9.11 x 10^{-31} kg

e = charge of electron = 1.6 x 10^{-19} C

3.0 Result

Table 1**:** Results of the energy and density of states for one dimension energy level

Energy Levels n_x,	**Energy (J)**	**Energy (eV)**	**Density of States ($m^{-3}J^{-1}$)**	**Density of States ($m^{-3}eV^{-1}$)**
1	6.0200 x 10^{-20}	0.37625	8.302x 10^{27}	3.320 x 10^{18}
2	2.4080 x 10^{-19}	1.50500	4.151x 10^{27}	1.660 x 10^{18}
3	5.4180 x 10^{-19}	3.38625	2.767x 10^{27}	1.107x 10^{18}

4	9.6320×10^{-19}	6.02000	2.076×10^{27}	8.302×10^{17}
5	1.5050×10^{-18}	9.40625	1.660×10^{27}	6.642×10^{17}
6	2.1672×10^{-18}	13.54500	1.384×10^{27}	5.535×10^{17}
7	2.9498×10^{-18}	18.43625	1.186×10^{27}	4.744×10^{17}
8	3.8528×10^{-18}	24.08000	1.038×10^{27}	4.157×10^{17}
9	4.8762×10^{-18}	30.47625	9.225×10^{26}	3.690×10^{17}
10	6.02×10^{-18}	37.62500	8.302×10^{26}	3.321×10^{17}

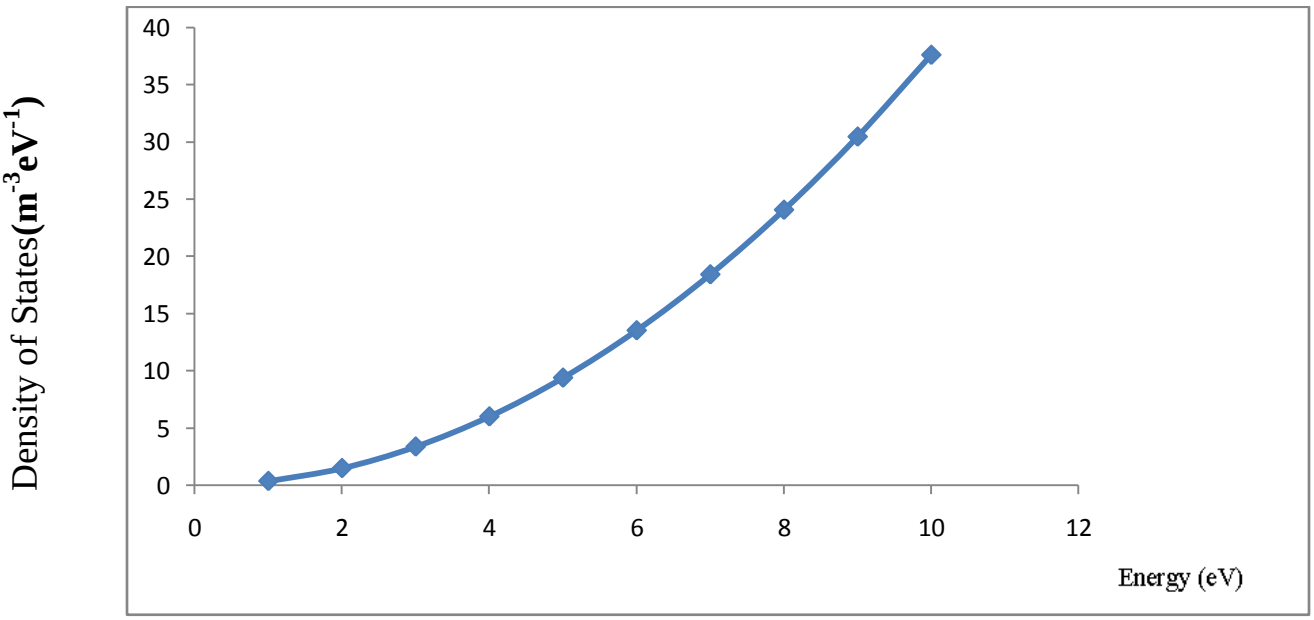

Figure 4: Variation of the density of states with energy for a 1- dimensional quantum dots

4.0 Discussion

From Figure 4 and Table, it shows that the density of states increases exponentially with energy.This suggests that the density of states depends on the quantum number with respect to the energy. Furthermore, the result reviews that energy levels with low energy (energy

quantization) has low density of states and vice versa.The results obtained in this work may slightly differ from real life situations because of the following reasons:

1. In computation, the electronic mass of the electron was used throughout and not the effective mass of the electron, which varies in the reciprocal space lattice of the solid.

2. The dimension of the well was kept constant at a value of 10 A^0 irrespective of the dimension under consideration. Changes with the dimension of the box will certainly cause a change in the energy level and hence the density of state of the system studied.

5.0 Conclusion

The assessment of energy and density of states of quantum dots has a tremendous impact in nano-electronics which may revolutionize technology. However, clear understanding of energy and density of states of quantum dots is necessary for it. In this paper, the energy and density of states for a quantum dots in one dimension were calculated and analyzed. The result showed the exponential relationship between energy and density of states of quantum dots in one dimension (1D).

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