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ENERGY OF A SINGLE ELECTRON IN GROUND STATE FOR A HETEROGENEOUS CYLINDRICAL DOT WITH FINITE CONFINEMENT ALONG AXIAL DIRECTION AND INFINITE CONFINEMENT IN TRANSVERSE PLANE

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ABSTRACT

This paper presents a simple theoretical study for cylindrical nano dot(CND) within the frame work of effective mass Schrödinger equation for investigating the motion of a single electron in the heterostructure with **GaAs** as well material embedded in $\mathbf{Ga_xAl_{1-x}As}$ matrix as barrier material having infinite band offset across their abrupt interface along transverse plane and finite band offset along the axial direction to obtain the energy Eigen values under the purview of effective mass approximation. The result shows that energy Eigen value of the single electron increases as the radius and the height of the dot decreases, which is in exact conformity with the Heisenberg's uncertainty principle.

Keywords: Size quantization; EMBC; Parabolic confinement; Effective mass Schrödinger equation; CND.

I. INTRODUCTION

Nano dot are low dimensional structures which exhibit exotic behaviours distinct from their bulk counterparts chiefly attributed due to size quantization effect, which is typical of a quantum confined system. In nanostructures, whenever the de-Broglie wavelength of electron exceeds the appropriate dimensions of the device structure, the quantum nature dictates the physical properties in them. As a result of which, the energy of the electrons in the confined directions become quantized and forms a discrete energy spectrum. For such size quantized electrons, the scattering probability is drastically suppressed [1].

The degrees of freedom for the electrons are restricted in the confined directions producing a system with reduced dimensionality. These low-dimensional systems with electron confinement in one, two and three dimensions are called **2-D** quantum wells (QW), **1-D** quantum wires (QWW) and **0-D** quantum dot (QD) or nano dot (ND) respectively. The energy quantization changes the band structure of such nano hetero systems and alters their optical, magnetic and electronic properties drastically. There have been recent studies on the ground state of electronic energy on QD considering conduction band with parabolic confinement [2] and with non-parabolic confinement [3]. Thus the effects of quantum confinement on low-dimensional systems are of both fundamental and of technological importance. The study of energy spectra of electron has also been extended for hole and exciton and the corresponding lifetimes of these quasi-particles has been studied in an open cylindrical quantum wire by others[4] in the framework of effective mass approximation.

In the following section, a theoretical work is presented for **0-D** cylindrical nano dot (CND) within the frame work of effective mass Schrödinger equation for investigating the band structure of the hetero system with abrupt interface between the materials to obtain the energy Eigen values. We have incorporated the motion of a single electron, which is assumed to be confined in a cylindrical well region formed by GaAs semiconductor (Region I) surrounded by a barrier semiconductor material $Ga_xAl_{1-x}As$ (Region II) with infinite band offset across the abrupt interface along the transverse plane and finite band offset along the axial direction.

In general for the structure under consideration, the boundary conditions to be satisfied across the well-barrier interface are the effective-mass boundary conditions (EMBC) which is also referred as Bastard boundary conditions [5,6,7]. Due to size quantization, quantum mechanical effects creep in and as a result, the Eigen values of the confined single electron become quantized forming a discreet energy spectrum. It is observed that on reducing the dot radius and the dot height the energy Eigen value of different states increases, which is in exact conformity with the Heisenberg's uncertainty principle.

II. MATHEMATICAL BASIS OF THE THEORY

The mathematical equation suitable for the analysis of single electron motion in microstructure as well as in semiconductor nano heterostructure under the effective-mass approximation satisfies the Schrödinger wave like equation[5,6,7,8] with the particular ordering of the two operators in the kinetic energy part of the effective mass

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Hamiltonian[9,10,11] preserving the Hermitian nature of the Hamiltonian with Bastard boundary conditions across the abrupt interface such that the probability current density is conserved across it.
The effective mass Schrödinger equation in such structure is represented by

$$\left[\frac{-\hbar^2}{2}\nabla.\left(\frac{1}{m^*}\nabla\right)+V\right]\Psi = E\ \Psi \qquad (1)$$

Where, m^* is the space dependent effective mass of the electron, V is the potential in the well region and E is the energy of the confined single electron in the nano dot.

If the semiconductor heterostructure remains region wise homogenous and uniform then the equation (1) reduces to

$$\left[\frac{-\hbar^2}{2m^*}\nabla^2+V\right]\Psi = E\Psi \qquad (2)$$

III. SOLUTION

In this section, we present a solution for the single electron assumed to have quantized motion in an all three dimensions of the **0-D** nano dot under consideration. We intend to solve the energy values of the electron confined in a CND along the transverse plane having infinite band offset and having finite band offset along the axial direction of the well-barrier interface.

If V_C describes the confining potential then the potential profile can be expressed as

$$V_C = \begin{cases} 0 & ; \quad \rho \le R \\ \infty & ; \quad \rho > R \end{cases} \qquad (3)$$

$$V_C = \begin{cases} 0 & ; \quad |z| \le d \\ V_o & ; \quad |z| > d \end{cases} \qquad (4)$$

$$m^* = \begin{cases} m_1^* & ; \quad \rho \le R \ \ \& \ |z| \le d \\ m_2^* & ; \quad \rho > R \ \ \& \ |z| > d \end{cases} \qquad (5)$$

The effective mass Schrödinger wave equation for the CND is expressed as

$$\frac{\hbar^2}{2m^*}\nabla^2\psi + (E - V_C)\psi = 0 \qquad (6)$$

Inside the CQD (i.e. $\rho \le R$ and $z \le d$) the effective mass Schrödinger wave equation is written as

$$\frac{\hbar^2}{2m_1^*}\nabla^2\psi + E\psi = 0 \qquad (7)$$

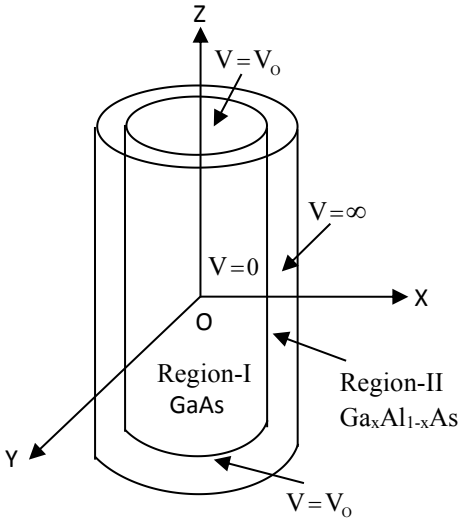

Fig:1.

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As the band- offset is infinite along transverse plane of the dot, hence no wave will exist in the outer region i.e. $\psi_{out} = 0$. The solution of the wave equation for transverse plane in CND in region I may be written as

$$f(\rho) = \sum A_m J_m(\Re_1 \rho) e^{im\phi} \quad \rho \le R \tag{8}$$

For the ground state $m = 0$

$$f(\rho) = A_o J_o(\Re_1 \rho) \text{ with } \Re_1 = \sqrt{\frac{2m_1^* E}{\hbar^2} - k_z^2}$$

The term k_z^2 becomes insignificant here as it represents the translational energy of the electron along z-axis but in this paper, we intend to determine the confined energy of the electron in transverse plane and in axial direction too.

Hence $\Re_1 = \sqrt{\frac{2m_1^* E}{\hbar^2}}$ (9)

Under the preview of effective mass approximation the Bastard boundary condition (EMBC) at $\rho = R$ are we found that

$$J_o(\Re_1 R) = 0 \tag{10}$$

If χ_{0s} are the zeros / roots of J-Bessel function [12] of zeroth order and 's' is the number of roots, then we may write energy Eigen value of ground state with respect to radius of the nano dot as

$$E_{0s} = \frac{\chi_{0s}^2 \hbar^2}{2m_1^* R^2} \tag{11}$$

The solution of the wave equation in axial direction of CND in region I $\left(|z| \le d, V_C = 0\right)$ may be written as

$$g_1(z) = Be^{i\Re_1 z} + Ce^{-i\Re_1 z}$$

where $\Re_1 = \sqrt{\frac{2m_1^* E}{\hbar^2}}$

Again $g_1(z)$ can be written as $g_1(z) = B\sin\Re_1 z + C\cos\Re_1 z$ (12)

The solution of the wave equation in axial direction of the CND in region II $\left(|z| > d, V_C = V_O\right)$ may be written as

$$g_2(z) = De^{-\Re_2 |z|} \tag{13}$$

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With $\Re_2^2 = \dfrac{2m_2^*(V_o - E)}{\hbar^2}$ (14)

The Eq^n (12) can be written as

i.e. $g_1(z) = M \sin(\Re_1 |z| + \phi_o)$ for $\phi_o = \begin{cases} 0 & \text{odd parity} \\ \dfrac{\pi}{2} & \text{even parity} \end{cases}$

Now applying 1st EMBC at $|z| = d$ for odd parity state, we get

$$M \sin \Re_1 d = D e^{-\Re_2 d}$$

$$\Rightarrow D = \frac{M \sin \Re_1 d}{e^{-\Re_2 d}}$$

Now substituting the value of D in Eq^n(13), We get

$$g_2(z) = M \sin \Re_1 d \; e^{-\Re_2(|z|-d)} \quad (15)$$

Now for the even parity state we get $g_2(z)$ as

$$g_2(z) = M \cos \Re_1 d \; e^{-\Re_2(|z|-d)} \quad (16)$$

Therefore $g_2(z)$ can be written as

$$g_2(z) \propto \sin(\Re_1 d + \phi_o)\, e^{-\Re_2(|z|-d)} \quad \text{for } \phi_o = \begin{cases} 0 & \text{odd parity} \\ \dfrac{\pi}{2} & \text{even parity} \end{cases}$$

Now applying 2nd EMBC at $|z| = d$ for odd parity state , we get

$$\tan \Re_1 d = -\frac{\Re_1 m_2^*}{\Re_2 m_1^*} \quad (17)$$

Now applying 2nd EMBC at $|z| = d$ for even parity state , we get

$$\cot \Re_1 d = \frac{\Re_1 m_2^*}{\Re_2 m_1^*} \quad (18)$$

Energy Eigen values are obtained by solving Eq^n (17) and Eq^n(18) either numerically or graphically. In a simplified approach, we have ignored variations in the effective masses of GaAs and $Ga_xAl_{1-x}As$ and keeping the mass same throughout the nano dot heterostructure.

i.e. $m_1^* = m_2^* = m^*$ (19)

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On the basis of Eq^n(19) , Eq^n(17) and Eq^n(18) take simplified form as

$$\Re_1 \cot \Re_1 d = -\Re_2 \qquad (20)$$

and

$$\Re_1 \tan \Re_1 d = \Re_2 \qquad (21)$$

Eq^n (20) and Eq^n (21) represent transcendental equations [13] for odd and even parity states.

The even parity solution of $\Re_1 d \tan \Re_1 d$ against $\Re_2 d$ can be achieved graphically with the circles of radii given by $\left(\frac{2m^* V_O d^2}{\hbar^2}\right)^{\frac{1}{2}}$. From the graph we find that for an electron, the number of confined states depend on the height of the barrier through the factor $V_o d^2$. It was found that the smallest height for the existence of a confined state is $d^2 = \frac{\pi^2 \hbar^2}{8 m^* V_O}$ [14].

The solution for confined state will exist only if

$$\frac{\pi^2 \hbar^2}{8 m^*} \le V_O d^2 \le \frac{9 \pi^2 \hbar^2}{8 m^*}$$

Plotting the graph of $\Re_1 d \tan \Re_1 d$ against $\Re_2 d$ from the transcendental Eq^n (21) ,we find that energy Eigen value of the ground state with respect to height of the nano dot as

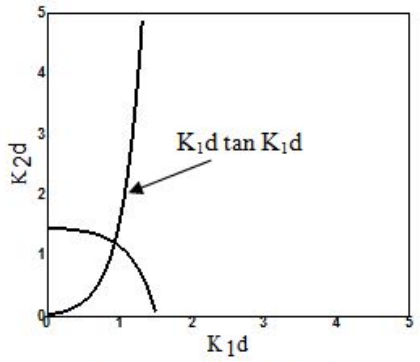

Fig2: Graph of $K_1 d \tan K_1 d$ against $K_1 d$

$$E_d = \frac{0.87\ \hbar^2}{2 m^* d^2} \qquad (22)$$

Hence the total energy Eigen value of the ground state is given by

$$E = E_{0s} + E_d$$

$$E = \frac{\chi_{0s}^2\ \hbar^2}{2 m^* R^2} + \frac{0.87\ \hbar^2}{2 m^* d^2}$$

$$E = \frac{\hbar^2}{2m^*}\left(\frac{\chi_{0s}^2}{R^2} + \frac{0.87}{d^2}\right) \qquad (23)$$

IV. RESULTS & DISCUSSION

The numerical analysis of the ground state energy has been computed for a heterogeneous CND composed of GaAs as well material, embedded in the surrounding barrier material of $Ga_{0.3}Al_{0.7}As$ in the CND with dot radius 'R' and dot height 'd'. The height of the dot varying from 2.58 nm to 20 nm, because this range of parameters

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represent strong confinement regime[15]. The band offset between the materials has been assumed to be infinite along the transverse plane and finite along the axial direction. The parameters taken in our calculation for energy Eigen value of the dot are given by $m^* = 0.067\, m_o = 6.097 \text{ x } 10^{-32}$ kg and $V_o = 190$ meV [16]. From Eq. (23), it can be inferred that the energy of ground state of CND is inversely proportional to the sum of the squares of the radius and the height of the dot. It was also found that the smallest height for the existence of a confined state is 2.5786nm[14]. The graphical representations of the ground state has been plotted as a function of height for three different radii of the nano dot.

V. CONCLUSION

The confined motion of an electron has been discussed in CND. The energy values have been obtained under the effective mass boundary conditions within the purview of effective mass theory. It has been observed in this case that the Eigen energy value of the confined electron increases as the radius and the height of the CND decrease. The reason may be attributed to strong confinement of the electron within the dot, which seems to be in exact conformity with the Heisenberg's uncertainty principle.

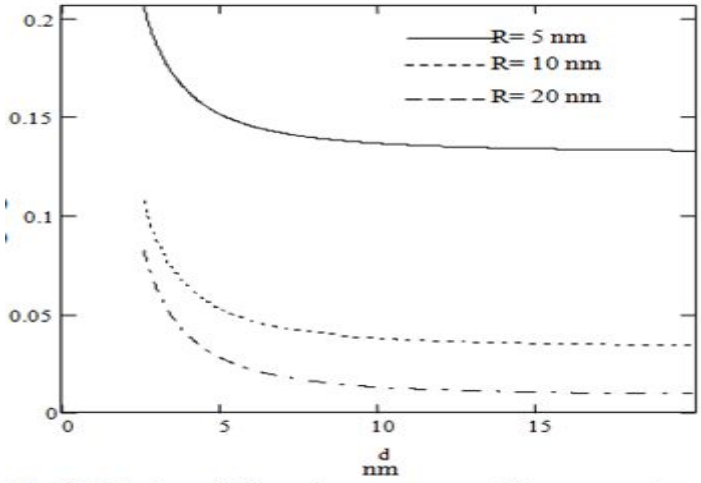

Fig:3 Variation of Ground state energy of electron against height of the CND for different dot radius.

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