ELECTRONIC STATES IN A PRISM SHAPED QUANTUM DOT

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ABSTRACT

This paper presents study of electronic states in a zero-dimensional equilateral prism shaped structure. The effective mass Schrödinger equation is applied in above structure to calculate energy eigenvalues. The variation in energy of electronic states with variation in volume is studied and observed to be decreasing with increase in volume. Further variation of ground state energy is studied by varyingaspect ratio keeping volume of the structure fixed which leads to an analytical comparison between effect of confinement along two mutually perpendicular directions.

Keywords*: Zero dimension structure, Effective mass Schrödinger equation, Aspect ratio.*

I. INTRODUCTION

In a three dimensional structure,electron can move along all three independent directions i.e. along all three axes. So, it has three degrees of freedom. If electron motion is restricted (up to nano-size regime) along any one of the three available degrees of freedom and is free along the rest two directions, it is a two-dimensional structure. If motion is restricted along any two degrees of freedom, it is a1-dimensional structure. If motion is restricted up to nano-size regime along all three degrees of freedom, it is a zero dimensional structure and is popular as a name quantum dot. The states of an electron in these structure shows various special properties like quantization of energy states, sharper density of states [1] etc.The electronic states in a equilateral triangular quantum wire is studied by many researcher by various methods [2-6]. In this paper, those result of two-dimensional structure is used to find the energy eigenvalues in equilateral prism using effective mass Schrödinger equation. Further the obtained energy eigenvalues are calculated in terms of volume and aspect ratio of the structure to study the variation in ground state energy of the structures with these two parameters analyzed theoretically. This will lead to increasing the efficiency of various quantum devices by helping in determinationof the semiconductor material of appropriate aspect ratio.

II. MATHEMATICAL MODEL

The effective mass Schrödinger equation in general in a semiconductor material is given by [7-8]

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

where $m^*(\vec{r})$ is effective mass of the electron, $V(\vec{r})$ is the potential function of structure, $\phi(\vec{r})$ is wave function and E is the total energy of the electron at position $\vec{r}$.

For completeconfinement inside the structure i.e., HWC, the potential inside structure should be finite and constant (for uniform structure) while outside it should be infinity. The constant potential here inside structure is taken to zero. For uniform mass distribution inside material, $m^*(\vec{r}) = m^*$ can be taken. Then, Eq (1) reduces to

$$-\frac{\hbar^2}{2m^*}\nabla^2\phi = E\phi \quad (2)$$

An equilateral prism structure is a prism which cross-section is an equilateral triangle. In Fig (1), the region of equilateral prism is taken as $0 \le x \le l, \sqrt{3x} \le y \le \sqrt{3l} - \sqrt{3x}$ and $0 \le z \le h$. The aspect ratio (AR) of the structure is defined as ratio of height of the structure (h) to the base length of its equilateral triangular cross-section (l) i.e.

$$\text{AR} = \frac{h}{l} \quad (3)$$

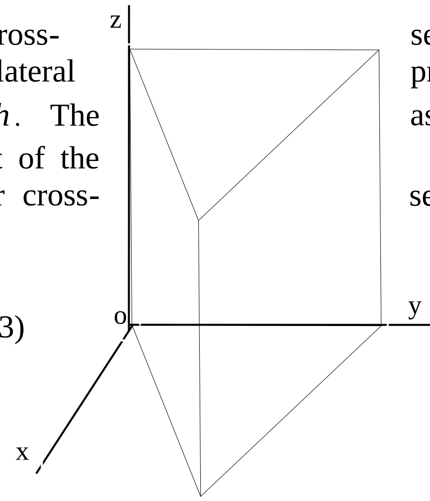

Fig.1

Let $\phi = \phi_{xy}(x,y)\phi_z(z)$ and substituting this in Eq (2) and dividing its both sides by $\phi_{xy}(x,y)\phi_z(z)$, it gave

$$-\frac{\hbar^2}{2m^*}\left\{\frac{1}{\phi_{xy}}\left(\frac{\partial}{\partial x^2}+\frac{\partial}{\partial y^2}\right)\phi_{xy}+\frac{1}{\phi_z}\frac{\partial\phi_z}{\partial z^2}\right\} = E \quad (4)$$

For an electron completely confined in atwo-dimensionalequilateral triangular planar structure is studied by many researchers by various methods and is given by [9-12]

$$E_{nm} = \frac{\hbar^2}{2m^* l^2}\left(\frac{4\pi}{3}\right)^2\left(n^2+m^2-nm\right) \quad (5)$$

with $n \ge 2m$ and n, m are positive integers.

Therefore, $\phi_{xy}(x,y)$ coming in Eq (4) must obey

$$-\frac{\hbar^2}{2m^*}\left(\frac{\partial}{\partial x^2}+\frac{\partial}{\partial y^2}\right)\phi_{xy}(x,y) = E_{nm}\phi_{xy}(x,y) \quad (6)$$

Substituting Eq(6) intoEq. (4) gave

$$-\frac{\hbar^2}{2m^*}\frac{1}{\phi_z}\frac{\partial^2\phi_z}{\partial z^2} + E_{nm} = E$$

$$\Rightarrow \frac{\partial^2 \phi_z}{\partial z^2} = -\frac{2m^*}{\hbar^2}\left(E - E_{nm}\right)\phi_z \qquad (10)$$

Let $\frac{2m^*}{\hbar^2}\left(E - E_{nm}\right) = \beta^2$, Eq (10) reduces to $\frac{\partial^2 \phi_z}{\partial z^2} = -\beta^2 \phi_z$,which general solution is

$$\phi_z = A\sin\left(\beta z + c\right) \qquad (11)$$

where A and c are constants. With the boundary conditions along z-axis: $\phi_z = 0$ at z = 0 and z = h, the Eq. (11) gives

$$E - E_{nm} = \frac{p^2\pi^2}{h^2} \text{ with } p = 1, 2, 3.... \qquad (12)$$

Substituting the value of E_{nm} from Eq. (5), the Eq. (12) gives

$$E = \frac{\hbar^2}{2m^*}\left\{\frac{\left(\frac{4\pi}{3}\right)^2\left(n^2 + m^2 - nm\right)}{l^2} + \frac{p^2\pi^2}{h^2}\right\} \qquad (13)$$

Using aspect ratio AR = $\frac{h}{l}$ and volume of square prism $V = \frac{\sqrt{3}}{4} l^2 h$, the energy eigenvalues given by Eq. (13) can be written in terms of volume and aspect ratio as

$$E = \frac{\hbar^2}{2m^*}\left(\frac{\sqrt{3}}{4}\frac{AR}{V}\right)^{2/3}\left\{\left(\frac{4\pi}{3}\right)^2\left(n^2 + m^2 - nm\right) + \frac{\pi^2 p^2}{(AR)^2}\right\} \qquad (14)$$

III. NUMERICAL RESULTS

The ground state energy was found with n=1, m=2 and p=1 in Eq. (14). The ground state energy is calculated for range of volume from 10 nm^3 to 1000 nm^3 at fixed aspect ratio 0.5. The result is plotted in Fig. 2. Again the ground state energy is calculated for range of aspect ratio from 0.2 to 2 at fixed volume 100nm^3.

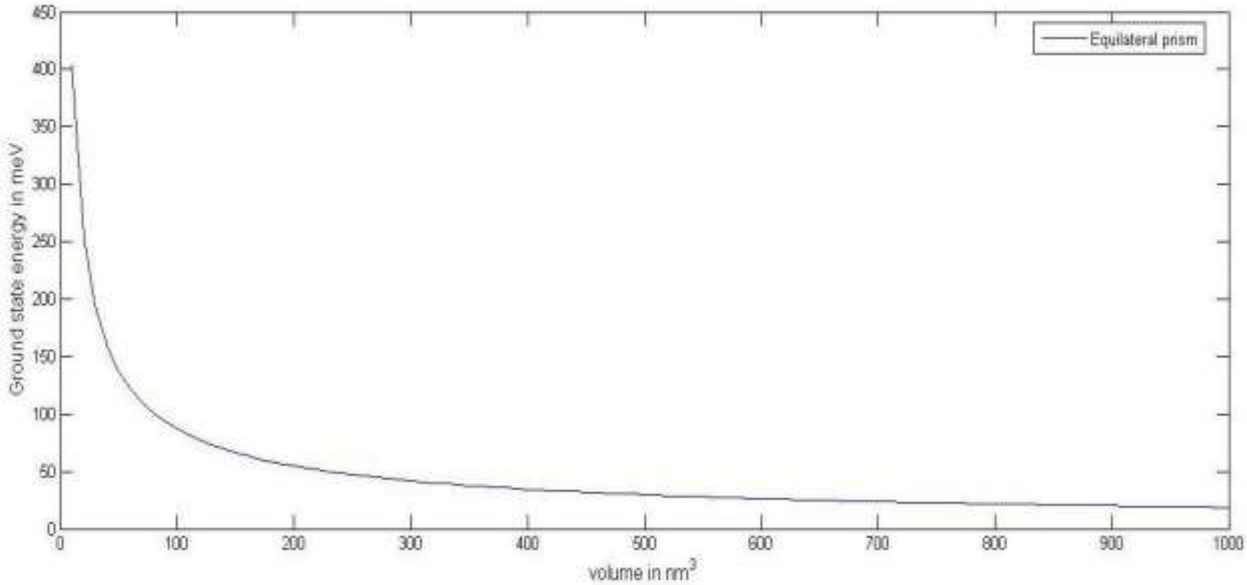

Fig.2: Variation of ground state energy with volume

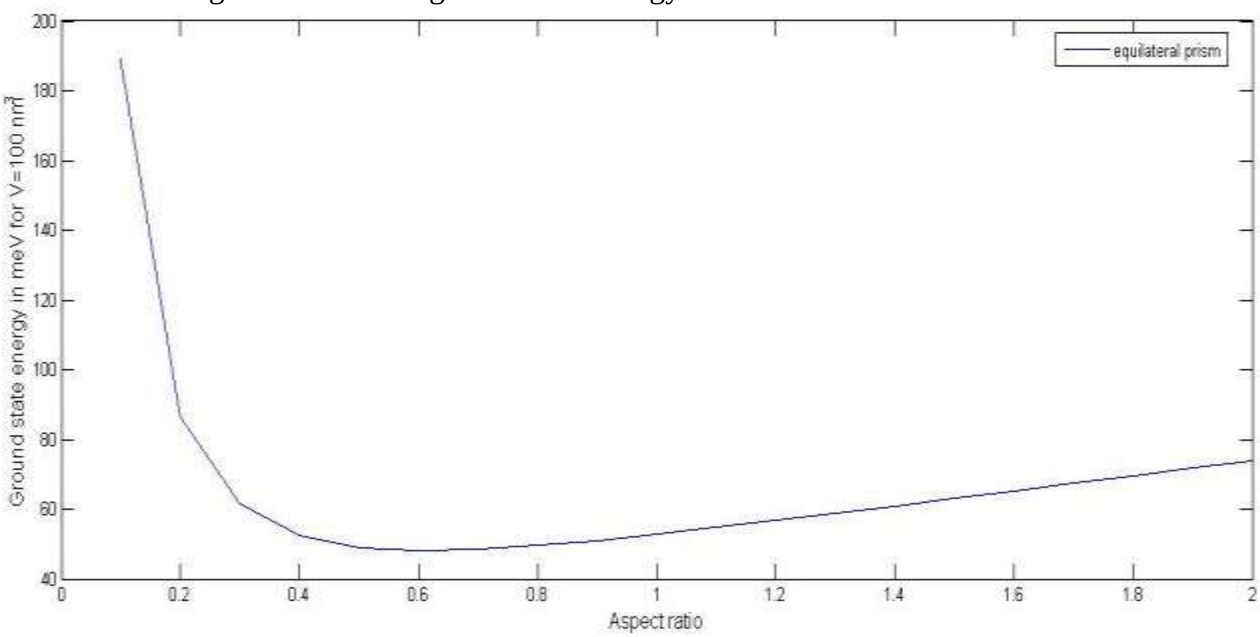

Fig. 3: Variation of ground state energy with aspect ratio

The range of parameters are chosen such that the value of volume and aspect ratio considered are useful for practical quantum devices [4]. Fig.2 shows that ground state energy decreaseswith volume. This result can be explained on basis of Uncertainty principle. When the volume of the structure is increased, the standard deviation accessible to position of the electron is increased. As a result of Uncertainty principle, it decreases the standard deviation accessible to its linear momentum which ultimately decreases the value of ground state energy with increase in volume.

IV. CONCLUSION

From the study of electronic states in triangular quantum wire, we can conclude that the energy eigenvalues of a quantum dot depends upon shape of cross-section, volume of the structure and aspect ratio of the structure. Ground state energy decreases monotonically with increase in volume at fixed aspect ratio while it first decreases rapidly with increase in aspect ratio and after attaining a minimum, it increases slowly with increase in aspect ratio.

V. REFERENCES

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