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Study of Effect of Shape, Size and Symmetry on Electronic States of Some Three-dimensional Structures in Mesoscopic Size Regime

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Abstract

This study presents theoretical study of effect of size and symmetry of different shaped three-dimensional GaAs structures in mesoscopic size regime. The effective mass Schrödinger equation is used in various shapes and its solution are modified as a function of volume and aspect ratio of structures. The calculated energy eigenvalues for square prism, equilateral prism, regular tetrahedral, cylindrical and spherical are comparatively analyzed to observe the effect of shape, size and symmetry on it. The result shows that energy eigenvalues decreases with increase in order of symmetry and volume. However, the energy eigenvalue doesn't vary monotonically with aspect ratio of structures. It decreases first rapidly and then increases with increase in aspect ratio of structures. Degeneracy of first excited state of different structures was found to depend upon both their order of symmetry and aspect ratio.

Keywords: *Confinement, aspect ratio, elements of symmetry, effective mass Schrödinger equation*

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INTRODUCTION

The theoretical study of low dimensional structures is of prime importance in research field of semiconductor. The low dimensional structures are those structures in which at least one spatial dimension has length in the nano-size domain, typically in the range 1–100 nm. This size regime is also called "mesoscopic size regime" and is studied by many researchers on its various properties like quantization of states [1], sharper density of states, quantized conductance [2, 3], reduction in electron-phonon coupling [2], etc. Electronic states of some of these structures of various shapes, like cuboid, cylindrical, pyramidal, conical and lens shaped [4–10] have been studied by various methods.

In present work, we will consider three-dimensional GaAs structures of square prism, equilateral prism, regular tetrahedron, cylindrical and spherical shaped collectively. Square prism is a prism whose base is a square and base of an equilateral prism is an equilateral triangle. Regular tetrahedron is a tetrahedron in which all four faces are same equilateral triangle. The potential inside each of the structure is taken as constant (zero) for uniform distribution of material with mass of electron equal to its effective mass and outside is infinity for complete confinement. This set of structures is interesting in sense that the order of symmetry, rotational and reflection symmetry both, varies over a wide range. Therefore, the comparative study of these-structure with complete confinement along all three dimensions shall give idea of effect of shape and size as well as symmetry of their electronic state in corresponding quantum dots, which are desired for construction of various semiconductor devices. For example, the knowledge of symmetry and size on electronic states is required for designing of active medium of a semiconductor laser in order to increase its efficiency.

MATHEMATICAL MODELS

The effective mass Schrödinger [11–12, 5] equation after taking into the operator ordering is written as

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

Where, $m^*(\vec{r})$ is effective mass of the electron, $V(\vec{r})$ is the potential function in the given region and E is the total energy of the particle. $\psi(\vec{r})$ is the wave function associated with the electron in material. As material is distributed uniformly and completely confined inside corresponding structures, $V(\vec{r})$ can be taken as

$V(\vec{r})=0$ at all points inside each of the structure
$=\infty$ at all points outside of each of the structure
and $m^*(\vec{r})=m^*$ as it is independent of $\vec{r}$.

m^* is effective mass of GaAs inside structure and is equal to 0.067 m_e, m_e = mass of an electron [5].

Therefore, the effective mass Schrödinger equation inside each of the considered structure takes the form

$$-\frac{\hbar^2}{2m^*}\nabla^2\psi=E\psi \quad (1)$$

Square Prism

Square prism is a prism with square cross-sectional base. In Figure 1, its base is xy plane and height is along z axis. Its region is given by $0\le x\le a, 0\le y\le a$ and $0\le z\le h$. To get energy eigenvalues of an electron completely confined in it, Eq. (1) is needed to solved with boundary condition that wave function $\psi(x,y,z)$ vanish at each point of the surface of the square prism.

Let $\psi=\psi_x\psi_y\psi_z$ and substituting this in Eq. (1) and dividing it's both sides by $\psi_x\psi_y\psi_z$, Eq. (1) reduces to

$$-\frac{\hbar^2}{2m^*}\left(\frac{1}{\psi_x}\frac{\partial^2\psi_x}{\partial x^2}+\frac{1}{\psi_y}\frac{\partial^2\psi_y}{\partial y^2}+\frac{1}{\psi_z}\frac{\partial\psi_z}{\partial z^2}\right)=E$$

Let $E=E_n+E_m+E_l\,(say)$ such that

$$-\frac{\hbar^2}{2m^*}\left(\frac{1}{\psi_x}\frac{\partial^2\psi_x}{\partial x^2}\right)=E_n \text{ with } \psi_x=0 \text{ at x=0 and x=a} \quad (2)$$

$$-\frac{\hbar^2}{2m^*}\left(\frac{1}{\psi_y}\frac{\partial^2\psi_y}{\partial y^2}\right)=E_m \text{ with } \psi_y=0 \text{ at y=0 and y=a} \quad (3)$$

$$\text{and } -\frac{\hbar^2}{2m^*}\left(\frac{1}{\psi_z}\frac{\partial^2\psi_z}{\partial z^2}\right)=E_l \text{ with } \psi_z=0 \text{ at z=0 and z=a} \quad (4)$$

Solution of Eq. (2), (3) and (4) gives $E_n=\frac{\hbar^2 n^2}{2m^*a^2}$, $E_m=\frac{\hbar^2 m^2}{2m^*a^2}$ and $E_l=\frac{\hbar^2 l^2}{2m^*h^2}$

Where, n, m and l are integers with condition: $n\ge1, m\ge1$ and $l\ge1$.

So, energy eigenvalues for square prism structure is given by

$$E_{nml}=E_n+E_m+E_l=\frac{\hbar^2}{2m^*}\left(\frac{n^2+m^2}{a^2}+\frac{l^2}{h^2}\right) \quad (5)$$

If $h\to0$ in the above equation, it can be used to calculate energy eigenvalues for square thin film. Using V as volume of structure and defining aspect ratio of structure as Q = $\frac{h}{a}$, h = height of structure and a = base length of structure, Eq. (5) is modified as function of aspect ratio and volume which gave.

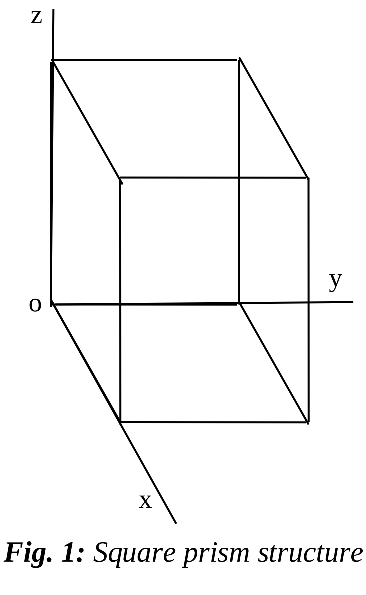

Fig. 1: *Square prism structure*

$$E_{nml} = \frac{\hbar^2\pi^2}{2m^*}\left(\frac{Q}{V}\right)^{\frac{2}{3}}\left(n^2 + m^2 + \frac{l^2}{Q^2}\right) \quad (6)$$

In Eq. (6), $n,m,l = (1,1,1)$ gives its ground state energy as

$$E_{GS} = \frac{\hbar^2\pi^2}{2m^*}\left(\frac{Q}{V}\right)^{\frac{2}{3}}\left(2 + \frac{1}{Q^2}\right) \quad (7)$$

and for $Q<1: n,m,l = (2,1,1)$ or $(1,2,1)$ gives twofold degenerate first excited state energy

$$E_{1st} = \frac{\hbar^2\pi^2}{2m^*}\left(\frac{Q}{V}\right)^{\frac{2}{3}}\left(5 + \frac{1}{Q^2}\right) \quad (8)$$

For $Q=1$, the square prism structure will be identical to cubic structure and $n,m,l = (2,1,1)$, $(1,2,1)$ or $(1,1,2)$ gives threefold degenerate first excited state degenerate. For $Q>1$, $n,m,l = (1,1,2)$ gives non-degenerate first excited state. This suggests that degeneracy of first excited state also depends upon aspect ratio of the structures.

Equilateral Prism

Equilateral prism is prism which base is an equilateral triangle. In Figure 2, its base is an equilateral triangle in xy plane and height is along z axis, i.e., its region is given as
$0 \le x \le a, \sqrt{3x} \le y \le \sqrt{3a} - \sqrt{3x}$ and
$0 \le z \le h$.

Let, $\psi = \psi_{xy}(x,y)\psi_z(z)$ and substituting this in Eq. (1) and dividing it's both sides by $\psi_{xy}\psi_z$, it gave

$$-\frac{\hbar^2}{2m^*}\left\{\frac{1}{\psi_{xy}}\left(\frac{\partial}{\partial x^2} + \frac{\partial}{\partial y^2}\right)\psi_{xy} + \frac{1}{\psi_z}\frac{\partial\psi_z}{\partial z^2}\right\} = E \quad (9)$$

The energy eigenvalues for complete confinement in a 2D equilateral triangular structure is studied by many researcher by various methods and is given by [13, 14]

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

Where, n,m are positive integers and $n \ge 2m$
So, ψ_{xy} appearing in eq.(9) must satisfy

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

Substituting it Eq. (9), we get

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

With the boundary conditions along z-axis: $\psi_z = 0$ at z = 0 and z = h, the solution of Eq. (10) gives

$$E - E_{nm} = \frac{l^2\pi^2}{h^2}$$ with l are integers and $l \ge 1$

Substituting the value of E_{nm}, energy eigenvalues came as

$$E = E_{nml} = \frac{\hbar^2}{2m^*}\left\{\frac{\left(\frac{4\pi}{3}\right)^2\left(n^2 + m^2 - nm\right)}{a^2} + \frac{l^2\pi^2}{h^2}\right\} \quad (11)$$

Where, n and m are distinct integer with $n \ge 2m$, $l \ge 1$.

As a function of aspect ratio and volume, it becomes

$$E_{nml} = \frac{\hbar^2}{2m^*}\left(\frac{\sqrt{3}}{4}\frac{Q}{V}\right)^{2/3}\left\{\left(\frac{4\pi}{3}\right)^2\left(n^2 + m^2 - nm\right) + \frac{\pi^2 l^2}{Q^2}\right\} \quad (12)$$

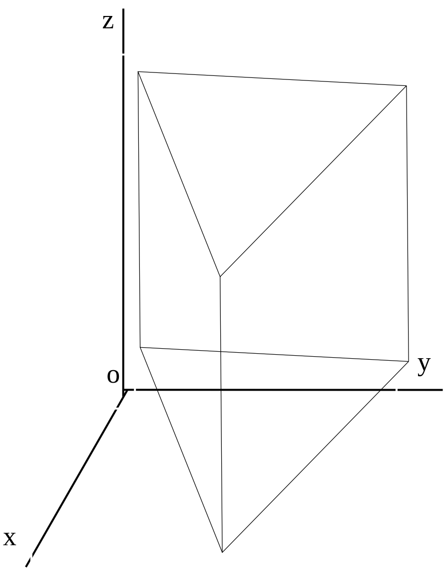

***Fig. 2:** Equilateral prism structure.*

In Eq. (12) $n,m,l=(1,2,1)$ gives its ground state energy

$$E_{GS}=\frac{\hbar^2}{2m^*}\left(\frac{\sqrt{3}}{4}\frac{Q}{V}\right)^{2/3}\left\{\left(\frac{4\pi}{3}\right)^2(3)+\frac{\pi^2}{Q^2}\right\} \tag{13}$$

and again degeneracy was found to depend upon aspect ratio. For $Q<1$, $n,m,l=(2,1,2)$ gives its first excited state energy

$$E_{1st}=\frac{\hbar^2}{2m^*}\left(\frac{\sqrt{3}}{4}\frac{Q}{V}\right)^{2/3}\left\{\left(\frac{4\pi}{3}\right)^2(3)+\frac{4\pi^2}{Q^2}\right\} \tag{14}$$

Cylindrical

Cylindrical structure with circular cross-section is considered In Figure 3, its circular base is xy plane as $0\le x^2+y^2\le\left(\frac{a}{2}\right)^2$ and its length is along z axis as $0\le z\le h$. Here we have taken 'a' as diameter of cylinder so that the parameter 'a' remains base length of this structures as well. Using cylindrical polar co-ordinates with $\rho=\sqrt{x^2+y^2}$, eq.(1) takes the form

$$-\frac{\hbar^2}{2m^*}\left\{\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial}{\partial\rho}\right)+\frac{1}{\rho^2}\frac{\partial^2}{\partial\phi^2}+\frac{\partial^2}{\partial z^2}\right\}\psi=E\psi$$

Using method of separation of variables, putting $\psi=\psi_\rho\psi_\phi\psi_z$, above equation reduces to

$$\frac{1}{\psi_\rho}\left(\frac{\partial^2\psi_\rho}{\partial\rho^2}+\frac{1}{\rho}\frac{\partial\psi_r}{\partial\rho}\right)+\frac{1}{\rho^2}\frac{1}{\psi_\phi}\frac{\partial^2\psi_\phi}{\partial\phi^2}+\frac{1}{\psi_z}\frac{\partial^2\psi_z}{\partial z^2}=\frac{-2m^*E}{\hbar^2}=-k^2 \tag{15}$$

Taking $\frac{1}{\psi_z}\frac{\partial^2\psi_z}{\partial z^2}=const.=-k_z^2(say)$ (16)

and $\frac{1}{\psi_\phi}\frac{\partial^2\psi_\phi}{\partial\phi^2}=const.=m^2$, (17)

Using Eq.(16) and (17), Eq.(15) reduces to

$$\frac{1}{\psi_\rho}\left(\rho^2\frac{\partial^2\psi_\rho}{\partial\rho^2}+\rho\frac{\partial\psi_\rho}{\partial\rho}\right)+\rho^2\left(k^2-k_z^2\right)=m^2 \tag{18}$$

Substituting $\rho\sqrt{k^2-k_z^2}=\alpha$ in Eq.(18), it gives

$$\alpha^2\frac{\partial^2\psi_\rho}{\partial\alpha^2}+\alpha\frac{\partial\psi_\rho}{\partial\alpha}+\left(\alpha^2-m^2\right)\psi_\rho=0 \tag{19}$$

which is cylindrical Bessel equation of order m.

Using the boundary condition $\psi_\rho=0$ at $\rho=0$ and $\rho=\frac{a}{2}$, we get $k^2-k_z^2=\frac{k_{mn}^2}{\left(\frac{a}{2}\right)^2}$

where k_{mn} is a n[th] zero of m[th] order cylindrical Bessel function with $n\ge1, m\ge0$.

Solving Eq. (15) with boundary condition $\psi_z=0$ at z = 0 and z=h gave $k_z=\frac{l\pi}{h}$, where l is any integer with $l\ge1$. So,

$$k^2=\frac{4k_{mn}^2}{a^2}+\frac{l^2\pi^2}{h^2}$$

$$\Rightarrow E=E_{nml}=\frac{\hbar^2}{2m^*}\left\{\frac{4k_{mn}^2}{a^2}+\frac{l^2\pi^2}{h^2}\right\} \tag{20}$$

In limit $h\to0$, the above equation can be used to find energy eigenvalues of an electron confined in a circular thin film. In terms of volume and aspect ratio, it can be modified as

$$E_{nml}=\frac{\hbar^2}{2m^*}\left(\frac{\pi Q}{4V}\right)^{2/3}\left(4k_{mn}^2+\frac{l^2\pi^2}{Q^2}\right). \tag{21}$$

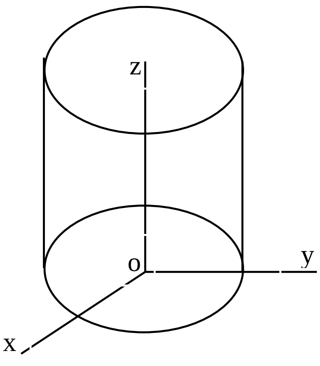

Fig. 3: *Cylindrical structure*

Using first zero of zeroth order Cylindrical Bessel function $k_{0,1} = 2.405$ [15, 16], i.e., n=1, m=0, and l =1, gives its ground state energy

$$E_{GS} = \frac{\hbar^2}{2m^*}\left(\frac{\pi Q}{V}\right)^{2/3}\left(4(2.405)^2 + \frac{\pi^2}{Q^2}\right) \quad (22)$$

and first zero of first order Cylindrical Bessel function $k_{1,1} = 3.832$ [15, 16], i.e., n=1, m=1, and l =1, first excited state energy comes as

$$E_{GS} = \frac{\hbar^2}{2m^*}\left(\frac{\pi Q}{V}\right)^{2/3}\left(4(3.832)^2 + \frac{\pi^2}{Q^2}\right) \quad (23)$$

Spherical

Taking center at origin, its region is given as $0 \le x^2 + y^2 + z^2 \le \left(\frac{a}{2}\right)^2$. Again, parameter 'a' is diameter of this structure so that it remains similar to base length (Figure 4). Obviously, the aspect ratio will be one as ratio of height and base length are same for spherical structure. Using the spherical polar co-ordinates, Eq.(1) reduces to

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

$$\Rightarrow -\frac{\hbar^2}{2m^*}\left\{\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \frac{\hat{L}^2}{\hbar^2 r^2}\right\}\psi = E\psi \quad (24)$$

Where, L^2 is an operator corresponding to magnitude of square of angular momentum of the electron confined in the spherical region.

Using variable separable form $\psi = R_{Elm}(r)Y_{lm}(\theta,\phi)$ and using the fact that

$$\hat{L}^2 Y_{lm}(\theta,\phi) = l(l+1)\hbar Y_{lm}(\theta,\phi), \quad (25)$$

Where, $Y_{lm}(\theta,\phi)$ is spherical harmonics with l is an integer and $l \ge 0, m = -l, -(l-1), ...(l-1), l$.

Substituting Eq.(25) in Eq.(24), it reduces to the differential equation for radial function as

$$-\frac{\hbar^2}{2m^*}\left\{\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}\right) + \frac{l(l+1)}{r^2}\right\}R_{El} = ER_{El} \quad (26)$$

As 'm' does not appear in Eq. (24), the radial function is independent of 'm'. So, we have written $R_{Elm} = R_{El}$. Taking $\frac{2m^*E}{\hbar^2} = k^2$, we get

$$\left\{\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}\right) + \frac{l(l+1)}{r^2} + k^2\right\}R_{El} = 0,$$

Substituting $\beta = kr$ in above equation gives,

$$\left\{\left(\frac{\partial^2}{\partial \beta^2} + \frac{2}{\beta}\frac{\partial}{\partial \beta}\right) + \left(1 - \frac{l(l+1)}{\beta^2}\right)^2\right\}R_{El}(\beta) = 0$$

which is spherical Bessel differential equation of order l. Using boundary condition that radial wave function should vanish at surface of the sphere, i.e., at r = a/2, we get $k\frac{a}{2} = p_{ln}$ where p_{ln} is n[th] zero of l[th] order spherical Bessel function with $n \ge 1, l \ge 0$.

Substituting the value of 'k', it gives energy eigenvalues as

$$E_{nl} = \frac{\hbar^2}{2m^*\left(\frac{a}{2}\right)^2}(p_{ln})^2, \quad (27)$$

As aspect ratio for spherical structure is always one, so in terms of volume

$$E_{nl} = \frac{\hbar^2}{2m^*}\left(\frac{4\pi}{3V}\right)^{2/3}(p_{ln})^2. \quad (28)$$

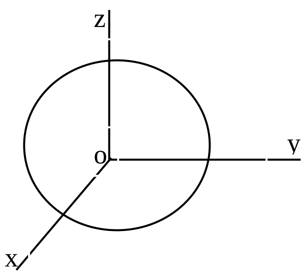

Fig.4: *Spherical structure.*

First zero of zeroth order Bessel function $p_{0,1} = \pi$, i.e., $l = 0, n = 1$ gives its ground state energy as

$$E_{GS} = \frac{\hbar^2}{2m^*}\left(\frac{4\pi}{3V}\right)^{2/3}(\pi)^2 \quad (29)$$

and first zero of first order spherical Bessel function [15] $p_{1,1} = 4.4934$, i.e., $l = 1, n = 1$ gives its first excited state energy

$$E_{1st} = \frac{\hbar^2}{2m^*}\left(\frac{4\pi}{3V}\right)^{2/3}(4.4934)^2. \quad (30)$$

Regular Tetrahedron

A regular tetrahedron is a tetrahedron which each side has equal length 'a' (Figure 5). The energy eigenvalues of an electron of mass 'm' confined in tetrahedral box of side length $\sqrt{3}\pi$ is given by [14]

$$E_{nml} = \frac{\hbar^2}{8m}\left\{3\left(n^2 + m^2 + l^2\right) - 2nm - 2ml - 2l\,\mathrm{n}\right\} \quad (31)$$

Where, n, m and *l* are distinct positive integers.

We have taken the above calculated energy eigenvalue for regular tetrahedron structure here only for its comparative study of effect of shape, size and symmetry on energy eigenvalues with other structures considered of different order of symmetries, viz. equilateral prism, square prism, cylindrical and spherical.

Using same method [14] for regular tetrahedron of any arbitrary side length 'a', the energy eigenvalues came as

$$E_{nml} = \frac{3\hbar^2\pi^2}{8m^*a^2}\left\{3\left(n^2 + m^2 + l^2\right) - 2nm - 2ml - 2l\,\mathrm{n}\right\} \quad (32)$$

Obviously substituting $a = \sqrt{3}\pi$ in Eq. (32) will give back the Eq. (31) [14]. Aspect ratio of a regular tetrahedron structure is always equal to fixed to $\sqrt{\frac{2}{3}}$, Eq.(32) can be modified as function of its volume as

$$E_{nml} = \frac{3\hbar^2\pi^2}{8m^*}\left(\frac{\sqrt{2}}{12V}\right)^{2/3}\left\{3\left(n^2 + m^2 + l^2\right) - 2nm - 2ml - 2l\,\mathrm{n}\right\} \quad (33)$$

$n, m, l = (1, 2, 3)$ in Eq.(32) gives its ground state energy and $n, m, l = (1, 2, 4)$ in Eq.(32) gives its first excited state energy

To make comparative studies of energy eigenvalues of these structure in terms of its volume and aspect ratio for different structures are summarized in Table 1.

DISCUSSION OF SYMMETRY OF STRUCTURES

Considering rotational and reflection symmetries of each of the above structures, order of symmetry is studied. For equilateral prism, we first observe symmetry of its base, which is an equilateral triangle. Equilateral triangle has C_{3v} group of symmetry, i.e., it has three rotational and three reflection symmetries.

Therefore, its order of symmetries is 6. Since D_3 is isomorphic to C_{3v}, $D_3 = C_{3v}$. As equilateral prism has two equilateral triangle and each one is reflection of other about mid horizontal plane, its symmetries will form a group that contain the elements of D_3 plus the horizontal reflection plane σ_h, i.e., group D_{3h} and it has twice as many elements as D_3 [17, 18]. So, equilateral prism has six rotational and six translational symmetries, which gives its order of symmetry equal to 12.

Similarly, C_{4v} symmetry of square leads to D_{4h} symmetry to square prism and it will have eight rotational and eight reflection symmetries giving order of symmetry equal to 16. Again using the symmetry of equilateral triangle, the symmetries of regular tetrahedral structure form T_d group in which include twelve reflection and twelve rotational symmetries giving order of symmetry to 24 [18]. These symmetries for discussed structures are summarized in Table 1.

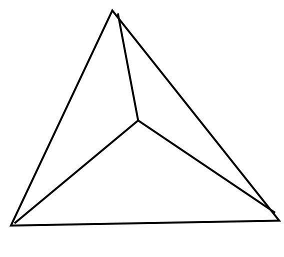

Fig.5: *Regular tetrahedral structure.*

Cylinder has its axis as ∞-fold rotational symmetry and ∞ axes of twofold symmetry (about perpendicular bisectors to its length) and these symmetry forms a group D_∞. Sphere has also ∞ axes (diameters) of ∞-fold symmetry. So, it has ∞ rotational and reflection symmetries. These forms a group O(3) [18].

The symmetries of structures impart degeneracy to electronic states. The structure belonging to D_{3h} and D_{4h} can have maximum twofold degeneracy while structure belonging to T_d can have threefold degeneracy [18]. After analyzing the energy expressions for various structures, it was observed that the ground state will be non-degenerate in all structures and degeneracy of first excited will depend upon order of symmetry as well as aspect ratio. For example, as observed in sec II(a), first excited state in square prism is doubly degenerate for aspect ratio less than one, triply degenerate for aspect ratio equal to one and non-degenerate for aspect ratio less than one. Increase in order of symmetries lead to increase in degeneracy of first excited state. Regular tetrahedral has threefold first excited state. Spherical structure has also threefold degeneracy to its first excited stated and in general its degeneracy will be $2l+1$ times for corresponding value of l

To study effect of order of symmetry on value of ground state energy, its value is calculated for considered structures at fixed volume and aspect ratio. It was observed that ground state energy decreases with increase in order of symmetry of structures at fixed volume and aspect ratio. For 100 nm^3 volume and aspect ratio 'one', the ground state energy variation is shown graphically in Figure 6.

DISCUSSION OF EFFECT OF SIZE AND ASPECT RATIO:

Ground state energy of each structure were calculated and plotted collectively. Range of volume 10 nm^3 to 10^7 nm^3 and range of aspect ratio (height to base length ratio) 0.1 to 2 have been considered. The above volume and aspect ratio range ensures that the dimension of structures remains nearly in mesoscopic regime [15, 5].

At first, we kept the aspect ratio of square prism, equilateral prism and cylindrical shapes fixed at 'one' as that of spherical structure. We calculated variation of ground state energy with volume for each of these three structures at fixed aspect ratio. The result is given graphically in Figure 7. Ground state energy variation with volume for square prism, equilateral prism, cylindrical and regular tetrahedral at fixed aspect ratio $\sqrt{\frac{2}{3}}$ (aspect ratio of a regular tetrahedron) is plotted in Figure 8.

Obviously, for each of the structures, ground state energy is decreasing with increase in volume. The first excited state energy was also found to be decreasing with increase in volume. This can be seen as a consequence of Uncertainty principle. Increase in volume leads to increase in allowed standard deviation in position of the electron, which decreases the standard deviation accessible to its linear momentum in accordance with Uncertainty principle. This lowers the value of ground state energy of the electron with increase in its volume.

In order to observe the effect of aspect ratio on electronic states, the variation of ground state energy is calculated for square prism, equilateral prism and cylindrical by varying aspect ratio and keeping the volume fixed at 100 nm^3. Spherical and regular tetrahedral structure is not included here as its aspect ratio is fixed. The result is shown graphically in Figure 9.

The results show that the energy eigenvalues doesn't vary monotonically with aspect ratio. It first decreases rapidly with aspect ratio and then increases gently with aspect ratio.

This can be seen analytically as result of two competing effect- one due to confinement along height and other due to confinement of base of the structure. When aspect ratio is small, increase in height leads to larger decrease in confinement with respect to increase in confinement due to decrease in base length. Thus an overall decrease in confinement leads to rapid decrease in ground state energy with increase in aspect ratio. For the larger aspect ratio, the above effect due to change in confinement along height and base are reversed, i.e., at larger aspect ratio, decrease in base leads slightly larger increase in confinement than decrease in confinement due to increase in height. So, an overall a slight increase in confinement with increase in aspect ratio leads to gentle increase in ground state energy. Obviously, the aspect ratio for which the effects cancel each other, the ground state energy is minimum.

Table 1: *Summary of Energy Eigen Values.*

Shape of structures	**Energy eigenvalues**	**Conditions on integers n, m and *l***
Equilateral prism	$E_{nml}=\frac{\hbar^2\pi^2}{2m^*}\left(\frac{\sqrt{3}}{4}\frac{Q}{V}\right)^{\frac{2}{3}}\left(n^2+m^2+\frac{l^2}{Q^2}\right)$	$n\geq1, m\geq1$ and $l\geq1$
Square prism	$E_{nml}=\frac{\hbar^2}{2m^*}\left(\frac{Q}{V}\right)^{2/3}\left\{\left(\frac{4\pi}{3}\right)^2\left(n^2+m^2-nm\right)+\frac{\pi^2 l^2}{Q^2}\right\}$	$n\geq2m, m\geq1$ and $l\geq1$
Cylinder	$E_{nml}=\frac{\hbar^2}{2m^*}\left(\frac{\pi Q}{V}\right)^{2/3}\left(4k_{mn}{}^2+\frac{l^2\pi^2}{Q^2}\right)$	$n\geq1, m\geq0$ and $l\geq1$
Sphere	$E_{nl}=\frac{\hbar^2}{2m^*}\left(\frac{4\pi}{3V}\right)^{2/3}\left(p_{ln}\right)^2$	$n\geq1 and\ l\geq0$
Regular Tetrahedron	$E_{nml}=\frac{3\hbar^2\pi^2}{8m^*}\left(\frac{\sqrt{2}}{12V}\right)^{2/3}\left\{3\left(n^2+m^2+l^2\right)-2nm-2ml-2l\,\mathrm{n}\right\}$	$n\geq1, m\geq1, l\geq1$ $and\ n\neq m\neq l$

***Table 2**: Symmetry Elements of Structures.*

Shape of structures	**Symmetry group**	**No. of rotational symmetries**	**No. of reflection symmetries**	**Order of symmetry**
Equilateral prism	D_{3h}	6	6	12
Square prism	D_{4h}	8	8	16
Regular Tetrahedron	T_d	12	12	24
Cylindrical	D_∞	∞	∞	∞
Spherical	O(3)	∞	∞	∞

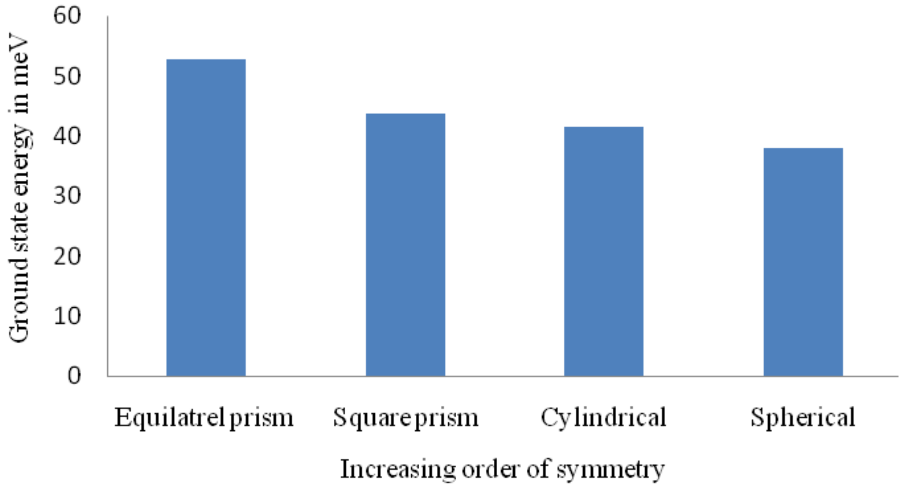

***Fig. 6**: Variation of Ground State Energy.*

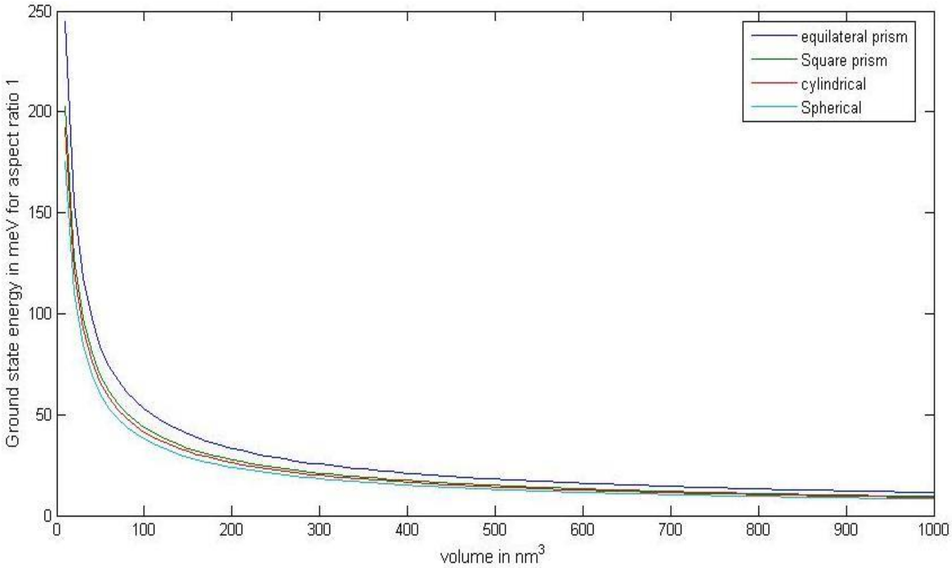

Fig. 7: *Ground State Energy for a Fixed Aspect Ratio 1.*

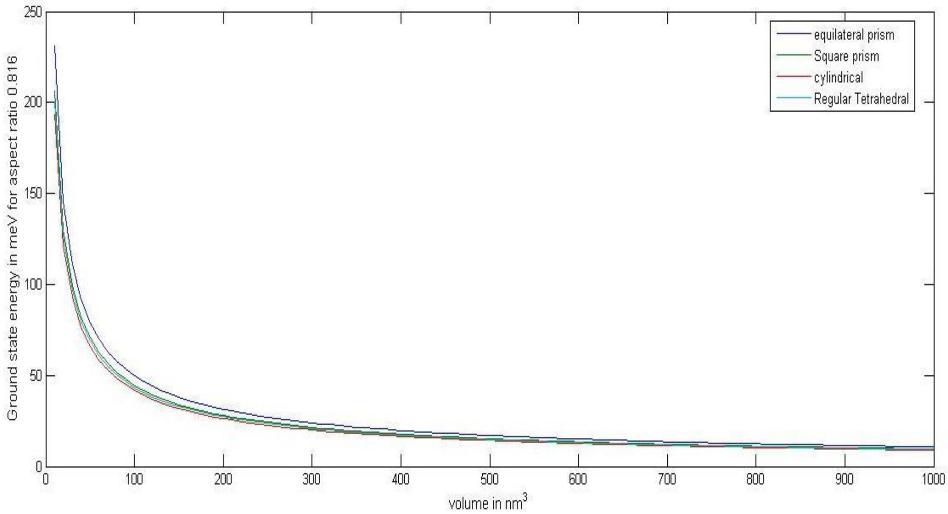

Fig. 8: *Ground State Energy for a Fixed Aspect Ratio 0.816.*

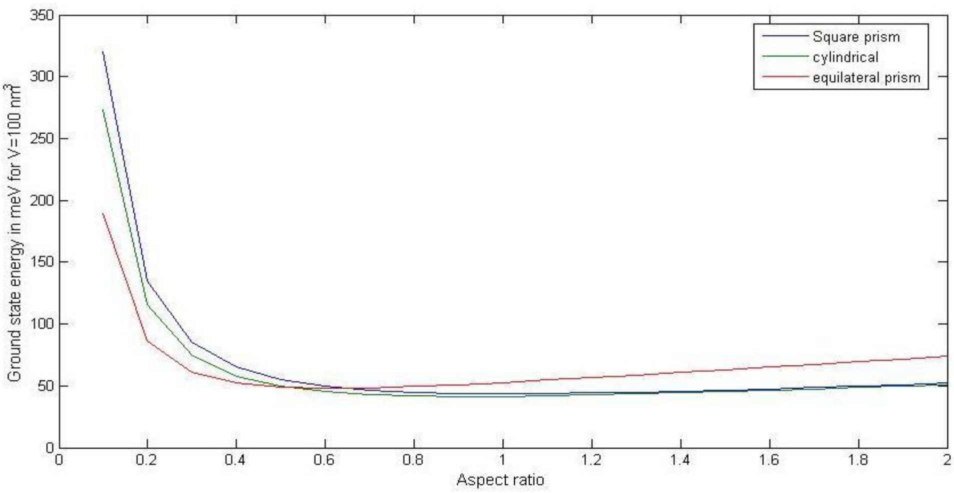

Fig. 9: *Variation of Ground State Energy at Fixed Volume.*

CONCLUSION

From this comparative study between energy eigenvalues in different structures, we can conclude following things:

1. For each shape for a given aspect ratio, the ground state energy and first excited energy decreases with increase in volume of the structure.
2. For each shape for a given volume, the ground state energy at first decreases rapidly with increase in aspect ratio and after attaining a minimum value, it increases gently with aspect ratio.
3. Ground state energy of different structures decreases with increase in the order of symmetry of structures.

The analytical reason of (1) and (2) are discussed in section IV, and that of (3) is discussed in section III. This study can also be extended to calculate the energy eigenvalues of corresponding quantum well by taking height of structure very small and restricting the motion along height of structure; and that of quantum well wire by taking base length very small and allowing the electron motion along only its height. The Knowledge of energy eigenvalues of various shaped structures can be used during development of quantum dot devices and related semiconductor devices. Further, the one can look to construct the wave packet in these three-dimensional structures to understand the effect of symmetry and size on time dependent electronic properties.

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