Report on

"Impact of Hydrostatic Pressure and Temperature on the matrix elements of a cylindrical Quantum wire"

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Submitted by:

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CANDIDATES' DECLARATION

We hereby declare that the project Dissertation II titled **"Impact of Hydrostatic Pressure and Temperature on the matrix elements of a cylindrical QW"** which is submitted by us to the Department of Applied Physics, Delhi Technological University, for the award of the degree of Master of Science, is carried under the supervision of **Professor Rinku Sharma.**

The work presented in this report has not been submitted and not under the consideration for the award of any other course / degree or any other Institute/University.

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To the best of my knowledge, the above work has not been submitted in part or full for any Degree or Diploma to this University or elsewhere. I, further certify that the publication and indexing information given by the students is correct.

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Supervisor

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THANK YOU

ABSTRACT

The matrix elements of a 2 – D electron gas restricted in a GaAs cylindrical quantum wire including Rashba Spin Orbit Interaction, under simultaneous effect of hydrostatic pressure and temperature is investigated. The strong dependency of hydrostatic pressure and absolute temperature, on energy band gap and effective mass of charge carriers of the quantum wire, have been found. Because of this, the linear and non-linear properties of the quantum wire also get affected. We also observed that under the influence of electric and magnetic field, the matrix elements get affected strongly with the change in Rashba spin orbit interaction and Magnetic field.

Pressure, temperature, and impurity effects on energy levels, binding energy, and linear and nonlinear optical properties of a modified Gaussian quantum wire are investigated in this article. In order to solve the single electron Schrodinger equation in the effective mass approximation, the finite element method is used. For a finite rectangular quantum wire in a transverse magnetic field, energy levels and Oscillator Strengths of an electron have been calculated. The results reveal that when the quantum wire has a certain width in one direction, the decoupled approximation, a numerical method for solving the Schrodinger equation, is not suitable for a quantum wire with a reduced cross section.

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Lists of Symbols and Abbreviation

Symbol/Index	Meaning/Abbreviation
QW	Quantum wire
2D	Two - dimensional
SOI	Spin Orbit Interaction
GaAs	Gallium Arsenide
nm	Nanometer
eV	Electron Volt
α	Rashba coefficient

Chapter 1

1.1 Introduction

A nanostructure is a structure that lies halfway between microscopic and molecular structures in terms of size. At the nanoscale, nano structural detail is microstructure.

When characterizing nanostructures, it's important to distinguish between the number of nanoscale dimensions in the volume of an object. On the nanoscale, nanotextured surfaces have only one dimension, i.e., the thickness of an object's surface is between 0.1 and 100 nm. On the nanoscale, nanotubes have two dimensions: their diameter is between 0.1 and 100 nm, and their length can be much longer. Finally, spherical nanoparticles have three dimensions on the nanoscale, with each spatial dimension ranging between 0.1 and 100 nanometers. Nanoparticles and ultrafine particles (UFP) are frequently used interchangeably.
A nanoparticle, also known as an ultrafine particle, is a small particle of matter with a dimension of 1 to 100 nanometers (nm). The name is sometimes applied to larger particles (up to 500 nm) or fibers and tubes with only two orientations of less than 100 nm. Metal particles less than 1 nm are commonly referred to as atom clusters instead.

Nanoparticles are distinguished from microparticles (1-1000 m), "fine particles" (sized between 100 and 2500 nm), and "coarse particles" (sized between 2500 and 10,000 nm) by their smaller size, which causes very different physical or chemical properties, such as colloidal properties, ultrafast optical effects, and electric properties.
Nanoparticles have features that differ significantly from larger particles of the same substance. Because an atom's usual diameter is between 0.15 and 0.6 nm, the nanoparticle's substance is concentrated within a few atomic diameters of its surface. As a result, the top layer's properties may take precedence over those of the bulk material. Because the interactions between the two materials at their interface become important, this effect is especially powerful for nanoparticles distributed in a medium of dissimilar composition.

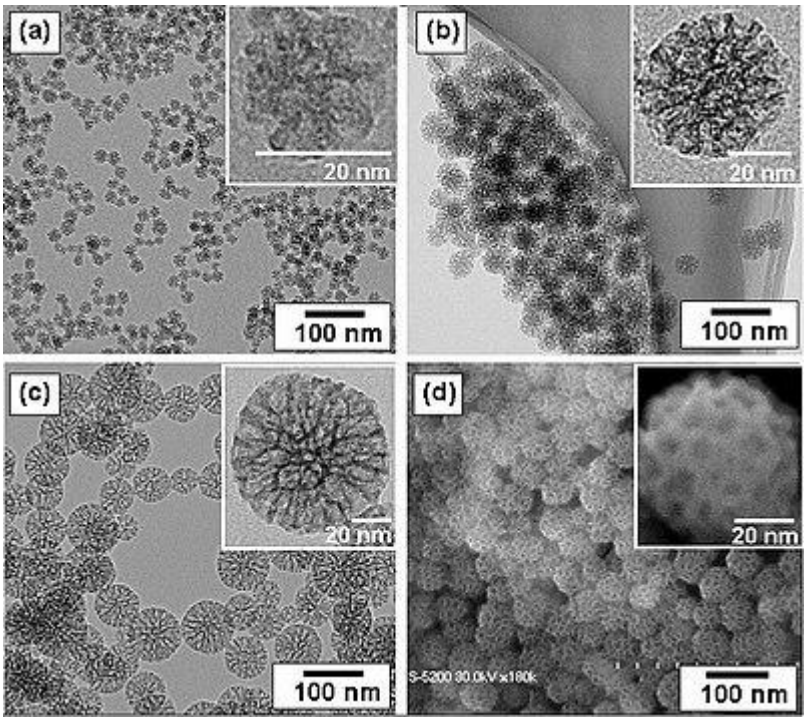


Fig.1. TEM (a, b, and c) images of prepared mesoporous silica nanoparticles with mean outer diameter: (a) 20nm, (b) 45nm, and (c) 80nm. SEM (d) image corresponding to (b). The insets are a high magnification of mesoporous silica particle.

A nanowire is a nanostructure that takes the shape of a wire and has a diameter on the order of a nanometer (109 meters). Nanowires, in a broader sense, are structures with a thickness or width restricted to tens of nanometers or less with an unconstrained length. Quantum mechanical phenomena are essential at these scales, hence the phrase "quantum wires."

1.2 What are low-dimensional structures?

The physicochemical properties of a solid differ noticeably from those of the bulk solid when one or more of its dimensions are decreased sufficiently. New electrical, mechanical, chemical, magnetic, and optical qualities can be introduced when the size of the component is reduced. A low-dimensional structure (or system) is the product of this process. The confinement of particles, particularly electrons or holes, to a low-dimensional structure causes a drastic shift in their behavior and the appearance of size effects that are commonly classified as quantum-size effects.
Low-dimensional materials have new physicochemical features that aren't seen in large-scale structures with the same composition. Nanostructures serve as a connection between molecules and bulk materials. Nanostructure features and responses can be controlled to create novel devices and technologies.

1.3 Classification of Low- Dimensional Materials

Low-dimensional structures are often classified based on how many reduced dimensions they have. The number of degrees of freedom in the particle momentum is referred to as dimensionality. Accordingly, depending on the dimensionality, the following classification is made:

Zero-dimensional (0D) structure or quantum dot (sometimes called “quantum box”): Quantization occurs in all three directions.

One-dimensional (1D) structure or quantum wire: Quantization occurs in two directions, leading to free movement along only one direction.

Two-dimensional (2D) structure or quantum well: Quantization of the particle motion occurs in one direction, while the particle is free to move in the other two directions.

Three-dimensional (3D) structure or bulk structure: No quantization of the particle motion occurs, i.e., the particle is free.

Source: https://en.wikipedia.org

Table 1. Nanostructures and their typical nanoscale dimensions

Nanostructures	Typical nanoscale dimension
Thin films and quantum wells (two-dimensional structures)	1–1000 nm (thickness)
Quantum wires, nanowires, nanorods and nanopillars (one-dimensional structures)	1–100 nm (radius)
Nanotubes	1–100 nm (radius)
Quantum dots, nanodots (zero-dimensional structures)	1–10 nm (radius)
Porous nanomaterials, aerogels	1–50 nm (particle size, pore size)
Sculptured thin films	10–500 nm

Tradition has determined that reduced-dimensionality structures are labeled by the remaining degrees of freedom in the particle motion, rather than by the number of directions with confinement.

Chapter 2

2.1 Quantum Confinement

Quantum confinement is a concept that refers to the energy of trapped electrons (electrons or electron hole). In comparison to bulk materials, the energy levels of electrons will not remain constant in nanocrystals. Furthermore, they become a discrete collection of energy levels after acquiring the restricted electron wave functions, as seen in Figure 1. When the dimensions of the potential approach the de Broglie wavelength of electrons, such phenomena occur, resulting in energy shifts or distinct levels. The phenomena are known as quantum confinement, and nanocrystals are frequently referred to as quantum dots (QDs). Additionally, the quantum dot effect has an impact on nanomaterial features such as electrical, optical, and mechanical behavior. Nanomaterials have higher energy electrons than bulk materials due to their unique nature.

Confined electrons have a higher energy than electrons in bulk materials, depending on the size of the QD. When the dimensionality of semiconductor nanomaterials is reduced from 2D to 1D or 1D to 0D, intriguing characteristics emerge. When the size and form of nanomaterials are reduced to less than 100–10 nm or even less, the quantum confinement phenomenon may occur. Size confinement results from these modifications caused by the discrete set of electron energy levels (Figures 1 and 2).

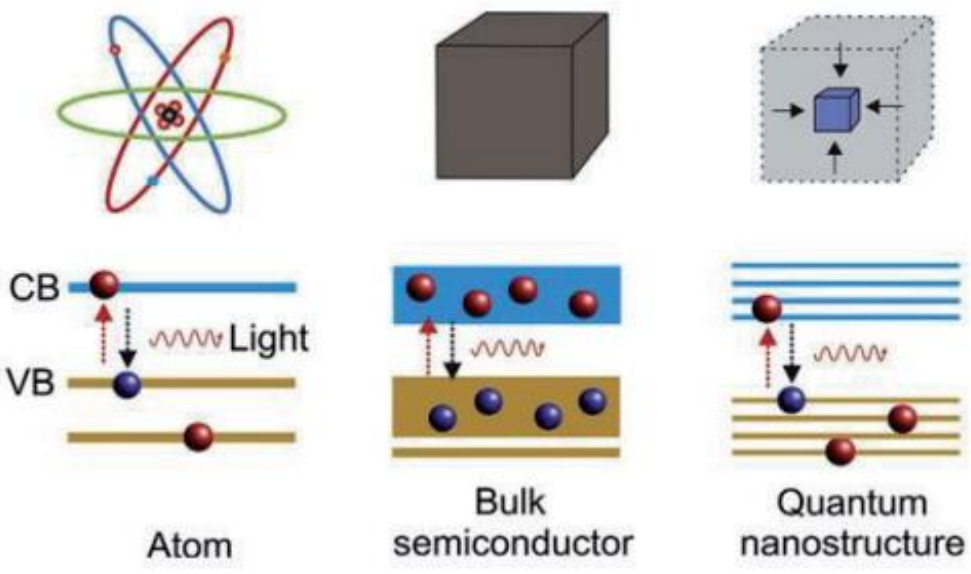


Fig.2 Schematic diagram showing energy band structures in atom, bulk semiconductor, and quantum nanostructure.

Source: https://cdn.intechopen.com

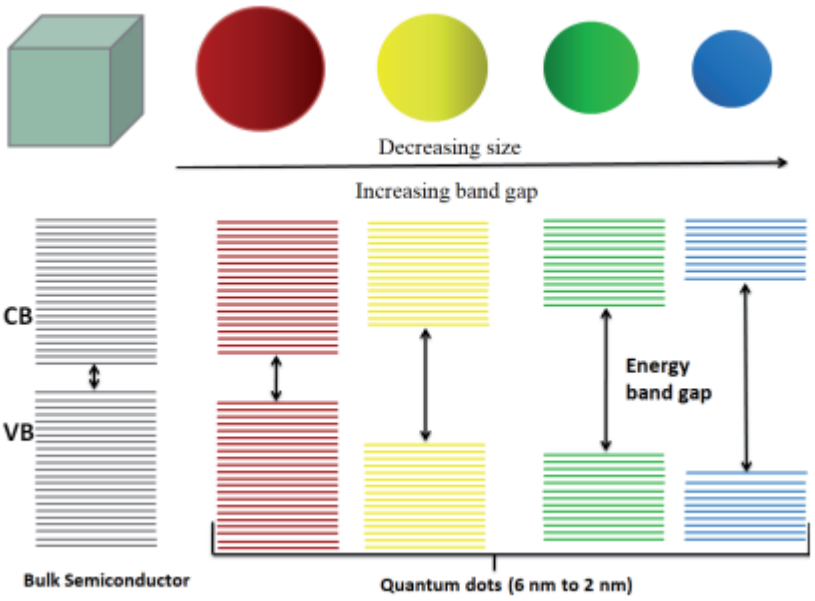


Fig.3 Schematic diagram showing energy band structures in atom, bulk material, and quantum nanostructure.

It is vital to understand the phenomenon of quantum dots in order to learn more about quantum confinement (QDs). QDs are a novel class of materials that exhibit quantum confinement effects. In all three dimensions, QDs are nanometer-sized semiconductor crystals, and molecules are tightly contained electrons or electron–hole pairs called "excitons" (described in the next section). Metals, insulators, semiconductors, and organic compounds all belong to the family of nanomaterials, which includes QDs. Because of their tunable bandgap nature, quantum confinement occurs only in semiconductor quantum dots, as opposed to metals, which have a zero bandgap. As previously stated, QD's unique tunable band gap features are made up of only.

2.2 Spin Orbit Interaction

The spin–orbit interaction (also known as the spin–orbit effect or spin–orbit coupling) is a relativistic interaction between a particle's spin and its motion inside a potential in quantum physics. The spin–orbit interaction, which causes alterations in an electron's atomic energy levels due to electromagnetic interaction between the electron's magnetic dipole, orbital motion, and the electrostatic field of the positively charged nucleus, is a good example of this phenomena. This phenomenon manifests itself as spectral line splitting, which can be thought of as a Zeeman effect consequence of two relativistic effects: the apparent magnetic field as perceived by the electron and the magnetic moment of the electron associated with its intrinsic spin. Protons and neutrons travelling inside the nucleus experience a comparable effect due to the link between rotational momentum and the strong nuclear force, resulting in a shift in their energy levels in the nucleus shell model. Spin–orbit phenomena for electrons in semiconductors and other materials are investigated for technological uses in spintronics.

Source: https://cdn.intechopen.com

2.2.a Rashba SOI

The Rashba effect, also known as the Bychkov–Rashba effect, is a momentum-dependent splitting of spin bands in bulk crystals and low-dimensional condensed matter systems (such as heterostructures and surface states), comparable to the Dirac Hamiltonian splitting of particles and antiparticles. The splitting is caused by a combination of spin–orbit interaction and crystal potential asymmetry, particularly in the direction perpendicular to the two-dimensional plane (as applied to surfaces and heterostructures).

The Rashba effect can be observed most clearly in the Rashba Hamiltonian, a basic model Hamiltonian

$$\widehat{H}_R = \frac{\alpha}{\hbar}\left(\vec{\sigma} * \left(\vec{p} + e\vec{A}\right)\right)$$

Where $\alpha = Rashba\ Coupling$
p = Momentum
$\sigma = Pauli\ matrix\ vector$

Chapter 3

Quantum Wire

3.1 How to prepare Quantum wire?

Photolithography or electron-beam lithography can be used to form a conventional quantum well layer, which can then be erased to leave a free-standing strip of quantum well material, which may or may not be filled in with an overgrowth of the barrier material (in this example, $Ga_{1-x}Al_xAs$). Any charge carriers are still restricted along the heterostructure growth (z-) axis, as they were in the quantum well, but they are also confined along an extra direction (if the strip is narrow enough), either the x- or y-axis, depending on the lithography.

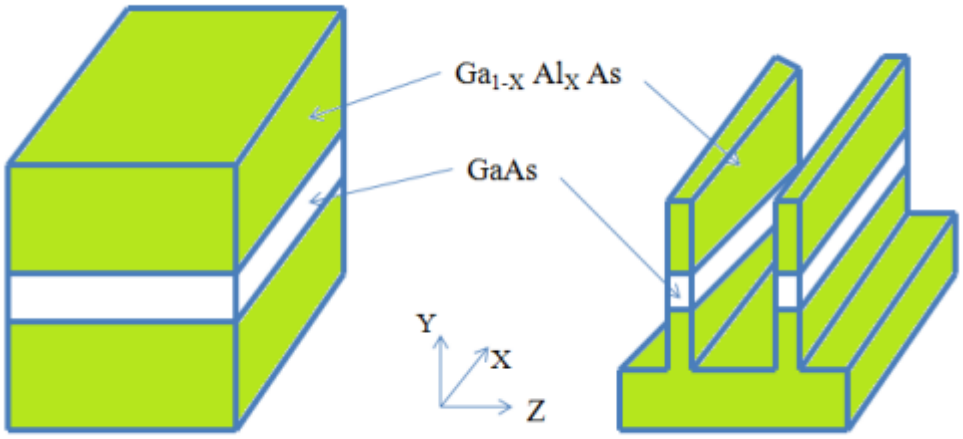


Fig.4 An expanded view of a single quantum wire, where clearly the electron (or hole) is free to move in only one direction, in this case along the y-axis.

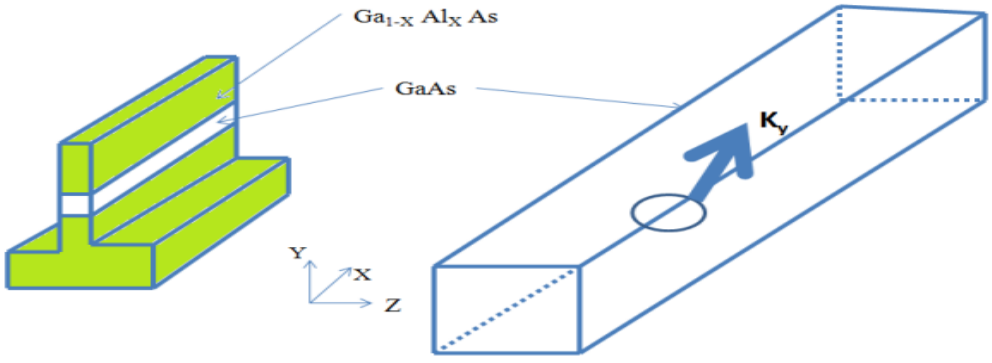


Fig. 5 GaAs Quantum Wire in which electron is moving in y direction.

Source: https://citeseerx.ist.psu.edu/

3.2 ONE-DIMENSIONAL STRUCTURES: QUANTUM WIRES AND NANOWIRES

It is feasible to decouple the motion along the length of the wire, which is taken to be along the x axis, for 1D structures—typically referred to as quantum wires, but other systems such as rods, belts, and tubes also fall into this category—as illustrated in Fig.

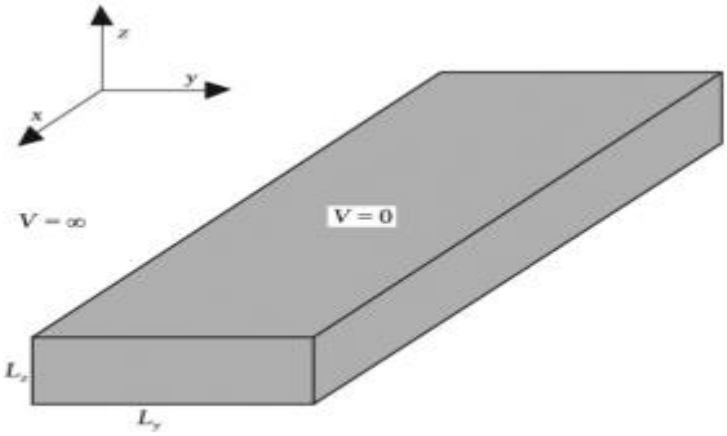


Fig. 6 Quantum wire at infinite potential

As a result, the potential V(r) is expressed as the sum of a two-dimensional confinement potential (yz plane) and a potential along the wire (x axis) as

$$V(\vec{r}) = V(x) + V(y,z)$$

As a result, the wave function is expressed as the following two-component product:

$$\psi(\vec{r}) = \psi(x)\psi(y,z)$$

We derive the time harmonic Schrodinger equation by substituting the above two equations.

$$\left\{-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)+V(X)+V(y,z)\right\}\psi(x)\psi(y,z) = E\psi(x)\psi(y,z)$$

The following two autonomous equations of motion can be deduced from this equation:

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi\,(\mathrm{x}) = E\psi(\mathrm{x})$$

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\psi(y,z)+V(y,z)\psi(y,z) = E\psi(y,z)$$

The above equation is satisfied by a plane wave of the form $\psi(x)\sim\exp(ik_x x)$, k_x being the particle's momentum along the x-axis, thus leading to the dispersion relationship

Source: https://citeseerx.ist.psu.edu

$$E = \frac{\hbar^2 k_x^2}{2m}$$

This equation, which resembles that of a 3D structure, specifies the energy level along the x axis, in which the particle is free to move (wherein confinement is not possible).

The potential $V(y,z)$ is given by:

$$V(y,z) = \{0\} \qquad \{0 < y < L_y\} \{0 < z < L_z\}$$

Otherwise ∞

The wave function ψ(y,z) is provided by outside the rectangular region is identically zero. As a result, the second equation of motion, which may be represented as, must be solved in the rectangular region.

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)\psi(y,z) = E\psi(y,z)$$

$$\{0 < y < L_y\} \{0 < z < L_z\}$$

The wave function dependencies on y and z can be dissociated thanks to the shape of the potential in this equation.

These equations have the same boundary conditions as the Schrodinger equation in the deep potential well and are subject to the same boundary conditions. Because the potential energy outside the wire is unlimited, the conventional boundary condition of wave function continuity at the walls dictates that the product of ψ (y) and $\psi(z)$ on the walls must be zero.

Hence, the Eigen solutions are

$$\psi_{n_y}(y) = \sqrt{\frac{2}{L_y}}\, sin\left(\frac{n_y \pi y}{L_Y}\right), \qquad n_y = 1,2,3, \ldots,$$

$$\psi_{n_z}(z) = \sqrt{\frac{2}{L_z}}\, sin\left(\frac{n_z \pi z}{L_z}\right), \qquad n_z = 1,2,3, \ldots.,$$

$$\psi_{n_y n_z}(y,z) = \sqrt{\frac{4}{L_y L_z}}\, sin\left(\frac{n_y \pi y}{L_y}\right) sin\left(\frac{n_z \pi z}{L_z}\right)$$

$$n_y = 1,2,3, \ldots., n_z = 1,2,3, \ldots..$$

Two main quantum numbers explain the quantum states in a quantum wire.

For a quantum well, just one principal quantum number is required.
The Eigen energy of a quantum wire grows as its size decreases, similar to that of a quantum well. In addition, for a given size, a smaller effective mass leads in a higher Eigen energy.

The corresponding Energy levels are given by

$$E_{n_y} = \frac{\hbar^2}{2m}\left(\frac{n_y\pi}{L_y}\right)^2, \qquad n_y = 1,2,3, \ldots.$$

$$E_{n_z} = \frac{\hbar^2}{2m}\left(\frac{n_z\pi}{L_z}\right)^2, \qquad n_z = 1,2,3, \ldots.$$

Where n_y and n_z are principal quantum number.

3.3 Optical properties of Nanomaterials

Nanomaterials' optical properties are among the most important, and they can be determined using a variety of spectroscopic techniques. The energies of the highest occupied molecular orbital, which is a valence band, and the lowest unoccupied molecular orbital, which is effectively the conduction band, are most affected by reduced dimensionality in the electronic structure of small nanoclusters. Nanomaterial optical properties, such as absorption, transmission, reflection, and light emission, are dynamic and can differ dramatically from bulk material properties. By simply altering its shape, size, and surface functioning, a wide range of optical effects can be created for a variety of purposes.
When electrons shift between these two states, optical characteristics like emission and absorption occur. The optical characteristics of semiconductors and certain metals change dramatically as particle size increases. The hue of various nanoparticle solutions is a basic illustration. The hue of the colloidal gold suspension changes from red to yellow as the size grows.

Table 2. Relation Between Size and Color of Nanoparticles

Nanoparticle	Size and Shape	Color
Gold	10–20 nm	Red
	2–5	Yellow
	> 20	Purple
Silver	40 nm	Blue
	100 nm	Yellow
	Prism shape	Red

The color of nanoparticles is caused by the surface plasmon resonance phenomenon, which is a resonance of the particles' outer electron bands with light wavelengths. When light photons excite the outer electrons of the particles, the metal particles' outer electrons jitter at specific wavelengths and absorb light corresponding to that resonance. The Mie's and Rayleigh scattering theories analytically quantify the link between particle size and color. Reduced dimensionality of nanoparticles affects properties such as photocatalysis, photoconductivity, photoemission, electroluminescence, and so on.

Chapter 4

4.1 Energy dispersion of quantum wire in external electric and magnetic field for an electron

Let us consider a two-dimensional GaAs quantum wire, with parabolic confined potential, given by:

$$V(x,y) = \frac{1}{2}m^*[P,T]\omega_0^2(x^2+y^2) \quad (1)$$

where $m^*[P,T]$ is the effective mass of electron under the influence of hydrostatic pressure and temperature. The Hamiltonian for a single electron in terms of mass can be given as

$$H_0(x,y)=\frac{1}{2m^*[P,T]}(p+eA)^2+\frac{1}{2}m^*[P,T]\omega_0^2(x^2+y^2) \quad (2)$$

When we consider the spin, two more terms will add up to the Hamiltonian in equation (2), where the first term is the Zeeman term and the second term is the spin orbit interaction term as:

$$H_{spin} = \frac{1}{2}g\mu_B B\sigma + H_{soi} \quad (3)$$

Where g represents the effective Lande factor for semiconductor. H_{soi} represents the spin orbit interaction term which consists of two terms as H_{soi}^R which is for Rashba spin orbit interaction and H_{soi}^D which is for Dresselhaus spin orbit interaction. Rashba term dominates over the Dresselhaus term that is why, here we will consider only the Rashba term, which is:

$$H_{soi}^R = \frac{\alpha}{\hbar}[\sigma * (p+eA)]_z \quad (4)$$

Where α is the Rashba coupling coefficient which can be controlled by applying the varying gate voltage in z-direction. Thus, the total Hamiltonian will be the combination of both the terms as H_0 and H_{soi}^R in the effective mass approximation and will be given as

$$H = \frac{p^2}{2m^*[P,T]} + \frac{e}{m^*[P,T]}A.p + \frac{e^2A^2}{2m^*[P,T]} + \frac{1}{2}m^*[P,T]\omega_0^2(x^2+y^2)+\frac{1}{2}g\mu_B B\omega+\frac{\alpha}{\hbar}(\sigma * p)_z+\frac{e\alpha}{\hbar}(\sigma * A)_Z \quad (5)$$

Now, the Hamiltonian gets transformed into the polar co-ordinates, so the eigen energy comes out as:

$$E_{n\sigma} = \hbar\omega\left(n+\frac{1}{2}\right) - \frac{e^2E^2}{2m^*(P,T)\omega^2} + \frac{\omega_0^2\hbar^2k_y^2}{\omega^2 2m*(P,T)} - \frac{e^2EB\hbar k_Y}{m*(P,T)^2\omega^2} + \frac{1}{2}g\mu_B\sigma B \quad (6)$$

Energy scale correlating with the confining potential and Rashba SOI are
Ep= $\hbar\omega_0$ and $\Delta_{so}=\frac{m(P,T)\alpha^2}{2\hbar^2}$ respectively. Expanding φ(x) in terms of

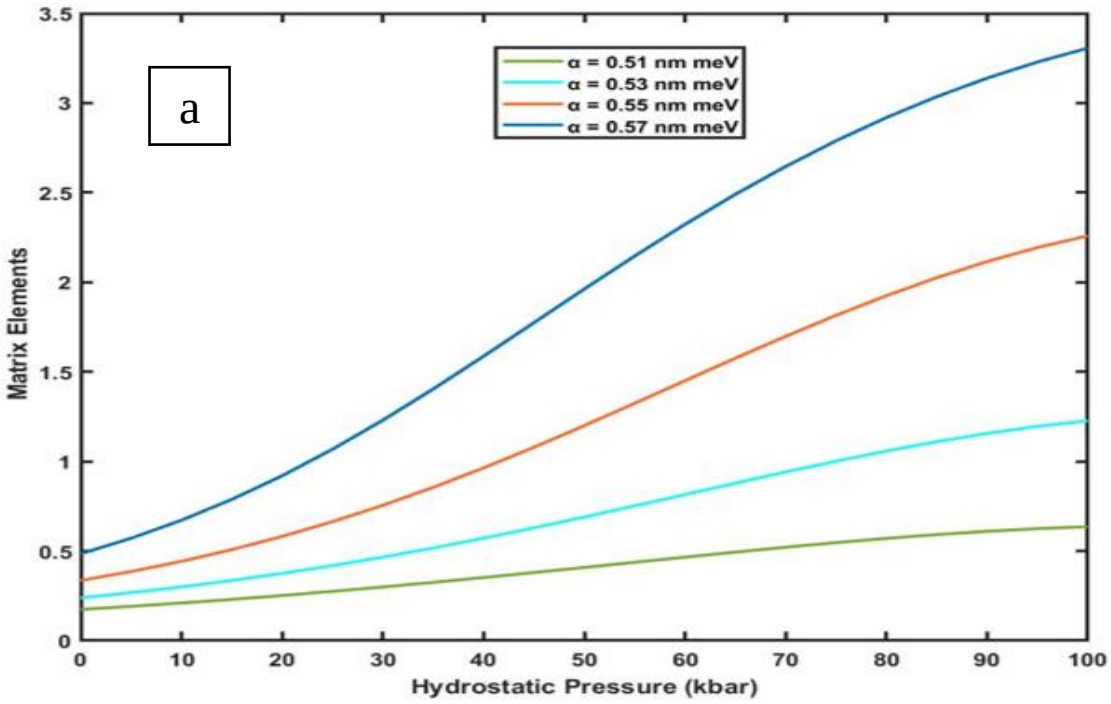
$\psi_{n\sigma}$(x) as φ(x) = $\Sigma_{n\sigma}a_{n\sigma}\psi_{n\sigma}$(x)

And using the condition of orthogonality, we have calculated the matrix elements $\left(M_{if} = |\langle \Phi_i | x, y | \Phi_j \rangle|\right)$ of a quantum wire by using the density matrix formalism.

4.2 Results

To calculate the eigenfunctions and eigenvalues for studying the purpose of hydrostatic pressure and temperature with spin orbit interaction, we have done the numerical calculations in this project. To look over the optical properties, we have used the calculated results. For the calculation of optical matrix elements of the GaAs quantum wire, we have taken the successive range of parameters as: magnetic field, $B = 1T\ to\ 2.5T$ and Rashba coupling coefficient, $\alpha = 0.51nmeV\ to\ 0.57nmeV$. Recently, J. R. Bindal et al., experimentally reported the higher values of Rashba SOI. For the computation, we have taken the material parameters of GaAs, for that an electron has the effective mass $0.03m_0$, where m_0 represents the rest mass of the electron.

In Fig.1, we showed the variation of matrix elements with hydrostatic pressure and the alteration of effective mass as a function of hydrostatic pressure for $P = 0Kbar\ to\ 100Kbar$. It is detected that the optical matrix elements go on increasing on increasing the pressure. From eq. (6), we can observe the dependence of energy band gap on hydrostatic pressure. This linear dependency of $E_{n\sigma}$ on hydrostatic pressure bring about the inflection in the graph among matrix elements and pressure as shown in fig. 1. With the increase in pressure, energy band gap also increases linearly and due to this reason, the effective mass of the electron also found to be increasing.



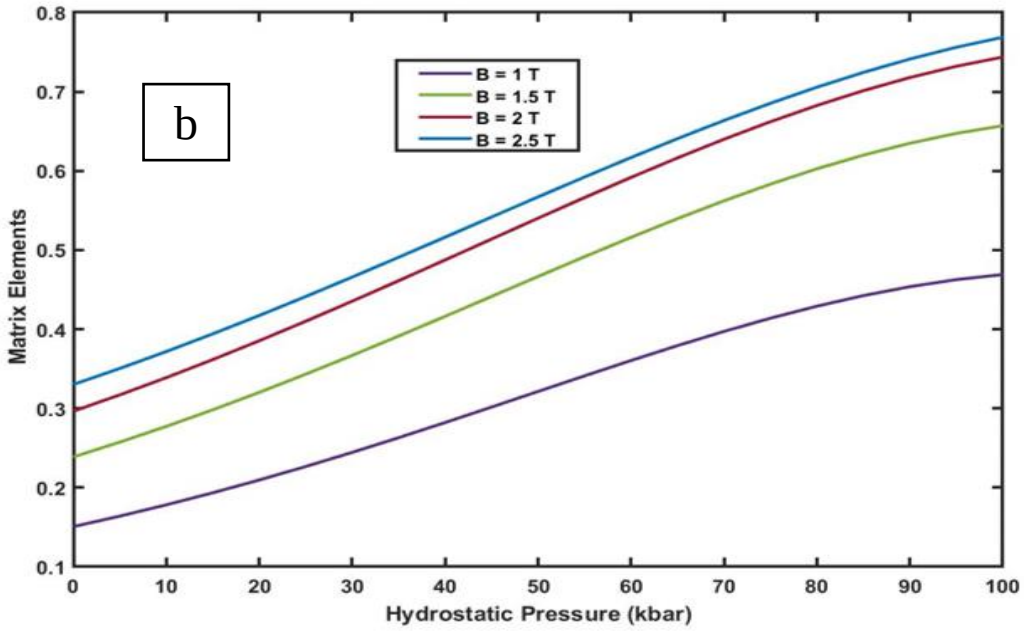
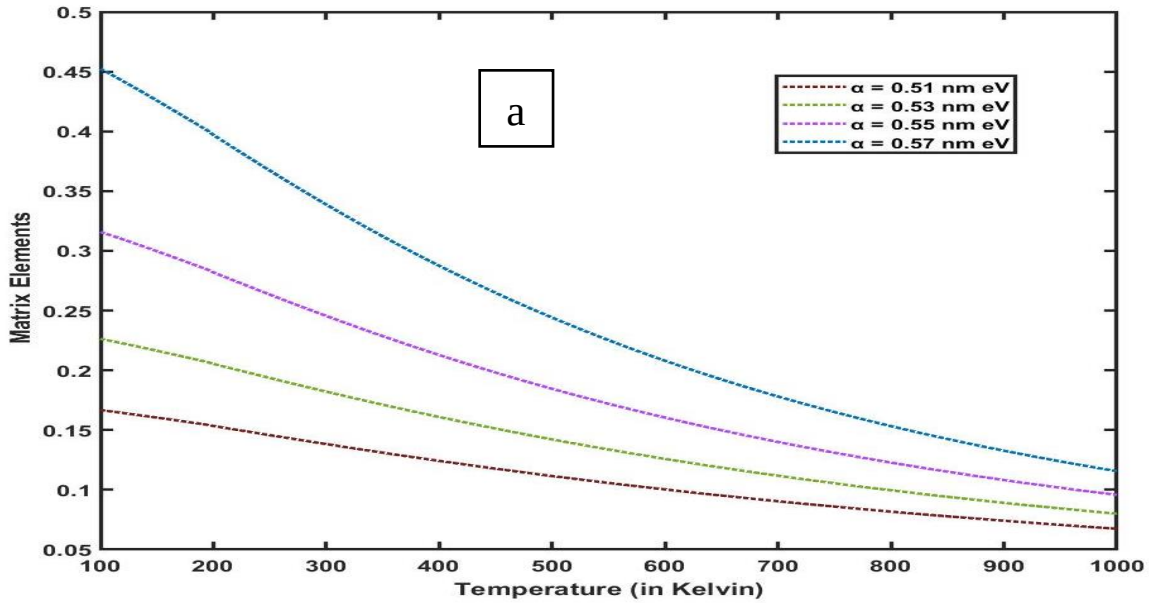


Fig.1. The matrix element variation with hydrostatic pressure at zero external electric field (E) for: (a) B = 1T, ∝ = 0.51nm eV to 0.57 nm eV (b) ∝ = 0.51 nm eV, B = 1 to 2.5 T.

In Fig.1(a), we have taken a constant value of magnetic field, $B = 1T$ and varied the value of Rashba coupling coefficient, $\alpha = 0.51$nm eV to 0.57nm eV and observed the linear dependency of matrix elements on the hydrostatic pressure. Then in fig.1(b), we have varied the value of magnetic field, B=1T to 2.5T and taken the constant value of the Rshba coupling coefficient, $\alpha = 0.51nm\ eV$.



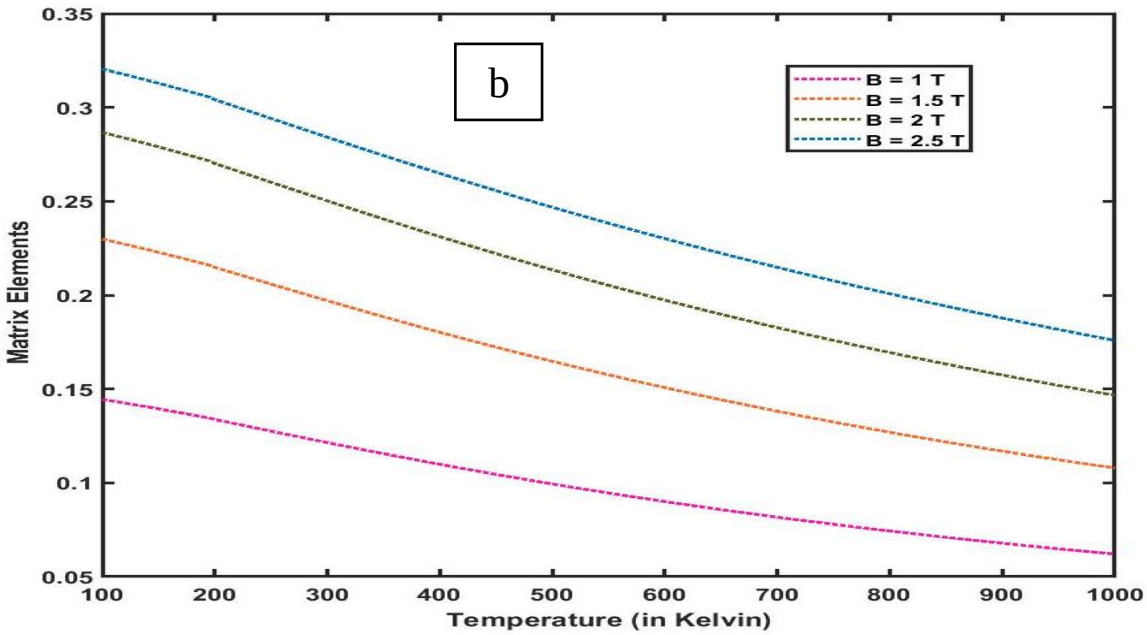


Fig.2. The matrix element variation with temperature at zero external electric field (E) for: (a) B = 0T, ∝ = 0.51 to 0.57 nm eV (b) ∝ = 0.51 nm eV, B = 1 to 2.5 T.

In Fig.2, we showed the variation of matrix elements with temperature and the alteration of effective mass as a function of temperature for $T = 100K\ to\ 1000K$. We observed that with increasing the temperature, the matrix elements found to be decreasing, it is also observed that on increasing the temperature, the band gap will decrease and because of this, the effective mass of the electron decreases.

In Fig.2(a), we have taken a constant value of magnetic field, $B = 1T$ and varied the value of Rashba coupling coefficient, $\alpha = 0.51$nm eV to 0.57nm eV and observed the inverse dependence of matrix elements on the temperature. On increasing the Rashba SOI factor, the transition energy is also found to increase. Then in fig.2(b), we have varied the value of magnetic field, B=1T to 2.5T and taken the constant value of the Rashba coupling coefficient, $\alpha = 0.51nm\ eV$.

4.3 Conclusion:

We presented the detailed inspection of the effect of hydrostatic pressure and temperature with spin orbit interaction on the linear and non-linear optical properties in case of a quantum wire. We have shown the results throughout the effective mass approximation using density matrix formalism. Before that, we have also investigated the influence of electric and magnetic field with Rashba spin orbit interaction in a quantum wire. We have also calculated the energy dispersion for a quantum wire.

We have found that the matrix elements depend linearly on pressure and inversely on temperature. Also, we observed that the energy band gap also varies linearly with pressure and inversely with temperature. Blue shifting in the peaks of absorption coefficient is detected with the increase in pressure and if the temperature is increased, a red shift in the peaks of absorption coefficient is observed. The transition energy is also found to be in linear dependence with the Rashba spin orbit interaction.

To sum up, the linear and non-linear properties of quantum wires are greatly influenced by the hydrostatic pressure and temperature, as well as the magnetic field with Rashba spin orbit interaction. Hence, hydrostatic pressure and temperature changed the energy eigenstates and eigenvalues, as done by all other parameters. By adjusting and regulating these parameters, we can tune and detune the THz laser in the low-dimensional structures so these characteristics would be extremely beneficial in the creation of tunable optoelectronic devices.

Impact of Hydrostatic pressure and Temperature on the matrix elements of a Cylindrical Quantum Wire

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I. **Abstract:** The matrix elements of a 2 – D electron gas restricted in a GaAs cylindrical quantum wire including Rashba Spin Orbit Interaction, under simultaneous effect of hydrostatic pressure and temperature is investigated. The strong dependency of hydrostatic pressure and absolute temperature, on energy band gap and effective mass of charge carriers of the quantum wire, have been found. Because of this, the linear and non-linear properties of the quantum wire also get affected. We also observed that under the influence of electric and magnetic field, the matrix elements get affected strongly with the change in Rashba spin orbit interaction and Magnetic field.

II. **Introduction:** Recently, the low dimensional semiconductor structures are attracting much attention e.g., quantum well, wire, dot etc. because of their applications in the area of optoelectronics [1][2][3][4]. Remarkable physical properties have been shown by the quantum wires of all these structures, in observing materiality in future automations [5]. Due to such discrete characteristics, scientists have been paid much attention to the nanostructures, as they provide a broad area for research to be aware of them [6]. Quantum wire which is a one-dimensional structure having the motion of electrons restricted in two directions, quantum effects get more obvious in comparison to the two-dimensional quantum structures [7].

Great interest has been shown in the learnings of spin-dependent phenomena of quantum confined structures due to their essential role in upcoming electronic devices with low power consumption, high speed and a high degree of performance [1][5][8][9][10]. These devices are based on the spin degree of freedom which is used for information processing including electron charge. The work of these proposed devices is manipulating the electron spin over spin orbit

interaction. Rashba spin orbit interaction has convenient benefits as it rely upon the electronic conditions of the quantum heterostructures and alternating the gate voltage exert influence on the strength of Rashba SOI, for managing the final spin orientation of electrons [11][12]. In this field, Datta-Das spin field effect transistor is one out of the innovative gadget idea. Many theoretical and experimental inspections have been done on the influence of Rashba SOI on the optical affections of nanostructures. However, from the experimental and theoretical viewpoints, the real existence of Rashba term in asymmetric quantum wires is still debatable. From the experimental standpoint, the trouble to discover the Rashba spin orbit coupling constant α, turn out the debate [13][14][15][16].

Optical properties possessed by quantum nanostructures, can be freely manipulated by apparently confined parameters that are hydrostatic pressure and temperature [17][18][19][20]. The optical matrix elements of the quantum wire structures depend on the direction of crystallographic wire and an optical anisotropy can appear there which will be in a perpendicular plane to the wire [21]. Recently, many researchers have investigated that in case of low-dimensional structures, the optical and electronic properties get influenced by hydrostatic pressure and temperature with varying confinement potential [22][23][24]. The optical properties of exciton with hydrostatic pressure was demonstrated by Duque et al., Ungan et al. investigated the effects of hydrostatic pressure in quantum well on the intersubband transitions [25]. Rezaei et al. reported that the linear and nonlinear properties get influenced extensively in case of quantum dot with the application of electric and magnetic fields [26]. In disc shaped quantum dot, the influence of hydrostatic pressure and temperature was investigated by Liang and Xie [27]. Mughnetsyan et al. have demonstrated the integrated effects of hydrostatic pressure and temperature in case of quantum ring. In low-dimensional structures, the impact of so many parameters on the optical properties have been investigated by a number of researchers, however, according to all the information till now, no one discussed the effects of pressure, temperature and external magnetic field with spin orbit interaction on the optical properties in a parabolic confinement of quantum wire. For quantum confined structures, the knowledge of Rashba SOI on the optical reciprocation is interesting and is going to be advantageous for many future applications namely quantum information systems and opt- spintronics devices [28][29]. Therefor, to learn about the optical properties under the effect of hydrostatic pressure and temperature with Rashba SOI in case of quantum wire is going to be fascinating.

In this conversation, we have used the density matrix formalism to compute the optical matrix elements for an electron applying electric and magnetic field both at the same time, under the influence of hydrostatic pressure and temperature for

a cylindrical quantum wire. From the results, we observed that matrix elements vary linearly with the pressure and inversely with temperature. We also detected that the peaks of absorption coefficient also behave in the same manner as the matrix elements, with the variation of hydrostatic pressure and temperature. In section III, the theory part is given, the result and conclusion of the conversation is mentioned in section IV and V.

Theoretical framework: Let us consider a two-dimensional GaAs quantum wire, with parabolic confined potential, given by:

$$V(x,y) = \frac{1}{2} m^*[P,T]\omega_0^2(x^2+y^2) \quad (1)$$

where $m^*[P,T]$ is the effective mass of electron under the influence of hydrostatic pressure and temperature. The Hamiltonian for a single electron in terms of mass can be given as

$$H_0(x,y) = \frac{1}{2m^*[P,T]}(p+eA)^2 + \frac{1}{2} m^*[P,T]\omega_0^2(x^2+y^2) \quad (2)$$

When we consider the spin, two more terms will add up to the Hamiltonian in equation (2), where the first term is the Zeeman term and the second term is the spin orbit interaction term as:

$$H_{spin} = \frac{1}{2} g\mu_B B\sigma + H_{soi} \quad (3)$$

Where g represents the effective Lande factor for semiconductor. H_{soi} represents the spin orbit interaction term which consists of two terms as H_{soi}^R which is for Rashba spin orbit interaction and H_{soi}^D which is for Dresselhaus spin orbit interaction. Rashba term dominates over the Dresselhaus term that is why, here we will consider only the Rashba term, which is:

$$H_{soi}^R = \frac{\alpha}{\hbar}[\sigma * (p+eA)]_z \quad (4)$$

Where α is the Rashba coupling coefficient which can be controlled by applying the varying gate voltage in z-direction. Thus, the total Hamiltonian will be the combination of both the terms as H_0 and H_{soi}^R in the effective mass approximation and will be given as

$$H = \frac{p^2}{2m^*[P,T]} + \frac{e}{m^*[P,T]} A.p + \frac{e^2A^2}{2m^*[P,T]} + \frac{1}{2} m^*[P,T]\omega_0^2(x^2 + y^2) + \frac{1}{2} g\mu_B B\omega + \frac{\alpha}{\hbar}(\sigma * p)_z + \frac{e\alpha}{\hbar}(\sigma * A)_Z \quad (5)$$

Now, the Hamiltonian gets transformed into the polar co-ordinates, so the eigen energy comes out as:

$$E_{n\sigma} = \hbar\omega\left(n+\frac{1}{2}\right) - \frac{e^2E^2}{2m^*(P,T)\omega^2} + \frac{\omega_0^2\hbar^2k_y^2}{\omega^2 2m*(P,T)} - \frac{e^2EB\hbar k_Y}{m*(P,T)^2\omega^2} + \frac{1}{2}\, g\mu_B\sigma B \quad (6)$$

Energy scale correlating with the confining potential and Rashba SOI are

Ep= $\hbar\omega_0$ and Δ_{so}=$\frac{m(P,T)\alpha^2}{2\hbar^2}$ respectively. Expanding φ(x) in terms of

$\psi_{n\sigma}$(x) as φ(x) = $\Sigma_{n\sigma}a_{n\sigma}\psi_{n\sigma}$(x)

And using the condition of orthogonality, we have calculated the matrix elements $\left(M_{if} = |\langle\Phi_i|x,y|\Phi_j\rangle|\right)$ of a quantum wire by using the density matrix formalism.

Result: To calculate the eigenfunctions and eigenvalues for studying the purpose of hydrostatic pressure and temperature with spin orbit interaction, we have done the numerical calculations in this project. To look over the optical properties, we have used the calculated results. For the calculation of optical matrix elements of the GaAs quantum wire, we have taken the successive range of parameters as: magnetic field, $B = 1T - 2.5T$ and Rashba coupling coefficient, $\alpha = 0.51nmeV - 0.57nmeV$. Recently, J. R. Bindal et al., experimentally reported the higher values of Rashba SOI [30]. For the computation, we have taken the material parameters of GaAs, for that an electron has the effective mass $0.03m_0$, where m_0 represents the rest mass of the electron.

In Fig.1, we showed the variation of matrix elements with hydrostatic pressure and the alteration of effective mass as a function of hydrostatic pressure for $P = 0Kbar - 100Kbar$. It is detected that the optical matrix elements go on increasing on increasing the pressure. From eq. (6), we can observe the dependence of energy band gap on hydrostatic pressure. This linear dependency of $E_{n\sigma}$ on hydrostatic pressure bring about the inflection in the graph among matrix elements and pressure as shown in fig. 1. With the increase in pressure, energy band gap also increases linearly and due to this reason, the effective mass of the electron also found to be increasing.

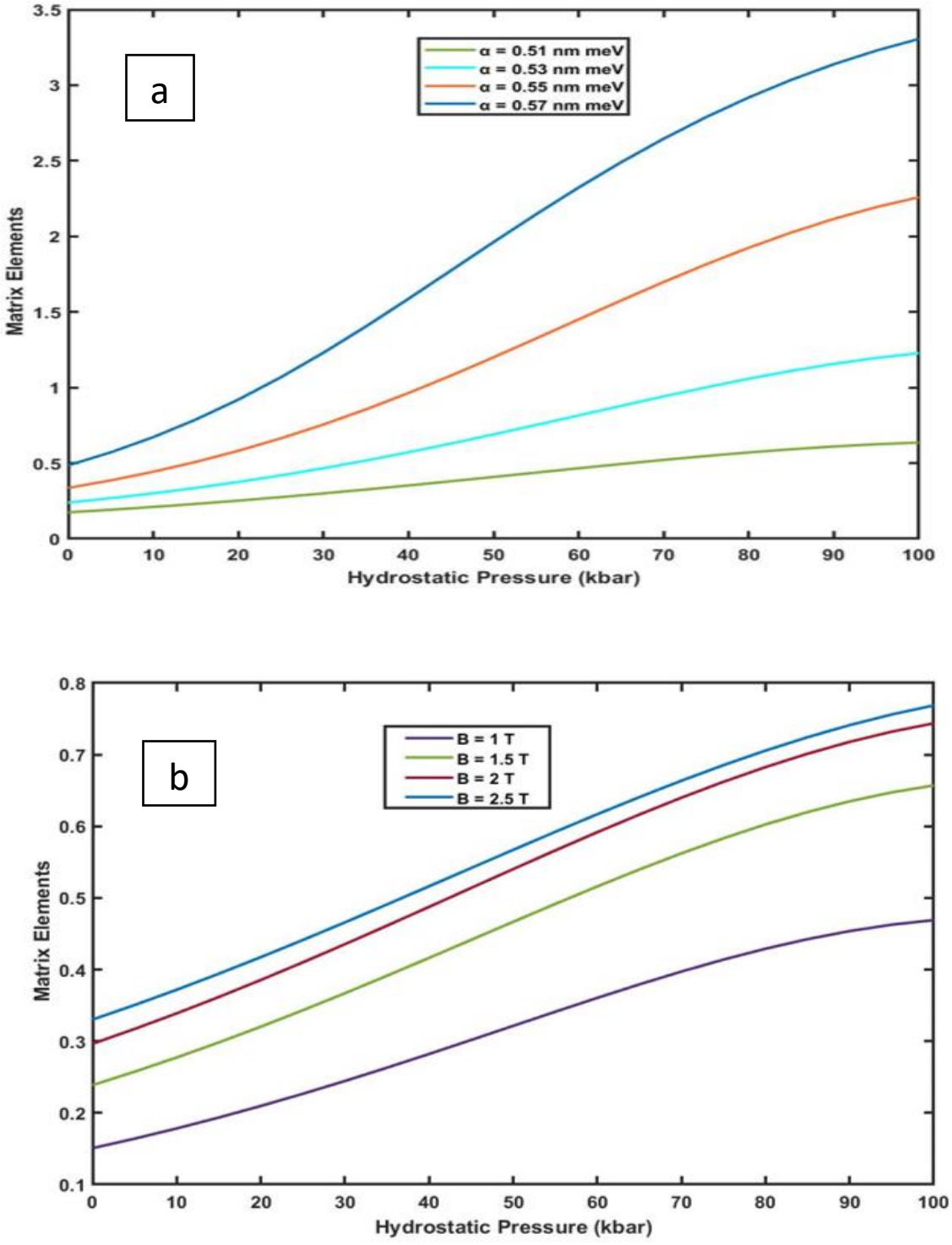

Fig.1. The matrix element variation with hydrostatic pressure at zero external electric field (E) for: (a) B = 1T, ∝ = 0.51nm eV to 0.57 nm eV (b) ∝ = 0.51 nm eV, B = 1 to 2.5 T.

In Fig.1(a), we have taken a constant value of magnetic field, $B = 1T$ and varied the value of Rashba coupling coefficient, $\alpha = 0.51$nm eV-0.57nm eV and observed the linear dependency of matrix elements on the hydrostatic pressure. Then in fig.1(b), we have varied the value of magnetic field, B=1T-2.5T and taken the constant value of the Rshba coupling coefficient, $\alpha = 0.51nm\ eV$.

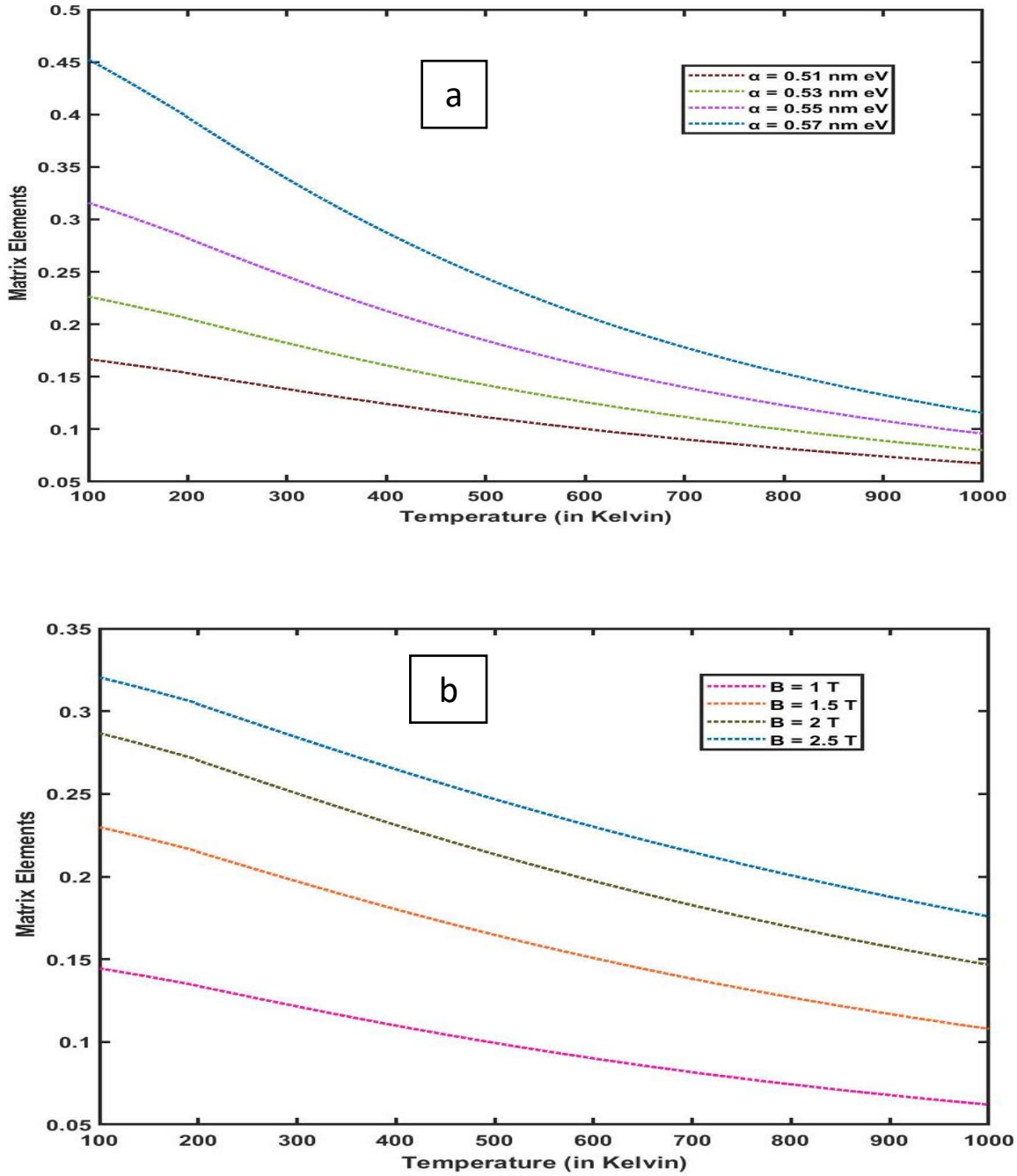

Fig.2. The matrix element variation with temperature at zero external electric field (E) for: (a) B = 0T, ∝ = 0.51 to 0.57 nm eV (b) ∝ = 0.51 nm eV, B = 1 to 2.5 T.

In Fig.2, we showed the variation of matrix elements with temperature and the alteration of effective mass as a function of temperature for $T = 100K - 1000K$. We observed that with increasing the temperature, the matrix elements found to be decreasing, it is also observed that on increasing the temperature, the band gap will decrease and because of this, the effective mass of the electron decreases.

In Fig.$2(a)$, we have taken a constant value of magnetic field, $B = 1T$ and varied the value of Rashba coupling coefficient, $\alpha = 0.51$nm eV-0.57nm eV and observed the inverse dependence of matrix elements on the temperature. On increasing the Rashba SOI factor, the transition energy is also found to increase. Then in fig.$2(b)$, we have varied the value of magnetic field, B=1T-2.5T and taken the constant value of the Rshba coupling coefficient, $\alpha = 0.51nm\ eV$.

Conclusion: We presented the detailed inspection of the effect of hydrostatic pressure and temperature with spin orbit interaction on the linear and non-linear optical properties in case of a quantum wire. We have shown the results throughout the effective mass approximation using density matrix formalism. Before that, we have also investigated the influence of electric and magnetic field with Rashba spin orbit interaction in a quantum wire. We have also calculated the energy dispersion for a quantum wire.

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