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## Research Paper

# Investigating the Effects of Electromagnetic Fields and Dimensions on the Electronic Properties of Gallium Arsenide Nanowire with Aluminum-Gallium Arsenide Coating in The Presence of Spin-Orbit Interaction

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### Abstract

In this research, the interaction of electromagnetic fields and sizes on the energy levels and specific functions of a GaAs nanowire coated with  $Al_{0.3}Ga_{0.7}As$ , along with the spin-orbit effect, has been carefully investigated. The magnetic field is applied in the direction parallel to the axis of the wire and the electric field is applied both in the plane perpendicular to the axis of the wire and in the direction parallel to it. To investigate the effects of the spin-orbit effect, in most cases, from the explicit form of the wave functions resulting from the solution of the Schrödinger equation Use related to the problem. We have shown that spin-orbit coupling together with external fields have a significant effect on the electronic properties of the wire. Since external magnetic field amplifies the intrinsic magnetic field, thus energy splitting due to SOI is bigger at higher B values. Because of the stronger role of magnetic field and weak effects of radial electric field on the SOI this phenomenon is not sensible when electric field is radial.

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## 1. INTRODUCTION

Considering the many experimental and theoretical activities on the spin-orbit effect, both in the field of spintronics and in the role it can have in bioelectronics [1,2,3], as well as its wide use in semiconductor lasers [4,5,6] and transistors [7] that work with this effect, and considering the great interest that has arisen in semiconductor nanocrystals [8,9], the importance of the combination of these two branches cannot be ignored.

Now, technologically, we are able to artificially control the  $\alpha$  spin coupling strength [10,11,12] and this will enable us to control the properties of nanostructures that depend on the spin-orbit [13, 14,15]. For this reason, in this article, we have investigated the spin-orbit effect on the energy levels of a cylindrical quantum dot with finite potential under the influence of magnetic and electric fields in different directions, and because Gallium arsenide and Aluminum-Gallium-Arsenide play an important role in transistor manufacturing technology [16], Therefore, we have chosen the first one for the nano wire and its coating from the second one.

The results show that the energy levels are split into two separate levels, one related to high spin and the other to low spin. Of course, this separation can be controlled by changing the direction of electric field radiation. The separation of energies and their changes strongly depend on the direction and intensity of external fields, as well as on the strength of spin-orbit coupling and the dimensions of the nanowire.

## 2. THEORY

For an electron that is confined inside a wire with a radius, in the framework of effective mass approximation, under the effect of external electric and magnetic fields, the Hamiltonian of the system is as follows [17,18]:

$$H_0 = \frac{1}{2m^*} [\vec{P} + e\vec{A}]^2 - e\vec{F} \cdot \vec{r} + V(\rho) \quad (1)$$

$$V(\rho) = \begin{cases} 0 & \text{if } 0 \leq \rho \leq R \\ V_0 & \text{if } \rho \geq R \end{cases} \quad (2)$$

where  $F$  is the electric field,  $A$  is the vector potential,  $P$  is the linear momentum operator, and  $m^*$  is the effective mass of the electron. In the gauge where the vector potential is in the form  $\vec{A} = \frac{B\rho}{2} \hat{\phi}$  and assuming that the electric field is in

the direction of the  $z$  axis, in the cylindrical coordinate system, the governing equation for the axial component of the wave function is as follows:

$$\frac{1}{Z(z)} \frac{\partial^2}{\partial z^2} - \frac{2m^* e}{\hbar^2} Fz = -k_z^2 \quad (3)$$

Where  $k_z$  is the axial component is the wave vector. The solution of the above equation that satisfies the boundary conditions on the axis is in the form of an Airy function.

$$Z(z) = C \text{ AiryAi} \left( \left( \frac{-2}{\hbar^2 e^2 m^{*2} F^2} \right)^{\frac{1}{3}} \left( \frac{\hbar^2 k_z^2}{2} - m^* e F z \right) \right) \quad (4)$$

Where C is the normalization factor. But  $\chi_{nm}(\rho)$ , which is the radial part of the wave function, applies in the following equation.

$$\frac{1}{\chi_{nm}(\rho)} \frac{\partial}{\partial \rho} \chi_{nm}(\rho) - \left[ \frac{m^2}{\rho^2} + \frac{eBm}{\hbar} + \left( \frac{eB\rho}{2\hbar} \right)^2 + \frac{2m^*}{\hbar^2} (V(\rho) - E) + k_z^2 \right] = 0 \quad (5)$$

$n$  is the radial quantum number,  $m$  is the azimuthal quantum number, and  $B$  is the intensity of the magnetic field. The answer to equation (5) is as follows:

$$\chi_{nm}(\rho) = \begin{cases} C_1 \frac{\mathcal{M}\left(\beta_1, \frac{|m|}{2}, \gamma\rho^2\right)}{\rho} & \text{if } 0 \leq \rho \leq R \\ C_2 \frac{\mathcal{W}\left(\beta_2, \frac{|m|}{2}, \gamma\rho^2\right)}{\rho} & \text{if } \rho \geq R \end{cases} \quad (6)$$

In the above expression,  $\mathcal{M}$  and  $\mathcal{W}$  are Confluent Hyper Geometric Functions. The coefficients  $C_1$  and  $C_2$  are obtained from the boundary conditions and  $\beta_i$  and  $\gamma$  are as follows:

$$\beta_i = -\frac{\hbar k_z^2}{2eB} - \frac{m}{2} + \frac{m^*}{eB\hbar} (E - V(\rho)), \quad \gamma = \frac{Be}{2\hbar} \quad (7)$$

So, the overall wave function of the system is as follows:

$$\psi_{nmk_z} = \frac{1}{\sqrt{2\pi}} e^{im\phi} Z(z) \chi_{nm}(\rho) \quad (8)$$

To obtain specific values, we can find the specific energy levels of their corresponding functions by using the continuity of wave functions and their

derivative at the boundary. When the electric field is in the radial direction  $\rho$ , the term  $-\frac{2m^*e}{\hbar^2}F\rho$  will be added to the relation (5). In this case, using explicit answers will be very complicated. Therefore, with the help of perturbation theory, we have obtained energy values and state functions of the system. In the presence of spin interaction, the spin-orbit Rashba Hamiltonian with the term

$$H_{SO} = \frac{\alpha}{\hbar} \left[ \vec{\sigma} \times (\vec{P} + e\vec{A}) \right] \cdot \hat{n} \quad (9)$$

will be given. where  $\vec{\sigma}$  is the Pauli matrix and  $\alpha$  is the spin-orbit interaction strength. In cylindrical coordinates, equation (9) becomes as follows[11].

$$H_{SO} = \begin{bmatrix} -\frac{i\alpha}{\rho} \frac{\partial}{\partial \varphi} + \frac{eB\rho}{\hbar} \alpha & \alpha e^{-i\varphi} \frac{\partial}{\partial z} \\ -\alpha e^{i\varphi} \frac{\partial}{\partial z} & \frac{i\alpha}{\rho} \frac{\partial}{\partial \varphi} - \frac{eB\rho}{\hbar} \alpha \end{bmatrix} \quad (10)$$

Now, taking into account the spin-orbit interaction of the total Hamiltonian, the following will be obtained.

$$H = H_{SO} + H_0 \quad (11)$$

By its effect on the special functions of the whole system, we reach the following matrix equation:

$$\begin{bmatrix} H, -\frac{i\alpha}{\rho} \frac{\partial}{\partial \varphi} + \frac{eB\rho}{\hbar} \alpha & \alpha e^{-i\varphi} \frac{\partial}{\partial z} \\ -\alpha e^{i\varphi} \frac{\partial}{\partial z} & H, +\frac{i\alpha}{\rho} \frac{\partial}{\partial \varphi} - \frac{eB\rho}{\hbar} \alpha \end{bmatrix} \begin{bmatrix} C_+ \psi^+ \\ C_- \psi^- \end{bmatrix} = E_{\pm} \begin{bmatrix} C_+ \psi^+ \\ C_- \psi^- \end{bmatrix} \quad (12)$$

Where  $C_{\pm}$  are the expansion coefficients of the overall wave function of the system and  $E_{\pm}$  is the energy corresponding to them. According to the cylindrical symmetry of the system and the constancy of the total motion, we can write:

$$\begin{bmatrix} C_+ \psi^+ \\ C_- \psi^- \end{bmatrix} = \begin{bmatrix} C_+ e^{-i\frac{\varphi}{\gamma}} \psi \\ C_- e^{+i\frac{\varphi}{\gamma}} \psi \end{bmatrix} \quad (13)$$

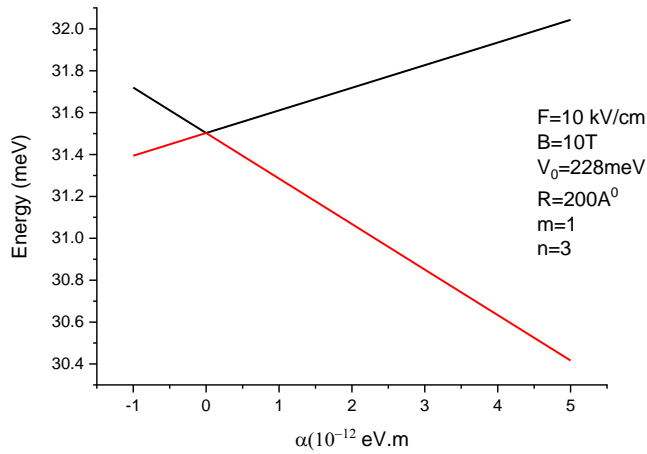
where  $\psi$  is given by expression (8). By inserting expression (13) in (12) and integrating over the entire space in the cylindrical coordinate system, we will reach the following integral equations:

$$\int \chi^*(\rho) \begin{bmatrix} E_0 - E_{\pm} + \frac{(2m-1)}{2\rho} \alpha + \frac{eB\rho}{2\hbar} \alpha & \alpha \frac{\partial}{\partial z} Z(z) \\ -\alpha \frac{\partial}{\partial z} Z(z) & E_0 - E_{\pm} - \frac{(2m+1)}{2\rho} \alpha + \frac{eB\rho}{2\hbar} \alpha \end{bmatrix} \begin{bmatrix} C_+ \\ C_- \end{bmatrix} \chi(\rho) \rho d\rho dz = 0 \quad (14)$$

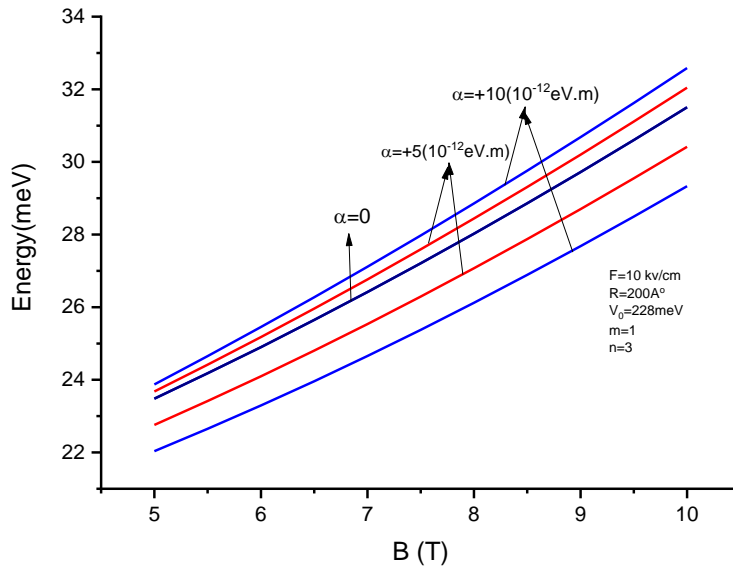
By solving these equations and integrating, their corresponding energies will be obtained.

### 3. DISCUSSION AND RESULTS

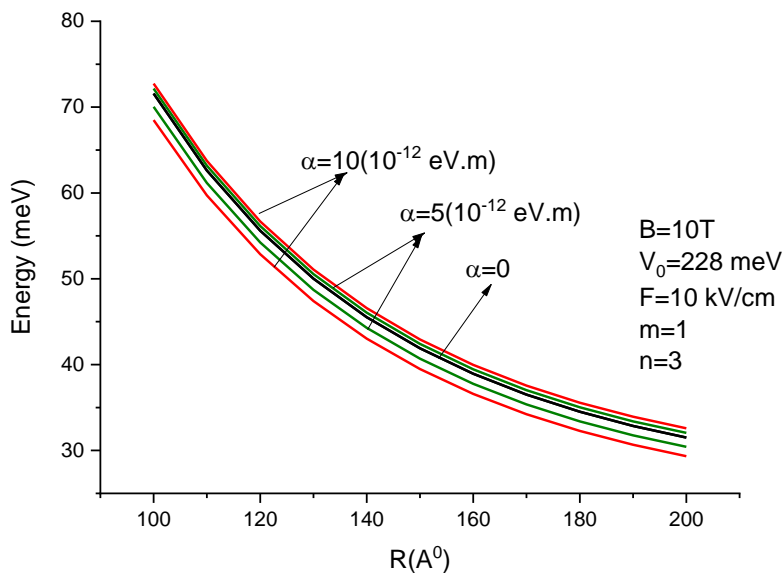
In this part, the results related to special calculations of system energy eigen values in a *GaAs* quantum wire covered with another layer of *Al<sub>0.3</sub>Ga<sub>0.7</sub>As* are given in figures (1) to (7) and according to different parameters.  $m^* = 0.067m_0$  ( $m_0$  rest mass of free electron) and  $V_0 = 228meV$  are considered in the calculations. In Figures (1) to (4), the electric field is axial, and in Figures (5) to (7), it is the radial electric field. In Figure (1), the energy is plotted in terms of the  $\alpha$  parameter, which shows the strength of the spin-orbit effect. As can be seen, the energy is divided into two branches, the energy of the high spin state increases with the increase of  $\alpha$  and the state with low spin decreases. The significant effect of this parameter is clearly shown in the figure. In figure (2), the energy is plotted in terms of the magnetic field for different  $\alpha$  values. As the intensity of the magnetic field increases, the energy increases and its effect is almost the same in different  $\alpha$  values. In figure (3), the energy is plotted in terms of the radius of the quantum wire. is drawn. As the radius increases and the quantum limit decreases, as expected, the energy decreases. In Figure (4), the energy is plotted in terms of the electric field. It can be seen that the effect of the electric field on the energy levels is insignificant and its effect in Different  $\alpha$ 's are the same. In figures (5) to (7) energy changes are plotted in terms of parameters similar to figures (2) to (4) when the electric field is radial. The interesting point in these figures is that when the electric field is radial, the energy levels are shifted and the effect of the spin-orbit interaction is different. In these cases, the electric field significantly affects the energy levels, so that with its increase, the energy decreases drastically.



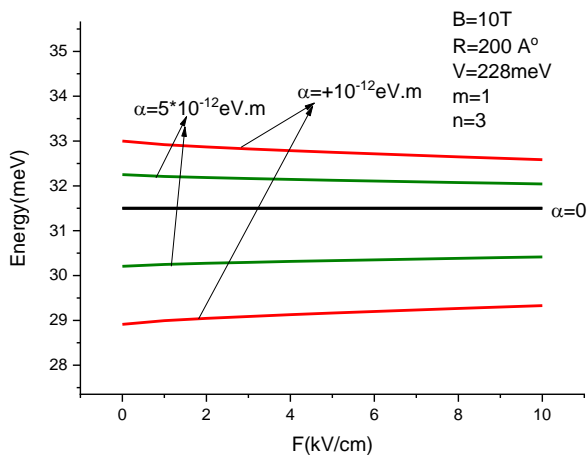
**Fig 1.** Energy level separation in the presence of axial electric field.



**Fig 2.** Energy change in terms of magnetic field changes when the electric field is axial.

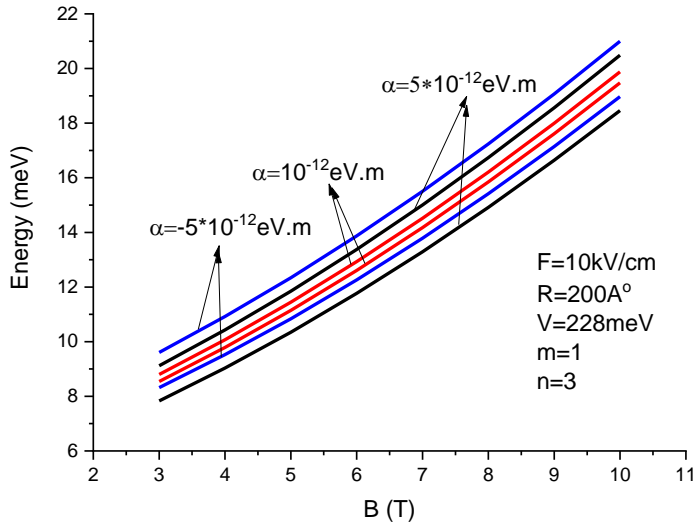


**Fig 3.** Energy change in terms of nanowire radius changes when the electric field is axial.

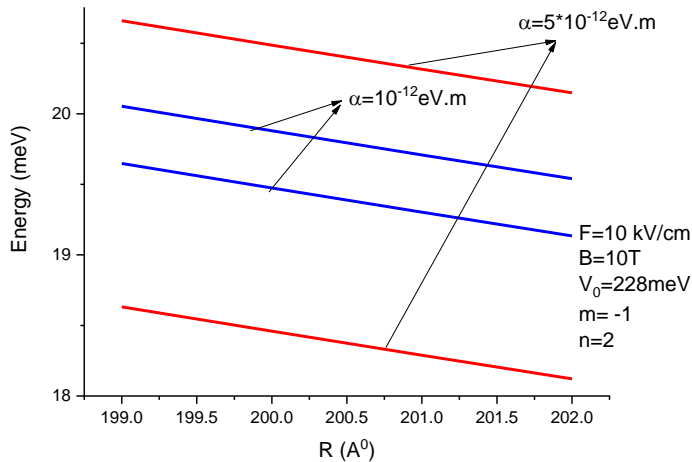


**Fig 4.** Energy change in terms of changes in the electric field intensity of the nanowire when the electric field is axial.

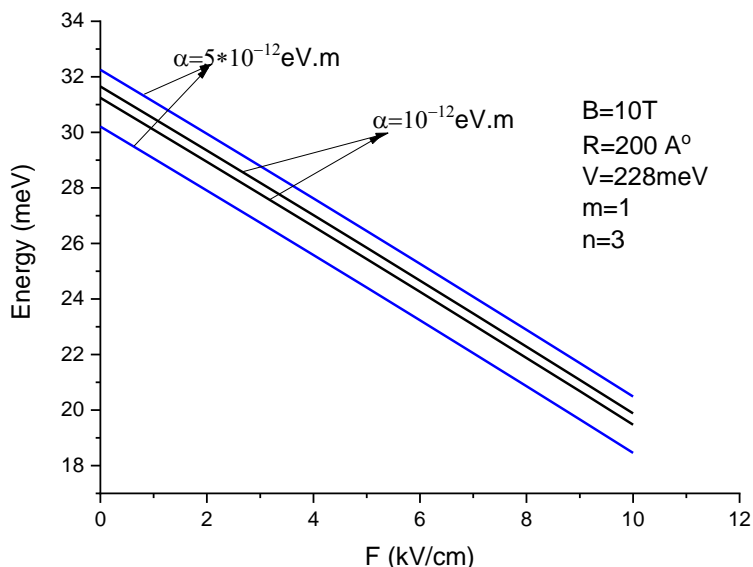




**Fig. 5** Energy change of the quantum wire in terms of changes in the magnetic field when the electric field is radial.



**Fig. 6** Energy change of the quantum wire as the radius increases when the electric field is radial.



**Fig. 7** The energy change of the quantum wire according to the increase of the electric field when the electric field is radial.

#### 4. CONCLUSION

In this article, we have studied the spin-orbit interaction and external fields, as well as the dimensions of the single-layer nanotube, on the eigenvalues and eigenfunctions. This problem is more complicated compared to other works done in this field due to the different boundary conditions of the system. Because the external field causes the symmetry of the system to be broken, we have shown that with the orientation of the electric field, the spin-orbit effects on the electronic structure will be important. Furthermore, we found a threshold for the value of the electric field when it is in the axial direction, on which the existence of the response depends. We also understood that this threshold value is also a function of the magnetic field and can act as a switch for the existence of the spin-orbit effect.

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