THE EFFECT OF TEMPERATURE ON THE SELF-POLARIZATION IN AN INFINITE GaAs/AlAs CYLINDRICAL QUANTUM WELL-WIRE

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Abstract

This work investigates the effects of temperature on self-polarization for different wire radii under an applied external magnetic field in an infinite GaAs/AlAs cylindrical quantum well-wire for the ground state. The variational method is used in the calculations by taking impurities in different positions from the centre to the edge of the wire. Self-polarization increases with increasing impurity atom distance from the centre, wire radius, and temperature. Moreover, as the magnetic field increases, self-polarization decreases. All calculations are in agreement with available data in the literature.

Keywords: self-polarization, temperature, well-wire, binding energy.

INTRODUCTION

Low-dimensional structures in modern technology and electronics are highly significant. Many electronic circuit elements are manufactured using low-dimensional structures by applying different potentials to different geometries. Various techniques, such as molecular beam epitaxy [1], chemical vapour deposition [2], and chemical etching [3,4], can be used to produce low-dimensional structures. Heterostructures allow electrons to be confined in one or more directions using a potential barrier. When this confinement is in three dimensions, quantum dots are formed, whereas when confinement is in two and one dimensions, quantum wires and wells are formed, respectively[5-11]. Many factors have a significant impact on the electronic properties of the system. These factors include temperature, hydrostatic pressure, electric and magnetic fields, optical effects, noise, and many other factors [12-15]. In addition, changing the applied potential geometries affects the electronic properties of the system. Therefore, it is very important to consider the issues present in the design of electronic systems.

In studying these various structures, it is essential to consider the influence of multiple factors, including electric field polarization, and self-polarization [16] due to potential barriers. Considering all these factors, we can better understand other calculated physical parameters and their importance in the overall analysis.

This study examines the influence of temperature, structure size, impurity position, and magnetic field on self-polarization within a cylindrical quantum well wire. The findings provide valuable insights into the fundamental properties of this system and may have practical applications in related areas.

THEORY

Within the effective mass approximation, the Hamiltonian of a system GaAs/AlAs cylindrical wire of radius d presence of a magnetic field parallel to the wire axis in cylindrical coordinates [17],

$$H = -\frac{1}{2m_e(T)}\left(\vec{P} + \frac{e}{c}\vec{A}\right)^2 - \frac{e^2}{\varepsilon(T)|\vec{r}-\vec{r}_i|} + V(\rho) \quad (1)$$

where $|\vec{r}-\vec{r}_i| = (|\vec{\rho}-\vec{\rho}_i|^2 + z^2)^{1/2}$ is the distance between electron and impurity atom (ρ_i is the impurity position). $\vec{P}$ is the momentum operator, $\vec{A}$ is the vector potential that generates a magnetic field in the direction of the wire axis. $m_e(T)$ and $\varepsilon(T)$ are the temperature dependent effective mass and dielectric constant for the electron respectively [18],

$$m_e(T) = \frac{m_0}{1+E^{\Gamma}\left[\frac{2}{E_g^{\Gamma}}+\frac{1}{E_g^{\Gamma}(T)+\Delta_0}\right]} \quad (2)$$

m_0 is the free electron mass and $E_g^{\Gamma} = 7.51\,eV, \Delta_0 = 0.341\,eV$ [19]. $E_g^{\Gamma}(T)$ the temperature dependent energy gap for GaAs structure is given by

$$E_g^{\Gamma}(T) = 1.519 - \frac{5.405\times10^{-4}T^2}{T+204}. \quad (3)$$

$E_g^{\Gamma}(T)$ and T are expressed in the eV and K unit. The temperature dependent static dielectric constant is given by [20,21]

$$\varepsilon(T) = \begin{cases} (12.74)e^{\left[9.4\times10^{-5}(T-75.6)\right]} & T<200K \\ (13.18)e^{\left[20.4\times10^{-5}(T-300)\right]} & T\geq300K \end{cases}. \quad (4)$$

Confining potential is express as for the cylindrical quantum well-wire,

$$V(\rho) = \begin{cases} 0, & 0 \leq \rho \leq d, \\ \infty, & \rho > d. \end{cases} \quad (5)$$

d is the radius of the cylindrical wire. Hamiltonian of the system in a cylindrical coordinate in the effective Rydberg unit can be express as without impurity [17],

$$H_1 = -\nabla^2 + \gamma L_z + \frac{1}{4}\gamma^2\rho^2 + V(\rho), \quad (6)$$

and with impurity [17]

$$H_2 = -\nabla^2 - \frac{2}{|\vec{r}-\vec{r}_i|} + \gamma L_z + \frac{1}{4}\gamma^2\rho^2 + V(\rho). \quad (7)$$

L_z is the z component of the angular momentum operator and γ is the dimensionless measure of the magnetic field ($\gamma = e\hbar B/2m_e(T)cR^*$). Effective Bohr radius and effective Rydberg energy can be written as $a^* = \frac{\varepsilon(T)\hbar^2}{m_e(T)e^2}$ and $R^* = \frac{m_e(T)e^4}{2\varepsilon^2(T)\hbar^2}$.

The trial wave function of the ground state without the impurity can be written as

$$\psi_1 = \begin{cases} N_1 J_0(r_{10}\rho), & \rho \leq d, \\ 0, & \rho > d, \end{cases} \quad (7)$$

$J_0(r_{10}\rho)$is an ordinary Bessel Function of order zero ($r_{10} = 2.4048/d$), N_1 is the normalization constant. The ground state energy of the system without impurity,

$$E_1 = \langle\psi_1|H_1|\psi_1\rangle. \quad (8)$$

The trial wave function of the ground state with the impurity can be chosen as,

$$\psi_2 = \begin{cases} N_2\psi_1(\rho)e^{(-\lambda|\vec{r}-\vec{r}_i|)}, & \rho \leq d, \\ 0, & \rho > d. \end{cases} \quad (9)$$

Here, N_2 is the normalization constant and λ is the variational parameter. We express the impurity position with a dimensionless impurity parameter c as follows,

$$c = \rho_i/d. \quad (10)$$

The ground state energy of the system with impurity

$$E_2 = \langle\psi_2|H_2|\psi_2\rangle_{\lambda_{min}}. \quad (11)$$

is defined as in Eq.(11). Variational parameter minimizes the system energy and electron-impurity binding energy is given as,

$$E_b = E_1 - E_2. \quad (12)$$

Self-polarization is the effect of the wire potential on the wave function is defined as [17,22],

$$\frac{SP}{e} = -\langle\psi_2|(\rho-\rho_i)\cos\varphi\,|\psi_2\rangle + \langle\psi_3|(\rho-\rho_i)\cos\varphi\,|\psi_3\rangle. \quad (13)$$

Here ψ_3 is the wave function of an electron in the absence of the wire potential and can be written as,

$$\psi_3 = N_3 e^{-\frac{|\vec{r}-\vec{r}_i|}{a^*}}. \quad (14)$$

This wave function is the ground state hydrogen atom's wave function.

RESULTS

In this study, we calculate the temperature dependence of self-polarization for an infinite cylindrical quantum well wire with varying impurity positions, magnetic fields, and wire radii. Temperature-dependent effective mass and dielectric constant are taken into account in all calculations.

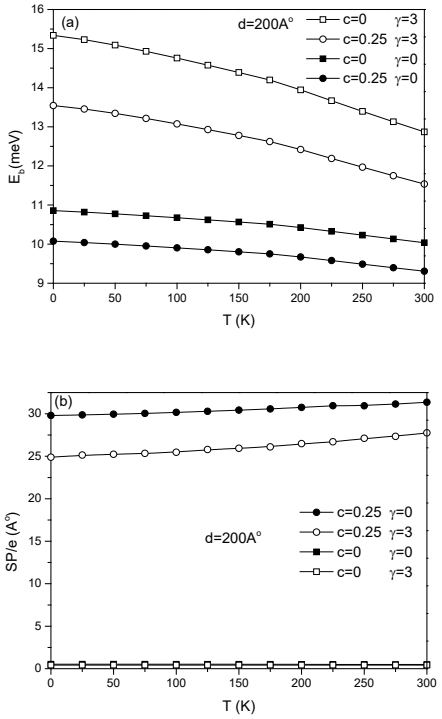

Fig.1. *Variation of binding energy (a) and self-polarization (b) according to temperature at fixed wire radius* $200A°$ *for different impurity positions and magnetic fields.*

In all representations in Fig.1., the wire radius is taken as $200A°$. The data presented in Fig.1.(a) clearly indicates that the binding energy decreases as temperature increases. This is because temperature increases the energy of the system but decreases the binding energy of the electron. Changes in binding energy affect the distance of the electron from the impurity atom, allowing changes in self-polarization to be detected. As the temperature increases, the self-polarization generated by the wire potential becomes more effective, which leads to an increase in self-polarization (Fig.1.(b)) due to the decrease in binding energy. By placing the impurity off-center, the wave function of the electron is not affected by the edges by the same amount. When the impurity is located in the centre, the electron is equidistant from the wire walls in a symmetric system, resulting in almost zero self-polarization (Fig.1.(b)). On the other hand, if there is an impurity located off-centre, the distance between the electron and the wire edges is not uniform. This creates an asymmetrical system where the electron is not affected by the edges in the same manner. As a result, non-zero self-polarizations can be computed. Moreover, a magnetic field creates an extra symmetric trapping potential, thus increasing the binding energy at all impurity positions. However, when the impurity is at the centre, the self-polarization is still around zero, as the magnetic field does not create a symmetry breaking.

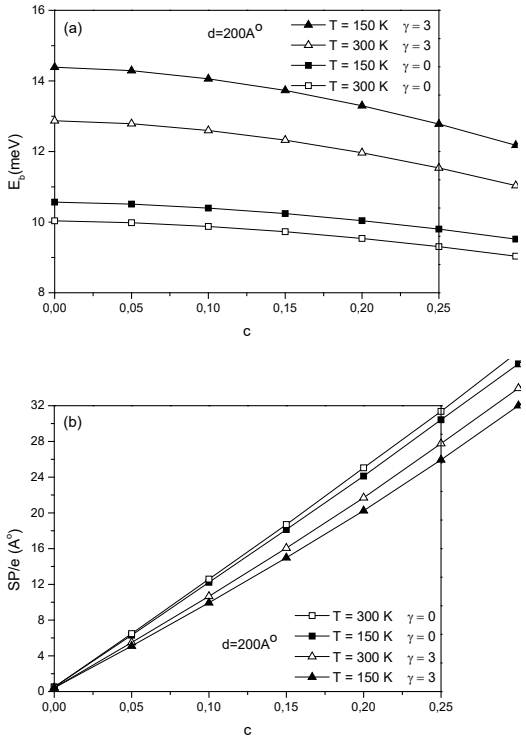

Fig.2. *Graph of the binding energy (a) and self-polarization (b) as a function of the impurity position with* $\gamma = 0; 3$ *and* $T = 150; 300K$ *values.* (d=200A°)

We have investigated the binding energies and self-polarizations of an electron when the impurity is located at different positions along the wire radius (200 Å) for different temperatures and magnetic fields, as shown in Fig.2. The movement of the impurity atom away from the centre weakens the Coulomb interaction and ultimately leads to a decrease in the binding energy. Although the binding energy is not zero (Fig.2.(a)), self-polarization can only take values other than zero as the impurity distance from the centre increases (Fig.2.(b)). Increasing the magnetic field leads to an increase in binding energies. However, this also leads to a decrease in self-polarization. Self-polarization does not occur when the impurity atom is at the centre, even with an increase in a magnetic field, confirming previous graphs. It is evident from Fig.2. (a) and (b) that temperature plays a crucial role in reducing the binding energies under all conditions. Additionally, it enhances self-polarization in cases where the impurity is off-centre.

In Fig.3., the effects of wire radius on binding energy and self-polarization are analyzed for different magnetic fields and temperatures, with an impurity atom at c=0.25. As the radius of the wire is increased, the binding energy of the electron decreases while the self-polarization effect becomes more pronounced. This phenomenon can be observed due to the increased distance between the impurity and the electron within the wire. As a result, this leads to a decrease in electrons in their attraction to the impurity. The variation of self-polarization increases gradually as the wire radius increases. Findings supporting the previous graphs were also obtained using previous temperature and magnetic field measurements. The most important observation in this graph is that the self-polarization shown in Fig.3.(b) never reaches zero. This is due to the fact that in these plots, the impurity is located at c=0.25, and there is no completely symmetric potential.

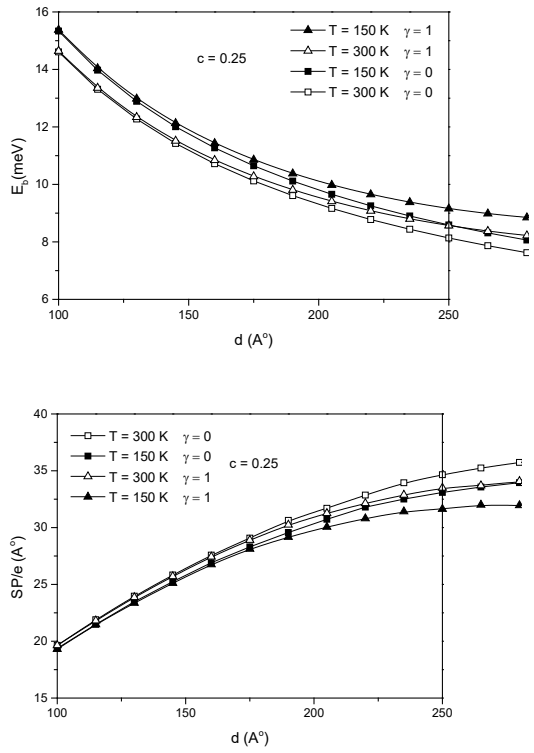

Fig.3. *Plot of binding energy (a) and self-polarization (b) for different temperatures and magnetic field values versus wire radius when the impurity position is fixed at c = 0.25.*

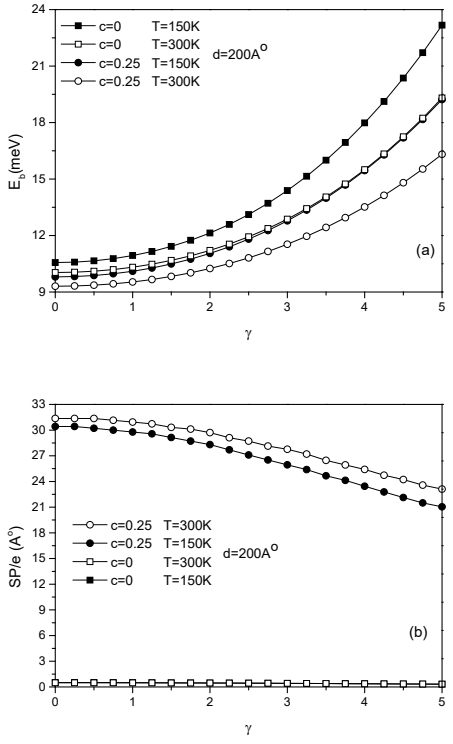

Fig.4. *Variations in binding energy and self-polarization based on magnetic field at fixed wire radius* $(200A°)$ *for different temperatures and impurity positions.*

Fig.4. shows the binding energy (a) and self-polarization (b) changes with the magnetic field at different temperatures and impurity positions with a fixed wire radius of $200A°$. As the magnetic field increases, an extra confinement potential occurs in the system and the binding energy increases for all conditions (Fig.4.(a)). Interestingly, when the impurity atom is placed in the centre, the system maintains its symmetry and self-polarization values close to zero are calculated at all temperatures, even with an increased magnetic field (Fig.4.(b)). However, if the impurity atom is off-centre, the symmetry is broken, leading to non-zero self-polarization values (Fig.4.(b)). On the other hand, an impurity atom far from the centre reduces the binding of the electron and causes increased self-polarization. An increased temperature makes the electron more energetic, causing it to bind more weakly to the impurity. As a result, the electron becomes more sensitive to the wire potential. After this, if the system is not symmetrical, self-polarization values other than zero are measured.

CONCLUSION

This study investigates the effect of temperature on self-polarization by considering various factors such as magnetic field, wire radius, and impurity atom locations. It aims to determine the relationship between these variables and self-polarization for a deeper understanding of the phenomenon. In a cylindrical quantum wire, the binding energy decreases with increasing temperature. But when the impurity is at the centre, the self-polarization is calculated to be almost zero, and its value does not change with changes in temperature, magnetic field and wire width. The self-polarization can be calculated when the impurity is not centred, and in this case, it is important to note that the self-polarization increases as the temperature increases. The findings of this research may have important implications for a variety of industries and scientific fields, including materials science, electrical engineering, and physics.

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