Temperature effect on the diamagnetic susceptibility of a shallow magneto-donor in GaAs/AlAs Quantum Box

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Abstract. In this paper, we have studied the influence of the temperature on the diamagnetic susceptibility of a shallow donor confined to move in a quantum box (QB) made out of GaAs/Ga$_{1-x}$Al$_x$As with a uniform magnetic field. The Hass variational method within the effective mass approximation is used in the case of finite barrier confining potential. In the calculation, we have taken account of the electronic effective mass, dielectric constant and conduction band offset between the dot and the barriers varying with the temperature. We present our results as a function of the size of the box and the magnetic field intensity. The results obtained show that the temperature and the magnetic field effects on the diamagnetic susceptibility are appreciable and more pronounced for large dot. A good agreement is obtained with the existing literature.

1. Introduction

The semiconductor structures with dimensionality reduced such as quantum wells, quantum dots, heterostructures and multilayers form a very interesting system for the fundamental study of the physical phenomena and a major area of research for over recent years, such as the observation of discrete electronic states in GaAs/GaAlAs nanostructures [1-4]. Investigations on impurity states in semiconductors are very essential as they govern the thermal, optical and electrical properties. The electronic and optical properties of the impurities in low dimensional systems such as GaAs/GaAlAs quantum dots are quite different from those in the bulk materials [5, 6].

After the pioneering work by Bastard [7], several investigators with various methods have studied hydrogenic donors under confined geometries in the presence of an electric field [8], magnetic field [9], crossed magnetic and electric fields [10] and under temperature and pressure effects [11-14]. EL Messoudi et al [15] have calculated the polarizability and diamagnetic susceptibility for a shallow donor confined to move in quantum box (QB) with a uniform magnetic field.

There are several works which study the diamagnetic susceptibility of a donor in nanostructures [9, 16]. Jeice et al [16] have studied the polaronic effects on diamagnetic susceptibility of a hydrogenic donor in nanostructures.
Nevertheless, to the best of our knowledge, there is no study on the effect of temperature on the diamagnetic susceptibility and polarizability of a donor in a quantum box.

In the present paper, we report the effect of the temperature on the diamagnetic susceptibility of a hydrogenic shallow donor impurity placed at the center of a quantum box (GaAs/Ga_{1-x}Al_{x}As) in the presence of a uniform magnetic field. The Hass variational method within the effective mass approximation is used in the case of finite barrier confining potential.

2. General formalism:
We consider a system consisting of a quantum box (QB) made out of GaAs surrounded by Ga_{1-x}Al_{x}As with a donor impurity located in the center of the box. In the presence of a weak applied magnetic field along the z direction. In the effective mass approximation, the Hamiltonian of magneto-donor is given by:

\( H = -\frac{1}{2m^* (T)} \left( \vec{p} - \frac{e}{c} \vec{A} \right)^2 - \frac{e^2}{\varepsilon_0(T)r} + V(r,T) \)  \( (1) \)

Where \( m^*(T) \) and \( \varepsilon_0(T) \) are the effective mass and static dielectric constant of GaAs at temperature \( T(\text{K}) \). The temperature dependent potential barrier height is:

\[
V(r,T) = \begin{cases} 
0 & |x| \leq \frac{L}{2}, |y| \leq \frac{L}{2}, |z| \leq \frac{L}{2} \\
V_0(T) & \text{elsewhere}
\end{cases}
\]  \( (2) \)

Where:

\[
V_0(T) = Q_c \Delta E_g^\Gamma (x,T)
\]  \( (3) \)

Is the barrier height [17]. \( Q_c \) is the conduction band offset parameter \( Q_c=0.60 \) [18]. \( \Delta E_g^\Gamma (x,T) \) is the difference in the QD band gap which depends on the concentration of aluminum \( x \) and the temperature in Ga_{1-x}Al_{x}As, given in ref [17]:

\[
\Delta E_g^\Gamma (x,T) = \Delta E_g^\Gamma (x) + TC(x)
\]  \( (4) \)

Where

\[
\Delta E_g^\Gamma (x) = 1.155x + 0.37x^2
\]  \( (5) \)

Is the variation of the energy gap difference with composition \( x \) [19] and the quantity of \( C(x) \) is defined as the temperature coefficient of band gap difference is given by [20]:

\[
C(x) = [-1 \times 10^{-4})x] \quad (eV.k^{-1})
\]  \( (6) \)

\( m^*_{d,b}(T) \) are the conduction electron effective mass:

\[
m^*(T) = \begin{cases} 
m^*_{b}(T) & \text{in GaAs} \\
m^*_{d}(T) & \text{in Ga_{1-x}Al_{x}As}
\end{cases}
\]  \( (7) \)

For GaAs quantum dot, the parabolic conduction effective mass is determined from the expression [20, 21]:

\[
\]
\[ m^*_d(T) = \frac{m_0}{1 + E^\Gamma_g \left( \frac{2}{E^\Gamma_g(T)} + \frac{1}{E^\Gamma_g(T) + \Delta_0} \right)} \] (8)

Where \( E^\Gamma_g = 7.51 \text{ eV} \) is the energy, which corresponds to the momentum matrix element. 
\( \Delta_0 = 0.341 \text{ eV} \) : The spin-orbit splitting. \( E^\Gamma_g(T) \) : The temperature dependence of the energy gap (eV) at the \( \Gamma \)-point given by [22]:

\[ E^\Gamma_g(T) = 1.519 - \frac{(5.405 \times 10^{-4})T^2}{(T + 204)} \text{ (eV)} \] (9)

The Ga\(_{1-x}\)Al\(_x\)As conduction effective mass is given by [20, 21]:

\[ m^*_c(T) = m^*_c(T) + 0.083m_0 \] (10)

\( \varepsilon_{db}(T) \) are the temperature dependent static dielectric of both materials respectively. In the GaAs, \( \varepsilon_d(T) \) is given by [23, 24].

\[ \varepsilon_d(T) = \begin{cases} 12.74 & \exp\left[9.4 \times 10^{-5}(T - 75.6)\right] \quad T \leq 200K \\ 13.18 & \exp\left[20.4 \times 10^{-5}(T - 300)\right] \quad T > 200K \end{cases} \] (11)

And the dielectric constant of Ga\(_{1-x}\)Al\(_x\)As is given by:

\[ \varepsilon_b(x,T) = \varepsilon_d(T) - 3.12x \] (12)

The temperature effect on lattice parameter is given by [25, 26]:

\[ a(x,T) = a(T) + 0.00809x \] (13)

\[ a(T) = 5.65325 + 3.88 \times 10^{-5}(T - 300) \] (14)

When the hydrogenic impurity is placed at the center of the dot. The Schrödinger equation for the Hamiltonian cannot be solved exactly, we follow the Hass variational method. For the ground state, we choose the trial wave function as [15]:

\[ \psi_0 = N\varphi(x)\varphi(y)\varphi(z)\exp\left[-\left(\frac{x^2 + y^2}{8b^2} + \frac{z^2}{8a^2}\right)\right] \] (15)

\[ \varphi(x) = \begin{cases} A_x \exp(K_{2x}x) & x \leq -\frac{L}{2} \\ \cos(K_{1x}x) & -\frac{L}{2} \leq x \leq \frac{L}{2} \\ A_x \exp(-K_{2x}x) & x \geq \frac{L}{2} \end{cases} \] (16)

Where:

\[ K_{1x} = \sqrt{\frac{2m^*_cE_x}{\hbar^2}} \quad \text{And} \quad K_{2x} = \sqrt{\frac{2m^*_c(V_0 - E_x)}{\hbar^2}} \] (17)

The parameters \( K_{1x}, K_{2x} \) and \( A_x \) are determined by using the appropriate current-conserving boundary conditions for the wave functions at the interfaces and must satisfy the following relations:
The functions $\varphi(y)$ and $\varphi(z)$ are taken in similar manner.

The variational method leads to the ground-state expectation of energy $E(T)$ for a hydrogenic donor as function of temperature which can be written as:

$$E(T) = \langle \psi | H | \psi \rangle$$

Which is minimized with respect to the variational parameters $a$ and $b$.

The temperature dependence of the donor binding energy is given by:

$$E_b(T) = E_{\text{sub}}(T) - \min_{a,b} E(T)$$

Where $E_{\text{sub}}(T)$ is the eigenvalue of Hamiltonian in Eq. 1 without the impurity potential.

The diamagnetic susceptibility ($\chi_{\text{dia}}$) of the donor impurity under the influence of temperature is given by:

$$\chi_{\text{dia}} = -\frac{e^2}{6m^*(T)c} \left\langle \frac{1}{r^2} \right\rangle$$

Where $c$ is the velocity of light ($c = 137$ and $e = 1$, $m_0 = 1$ in a.u.) and $\left\langle \frac{1}{r^2} \right\rangle$ is the mean square distance of the electrons from the nucleus.

In our calculations, we use the reduced units: the effective Bohr radius $a^* = \frac{\hbar^2 \varepsilon_0}{m^* e^2}$ as unit of length

and the effective Rydberg $R^* = \frac{e^2}{2\varepsilon_0 a}$ as unit of energy $\gamma = \frac{\hbar \omega_c}{2R^*}$ is a dimensionless measure of magnetic field where $\omega_c = \frac{eB}{m^*(T)c}$ is the effective cyclotron frequency.

3. Results and Discussion

The various parameters values used in the calculations are given in table 1. Therefore, the results are presented in reduced atomic units.

In figure 1, we present the variation of the potential barrier height as function of temperature for different values of concentration. We can see that the potential barrier height decrease with the temperature for all values of concentration $x$. We explain this that when the temperature increase, the effective mass $m^*$ decrease, which lead to the increase of Bohr radius $a^*$ and reduces the value of the effective Rydberg $R^*$. This makes the potential barrier height decrease with temperature. Ours results are in good agreement with [17].
Table 1. The variation of effective mass, dielectric constant, effective Bohr radius, effective Rydberg, and potential barrier height with temperature.

| T(k) | \( m^*_d(T) \) | \( \epsilon_d(T) \) | \( a^* \) | \( R^* \) | \( V_0 \) | \( m^*_b(T) \) | \( \epsilon_b(T) \) | \( V_0 \) | \( m^*_b(T) \) | \( \epsilon_b(T) \) |
|------|---------------|----------------|-------|-------|--------|---------------|----------------|--------|---------------|----------------|
|      | \( m_0 \)    | (Å)            | (meV) | (meV) |         | \( m_0 \)    | (Å)            | (meV) | \( m_0 \)    | (Å)            | (meV) |
| 77   | 0.0665        | 12.50          | 99.3  | 5.83  | 99.8437 | 0.0748        | 12.188         | 445.3117 | 0.0997        | 11.252         |
| 150  | 0.0657        | 12.85          | 103.4 | 5.42  | 99.8537 | 0.0748        | 12.538         | 443.7549 | 0.0989        | 11.602         |
| 250  | 0.0641        | 13.05          | 107.6 | 5.13  | 98.8761 | 0.0724        | 12.738         | 443.2449 | 0.0973        | 11.802         |
| 300  | 0.0632        | 13.18          | 110.2 | 4.96  | 98.3875 | 0.0715        | 12.868         | 431.2898 | 0.0964        | 11.932         |
| 400  | 0.0613        | 13.45          | 115.9 | 4.62  | 97.4100 | 0.0696        | 13.138         | 427.3800 | 0.0945        | 12.201         |
| 500  | 0.0594        | 13.73          | 122.2 | 4.29  | 96.4325 | 0.0677        | 13.418         | 423.4700 | 0.0926        | 12.482         |

The figure 2, and figure 3 present the variation of lattice parameter as a function of temperature for different values of Aluminum composition x. We notice that the lattice parameter increases with temperature for all values of concentration x. Indeed that when increasing the temperature, the interatomic distance in the cubic lattice increases. This has the effect of increasing the lattice parameter and lower the gap.

In order to evaluate the temperature effect on the diamagnetic susceptibility \( \chi_{\text{dia}} \) of a hydrogenic donor impurity, we plotted in figure 4 and figure 5 the variation of the diamagnetic susceptibility as a function of the temperature and the size of the quantum box.

From figure 4, we can observe that the absolute value of the diamagnetic susceptibility \( |\chi_{\text{dia}}| \) increases with QD width (L) for different temperature values, T=150K, 300K and 500K. It is to be noted that, for a fixed temperature the absolute value of the diamagnetic susceptibility increase as the QD width increase. This is related to the fact that, at a specific temperature, the wave function is more compressed for small QD.

From figure 5, we remarque that the influence of the temperature is appreciable only for large QD (L \( \geq 3a^* \)). For small QD (L \( \leq 2a^* \)), the geometric confinement is more pronounced and the temperature effect is negligible. For large dots, we notice that when the temperature increase, the absolute value of the diamagnetic susceptibility \( |\chi_{\text{dia}}| \) increases. This increase is due to the fact of the increase in temperature. Because the effective mass of electrons decrease and the dielectric constant increases so the potential barrier height decreases (as presented in table 1) leading to a decrease in Coulomb interaction between the electron and impurity for all quantum dot sizes which increase the absolute value of the diamagnetic susceptibility.

In order to study the magnetic field effect on the diamagnetic susceptibility, we plotted in the figure 6, the variation of the diamagnetic susceptibility \( \chi_{\text{dia}} \) as a function of magnetic field, for different values of QD width L (L=0.1a*, 1a* and 3a*). Our results show that, in the absence of temperature, the magnetic field effect on the diamagnetic susceptibility is remarkable only for large QD (L \( \geq 3a^* \)) and when the magnetic field increase the absolute value of the diamagnetic susceptibility \( |\chi_{\text{dia}}| \) decreases. For small values of QD width (L \( \leq 2a^* \)) the influence of the magnetic field is masked because the geometric confinement is more pronounced. Ours results are in good agreement with Mmadi et al [27].
Figure 1. Variation of the potential barrier height as function of temperature for different values of concentration (x=0.1, 0.3 and 0.4).

Figure 2. Variation of the lattice parameter as a function of temperature, for different values of concentrations (x=0.1, 0.3 and x=0.45).
**Figure 3.** Variation of the lattice parameter as a function of concentration, for different values of temperature (T=150K, 300K and T=400K).

**Figure 4.** Variation of the diamagnetic susceptibility $\chi_{\text{dia}}$ as a function of QD width L, for different values of temperature (T=150, 300 and 500K) with x= 30%.
Figure 5. Variation of The diamagnetic susceptibility $\chi_{\text{diam}}$ as a function of temperature, for different values of QD width $L$ ($L_x=1a^*$, $2a^*$ and $3a^*$).

Figure 6. Variation of the diamagnetic susceptibility $\chi_{\text{diam}}$ as a function of Magnetic field, for different values of QD width $L$ ($L_x=0.1a^*$, $1a^*$ and $3a^*$).
4. Conclusion
In this study, the temperature effect on the diamagnetic susceptibility and on the polarizability of a hydrogenic donor placed at the center in a cubic quantum dot (QD) in the presence of an uniform magnetic field are investigated. It’s observed that the effect of temperature on the diamagnetic susceptibility in zero dimensional semiconductors is appreciable for large QD. The temperature increases, the absolute value of the diamagnetic susceptibility $|\chi_{dia}|$ increases. On the other hand, the susceptibility decreases by increasing the magnetic field. Its effect is recorded for large QD.

According to the results obtained from the present work, we have found that the temperature and the magnetic field play important roles on the diamagnetic susceptibility of quantum dots in the presence of a donor impurity.

In summary, the temperatures and the magnetic field have a great influence on the fabrication of semiconductors in the presence of a donor impurities in a QD.

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