The hydrostatic pressure and magnetic field effect on the diamagnetic susceptibility of a shallow donor in GaAs/AlAs Quantum Box

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Abstract. We investigated the simultaneous effects of the hydrostatic pressure and magnetic field on the diamagnetic susceptibility of shallow donor confined to move in GaAs/Ga₁₋ₓAlₓAs Structure. The Hass variational method within the effective mass approximation used as the framework. We describe the quantum confinement by a finite barrier deep potential. The diamagnetic susceptibility computed as a function of the hydrostatic pressure, box size and the magnetic field intensity. Our results show that the absolute value of the diamagnetic susceptibility decreases with increasing hydrostatic pressure or magnetic field intensity. It effects is more pronounced for large Quantum Box. Hydrostatic pressure and magnetic field introduce an additional confinement on the donor inside the Quantum Box. Which can be used in semiconductors design.

1. Introduction
Small-scale semiconductor systems, such as Quantum Dots (QDs), experience an increase in quantum compliance compared to bulk materials because of their small dimensionality. They confine electrons and holes in all three directions, and this property is making them very attractive to optoelectronic devices. The existence of impurities in those nanostructures changes certain physical properties such as optical phenomena, the conductivity and transport at low temperature [1-5]. During the last few decades, the effects of hydrostatic pressure on the optical properties of those semiconductor systems have attracted a lot of attention because of technical points of view. Hydrostatic pressure effects on hydrogen impurity states in GaAs QD have been studied [6-9]. Recently John Peter et al [10] studied the effect of hydrostatic pressure and magnetic field on a confined impurity in a Quantum Dot. It showed that the binding energy of the impurity increases with reduction size, and increase in the
presence of the magnetic field. There is an increase in the size of the impurity in the presence of pressure and magnetic field simultaneously. Rezaei et al [11] studied the effect of hydrostatic pressure and electric field on the binding energy and the diamagnetic susceptibility of contained impurity in QD. They found that the confinement potential is reduced and the test function expansion zone increases with increasing the applied electric field, this leads to decrease the binding energy and increases the diamagnetic susceptibility. And Messoudi et al [8] have calculated the polarizability for a shallow magneto-donor confined to move in Quantum Box (QB).

In this letter, we present our studies about the Diamagnetic Susceptibility of shallow magneto-donor located at the center in GaAs/Ga_{1-x}Al_xAs Quantum Dot, under the joint action of hydrostatic pressure and magnetic fields. Calculations are made using the variational method within the effective mass approximation. These results are used to explain the behavior of the diamagnetic susceptibility in nanostructure devices, and we show that the diamagnetic susceptibility is modified under the external constraints.

2. General formalism

Under the effective mass approximation, the Hamiltonian of a donor impurity located at the center of the Quantum Box (QB) of GaAs surrounded by Ga_{1-x}Al_xAs in the presence of magnetic field applied along the z direction, given by:

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

(1)

Where \( m^*(P) \), \( \varepsilon_0(P) \) and \( V(r, P) \) are respectively the effective mass, the static dielectric constant of GaAs and the potential barrier height.

![Figure 1. Schematic of Cubical quantum dot with a donor impurity located at the center.](image)

The variation of dielectric constant of GaAs with pressure at T=300K is given by [10-13]:

\[ \varepsilon(P) = 13.18 - 0.088P \]  

(2)

Where \( P \) is in GPa.
$m^*_{d,b}(P)$ are the hydrostatic pressure dependent conduction effective mass for the electron of the Quantum Box and barrier layer, respectively [14].

$$m^*_{d,b}(P) = m^*_{d,b}(0) \exp(0.078P) \quad (3)$$

$$m^*_{d,b}(0) = \begin{cases} m^*_d(0) = 0.067m_0 & \text{in GaAs} \\ m^*_b(0) = (0.067 + 0.083x)m_0 & \text{in Ga}_{1-x}Al_xAs \end{cases} \quad (4)$$

Where $m_0$ is the free electron mass.

The hydrostatic pressure dependent potential barrier height is:

$$V(r, P) = \begin{cases} 0 & |x| \leq \frac{L_x(P)}{2}, \ |y| \leq \frac{L_y(P)}{2}, \ |z| \leq \frac{L_z(P)}{2} \\ V_0(P) & \text{elsewhere} \end{cases} \quad (5)$$

The potential barrier as a function of the Aluminum concentration $x$ is given by [15]:

$$V_0(P) = 0.685 \ \Delta E_g(x, P) \quad (6)$$

The total band gap difference between GaAs and Ga$_{1-x}$Al$_x$As as a function of the aluminum concentration $x$, given by [14]:

$$\Delta E_g(x, P) = \Delta E_g(x) + PD(x) \quad (7)$$

$$\Delta E_g(x) = 1.155x + 0.37x^2 \quad (8)$$

Is the variation of the energy gap difference [10].

$D(x)$ is the pressure coefficient of the band gap, given by [11]:

$$D(x) = [-(1.3 \times 10^{-3})x] \quad (9)$$

With 1Kbar= 0.1 GPa.
Table 1. The variation of effective mass, dielectric constant, effective Bohr radius, effective Rydberg and potential barrier height with hydrostatic pressure.

| P (GPa) | \( \frac{m_d^*(P)}{m_0} \) | \( \varepsilon_d(P) \) | \( a^*(\text{Å}) \) | \( R^* \) (meV) | \( \frac{m_x^*(P)}{m_0} \) | \( \varepsilon_x(P) \) | \( V_0 \) (meV) | \( \frac{m_y^*(P)}{m_0} \) | \( \varepsilon_y(P) \) |
|---------|------------------|-----------------|-----------------|--------------|------------------|-----------------|-------------|------------------|-----------------|
| 0       | 15.830           | 13.18           | 110.2           | 4.96         | 214.2556        | 15.8383         | 12.868      | 328.443         | 15.855          |
| 1       | 14.867           | 12.95           | 101.93          | 5.43         | 213.6235        | 14.8753         | 12.638      | 329.073         | 14.8925         |
| 2       | 14.090           | 12.73           | 93.02           | 5.95         | 213.6200        | 14.0983         | 12.418      | 327.8089        | 14.1154         |
| 3       | 13.448           | 12.51           | 85.46           | 6.53         | 213.2512        | 14.4563         | 12.198      | 327.8074        | 13.4732         |
| 4       | 12.914           | 12.29           | 78.51           | 7.15         | 213.1145        | 12.9223         | 11.978      | 327.8078        | 12.9391         |
| 5       | 12.468           | 12.08           | 72.12           | 7.84         | 212.9854        | 12.4763         | 11.768      | 326.6151        | 12.4932         |

We use the Hass variational method and we estimate the following wave function [12]:

\[
\psi_0 = N \varphi(x) \varphi(y) \varphi(z) \exp \left[ -\left( \frac{x^2 + y^2 + z^2}{8b^2} \right) \right] \tag{10}
\]

With

\[
\varphi(x) = \begin{cases} 
A_x \exp(K_{1x}) & x \leq -\frac{L_x}{2} \\
\cos(K_{1x}) & -\frac{L_x}{2} \leq x \leq \frac{L_x}{2} \\
A_x \exp(-K_{1x}) & x \geq \frac{L_x}{2} 
\end{cases} \tag{11}
\]

Where \( N \) is a normalization factor and \( a, b \) are the variational parameters.

\[
K_{1x} = \sqrt{\frac{2m_d^*E_x}{\hbar^2}} \quad \text{And} \quad K_{2x} = \sqrt{\frac{2m_b^*(V_0-E_x)}{\hbar^2}} \tag{12}
\]

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:

\[
\tan \sqrt{2m_d^*E_x} \frac{L_x}{2\hbar} = \sqrt{\frac{m_d^*}{m_b^*}} \left( \frac{V_0}{E_x} - 1 \right) + \frac{L_x \hbar}{8b^2 \sqrt{2m_d^*E_x}} \left( \frac{m_d^*}{m_b^*} - 1 \right)
\]

\[
A_x = \cos \left( k_{1x} \frac{L_x}{2} \right) \exp \left( k_{2x} \frac{L_x}{2} \right)
\]

The functions \( \varphi(y) \) and \( \varphi(z) \) they taken in similar manner.
Matching the test function and its derivatives at the borders of the cubic box and standardization, we set all the constants except [17]. In presenting the Rydberg \( R^*(P) = \frac{m^*(P)e^4}{2\hbar^2 \epsilon^2} \) as a unit of the energy and the Bohr radius \( a^*(P) = \frac{\hbar^2 \epsilon(P)}{m^*(P)e^2} \) as the unit of length, and \( \gamma = \frac{\hbar \omega_c}{R^*} \) characterizing the magnetic field strength. \( \omega_c = \frac{eB}{mc} \) is the effective cyclotron frequency.

The diamagnetic susceptibility of an impurity confined in a quantum box in atomic unit (a.u), given by [15]:

\[
\chi_{\text{dia}} = -\frac{e^2}{6m^*(P)e(P)c^2} \langle r^2 \rangle
\]

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

The results obtained for the diamagnetic susceptibility was determined after the numerical minimization of the expression of energy:

\[
E = \min_{a,b} \langle \psi(r, P) | H | \psi(r, P) \rangle
\]

3. Results and Discussion

We have calculated the Diamagnetic Susceptibility of a magneto-donor placed at the center of the Quantum Box (QB) and we have evaluated the influence of the hydrostatic pressure and the magnetic field. We have applied this model to the boxes made out of the GaAs surrounded by Ga\(_{1-x}\)Al\(_x\)As, where \( x \) is the Aluminum concentration.

In figure 2, we represent the variation of the barrier height depending on the hydrostatic pressure. We note that for different values of the Aluminum concentration, the height of the barrier depends on the applied hydrostatic pressure. The height of the barrier decreases with increasing hydrostatic pressure.

Figure 3 shows the variation of the diamagnetic susceptibility of a hydrogenic impurity as function of the length of the box for different values of the hydrostatic pressure. We can observe that the absolute value of the diamagnetic susceptibility \( |\chi_{\text{dia}}| \) increases with increasing the width of the box. The effect of the hydrostatic pressure is more important for larges Quantum Box and neglected for small QB. For larges Quantum Box, when the hydrostatic pressure increases, the absolute value of the diamagnetic susceptibility \( |\chi_{\text{dia}}| \) decreases. This is because that the wave function is more localized, and thus the value of \( \langle r^2 \rangle \) is diminished with increasing the pressure, which leads to modify the value of the diamagnetic susceptibility \( |\chi_{\text{dia}}| \).

We remark in Table.1 that the expressions \( m^*(P) \) and \( \epsilon(P) \) increases and consequently \( |\chi_{\text{dia}}| \) decreases with increasing the pressure. Our results are in good agreement with reference [10, 11, 18, 19].

Figure 4 present the variation of the diamagnetic susceptibility as a function of the magnetic field for different widths of the box in the absence of the hydrostatic pressure. We can observe that the absolute value of the diamagnetic susceptibility \( |\chi_{\text{dia}}| \) increases as the width of the box increases. For small QB \( (L=1 \, a^* \) and \( L=1.25 \, a^* \)), the magnetic field effect is neglected and becomes more pronounced for larges QB \( (L=2 \, a^* \) and \( L=3 \, a^* \)). When the magnetic field increases the absolute value
of the diamagnetic susceptibility $|\chi_{\text{dia}}|$ decreases. It’s due to the stronger confinement effect of the magnetic field and the spatial confinement. We can say that in the low dimensional nanostructures, when the size of the structure is large, the induced confinement by the effect of the magnetic field becomes dominant. Which are important in device applications based on the low dimensional nanostructures. Ours results are in good agreement with reference [10, 18, 19].

Figure 5 shows the variation of the diamagnetic susceptibility as a function of the length of the box for different values of hydrostatic pressure and under magnetic field applied simultaneously ($\gamma=2$). It’s seems that the absolute value of diamagnetic susceptibility decreases as the length of the box increases as expected, and it’s noticed that the variation of $|\chi_{\text{dia}}|$ is not pronounced for smaller Quantum Box due to the domination of geometrical confinement. For larger Quantum Box, it is clear that the geometric confinement induced by a magnetic field is dominant in which that the wave function is more concentrated around the impurity. The results shows that for larger Quantum Box the effect of both external perturbations seems to take part equally, which is induced to a strong confinement and a more impressive decrease of the absolute value of the diamagnetic susceptibility $|\chi_{\text{dia}}|$.

![Figure 2](image-url)

**Figure 2.** Variation of the barrier function on the hydrostatic pressure for different values of the aluminum concentration $x=0.2; x=0.3$ and $x=0.4$. 
Figure 3. The diamagnetic susceptibility as function of the length unit of the quantum box for different values of the hydrostatic pressure $P=0; 1; 2; 3\text{GPa}$ and $P=4\text{GPa}$.

Figure 4. The diamagnetic susceptibility as a function of the magnetic field for various values of the widths $L_x=L_y=L_z=0.1a^*,$ $1a^*, 1.25a^*, 2a^*$ and $L_x=L_y=L_z=3a^*$. 
Figure 5. The diamagnetic susceptibility as function of the length unit of the cubic box for different values of the hydrostatic pressure $P = 0\text{GPa}$, $P = 1\text{ GPa}$, $P = 2 \text{ GPa}$, $P = 3 \text{GPa}$ and $P = 4\text{GPa}$ in under the influence of the magnetic field ($\gamma = 2$).

4. Conclusion

In this work, we have studied the effect of the hydrostatic pressure and the magnetic field on the diamagnetic susceptibility of an impurity confined to move in a Quantum Box. We have solved analytically the Schrödinger equation using variational method of Hass and got the eigenvalues. The diamagnetic susceptibility decreases with increasing hydrostatic pressure or the magnetic field. For small Quantum Box, the diamagnetic susceptibility remains independent for hydrostatic pressure and the magnetic field.

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