Temperature effect on the binding energy and the diamagnetic susceptibility of a magneto-donor in Cylindrical Quantum Dot (GaAs/GaAlAs)

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Abstract. In this work, the effect of the temperature on the binding energy and the diamagnetic susceptibility of a shallow magneto-donor confined to move in a cylindrical quantum dot made out of GaAs/GaAlAs is studied within the effective mass approximation. We describe the quantum confinement by an infinite deep potential. The results show that when the temperature or the magnetic field increases, (i) the binding energy increases and (ii) the absolute value of the diamagnetic susceptibility decreases. Its effects depend strongly on the size of the CQD.

1. Introduction
In recent years, nanostructures such as quantum well (QW), quantum well wire (QWW) and quantum dot (QD) heterostructures and multilayers become a major research area in the field of nanoscience. The problem of shallow donor impurities confined to a semiconductor structure has been studied extensively during the last decade [1–6]. Investigations on impurity states in semiconductors are very essential not only for academic interest, but also because of the necessity to take into account the Coulomb effects at experimental analysis of optical and kinetic properties of semiconductor structures. Hitherto, many works have been done on the impurity states in quantum dots. For example, El-Yadri et al [7] have studied temperature and hydrostatic pressure effects on single dopant states in hollow cylindrical core-shell quantum dot. The results show that the temperature and hydrostatic pressure have significant influences on the impurity binding energy for large shell quantum dot. It will be shown that the binding energy is more pronounced with increasing pressure and decreasing temperature for any impurity position and quantum dot size. Surajit Saha et al [8] have investigated the simultaneous influence of hydrostatic pressure and temperature on diamagnetic susceptibility of impurity doped quantum dots under the aegis of noise. The results show that the application of
hydrostatic pressure and temperature invites greater delicacies in the observed DMS profiles. However, whereas the interplay between T and noise comes out to be extremely sensitive in fabricating the DMS profile, the pressure noise interplay appears to be not that much noticeable. Chu et al. [9] have studied the energy of hydrogenic impurity states with an impurity atom located at the center of a quantum dot and on the axis of a quantum-well wire. They assumed the two systems to have an infinite confining potential. Zhu [10] obtained exact solutions of donor states in a spherically rectangular quantum well using different series forms in different regions of the radial equation. Jayam and Navaneethakrishnan [11] calculated the binding energy of a hydrogenic donor in a GaAs spherical quantum dot with assuming parabolic confinement. They discussed the effects of hydrostatic pressure and electric field on the results obtained using a variational method. To obtain more information about impurity states in quantum dots, reader can refer to Refs [12].

In the present paper, we report the effect of the temperature on the diamagnetic susceptibility and the binding energy of a hydrogenic shallow donor impurity placed at the center of a quantum dot (GaAs/Ga1-xAlxAs) in the presence of an uniform magnetic field. The Hass variational method within the effective mass approximation is used in the case of infinite confining potential.

2. Formalism General

We consider a donor impurity located at the center of the cylindrical quantum dot “CQD” with radius \( R \) and length \( H \) in the presence a magnetic field \( \vec{B} \) one along the \( z \)-direction (see figure 1). In the effective mass approximation, the Hamiltonian can be written in cylindrical coordinates and reduced units as [11]:

\[
H = -\nabla^2 - \frac{2}{\sqrt{\rho^2 + z^2}} + \frac{\gamma^2}{4} \rho^2 + \gamma L_z + V(\rho, z)
\] (1)

![Figure 1. Schema of a cylindrical quantum dot with infinite confinement potential](image)

Where \( \rho \) and \( z \) are the electron coordinates in the plane perpendicular and along the cylinder axis respectively. \( L_z \) is the \( z \) component of the angular momentum operator. \( V(\rho, z) \) is the confining potential given by:

\[
V(\rho, z) = \begin{cases} 
0 & \text{for } \rho < R \text{ and } \left| z \right| < \frac{H}{2} \\
\infty & \text{for } \rho > R \text{ and } \left| z \right| > \frac{H}{2}
\end{cases}
\] (2)

Since the Schrödinger equation cannot be solved exactly, we follow the Hass variational method. We choose the wave function for the impurity ground-state as [13]:
\[ \psi(\rho,z) = \begin{cases} N J_0 \left( \frac{\rho}{\rho_0} \right) \cos \left( \frac{\pi z}{H} \right) \exp \left( - \frac{\rho^2}{8 \alpha^2} - \frac{z^2}{8 \beta^2} \right) & \text{for } \rho < R \text{ and } |z| < \frac{H}{2} \\ 0 & \text{for } \rho > R \text{ and } |z| < \frac{H}{2} \end{cases} \]  

(3)

Where \( J_0 \) is the Bessel function of zero order; \( \theta_0 = 2.40482 \) is its first zero, \( \alpha \) and \( \beta \) are variational parameters and \( N \) is the normalization constant. The corresponding energy is obtained by minimization with respect to the variational parameters \( \alpha \) and \( \beta \).

We use the effective Bohr radius \( a_\text{B}^*(T) = \hbar^2 \varepsilon(T) / m^*(T) e^2 \) and the effective Rydberg \( R_\text{B}^*(T) = m^*(T) e^4 / 2 \hbar^2 \varepsilon^2(T) \) as the units of length and energy. Furthermore, we introduce the dimensionless parameter \( \gamma = \hbar \omega_\gamma / R^* \) and \( \omega_\gamma = eB / m^*c \) characterizing the strength of the magnetic field and the effective cyclotron frequency respectively.

The application of temperature modifies the lattice constants, the effective Rydberg, the Bohr radius the effective masses and the dielectric constants. These values are obtained in the following way. The variation of dielectric constant with pressure is given by [13]:

\[ \varepsilon(T) = 13.13 - 0.088T \]  

(4)

The effective mass in the well (GaAs) changes as:

\[ \begin{align*}
 m^*(T) &= m^*(0) \exp(0.078T) \\
 m^*(0) &= 0.067m_0
\end{align*} \]  

(5)

Where \( m^*(0) = 0.067m_0 \) is the effective mass without pressure and \( m_0 \) is a free electron mass. The final results on the diamagnetic susceptibility are obtained by numerical minimization of the energy expression with respect to the parameters \( \alpha \) and \( \beta \) for CQD. The binding energy of the donor impurity located at the center of a Cylindrical Quantum Dot is given by:

\[ E_b = E_{Sub} - \langle H \rangle_{\text{min}} \]  

(6)

Where \( \langle H \rangle_{\text{min}} \) is the minimum of the expectation value of the Hamiltonian obtained by varying the variational parameters \( \alpha \) and \( \beta \).

The Schrodinger equation is solved variationally to find the ground state wave function, which has been used in the computation of diamagnetic susceptibility \( \chi_{\text{dia}} \) of the hydrogenic donor given as [13]:

\[ \chi_{\text{dia}} = -\frac{e^2}{6m^*(T)\varepsilon(T)c^2} <(\vec{r})^2> \]  

(7)

Where \( c \) is the velocity of light and \( <(\vec{r})^2> \) is the mean square distance of the electrons from the nucleus. The hydrostatic pressure effect on the \( \chi_{\text{dia}} \) of a hydrostatic impurity confined in a cylindrical quantum dot (CQD) in the presence of a uniform magnetic field is evaluated.

3. Results and Discussion
For the GaAs material, we have the effective mass $m^*=0.067 \, m_0$ and $\varepsilon_0=13.13$. The effective Bohr radius $a_B^*=98.6 \, \text{Å}$, the effective Rydberg $R_B^*=5.85 \, \text{MeV}$.

The binding energy versus radius $R$ for different temperature ($T= 200\,\text{K}, 300\,\text{K}, 400\,\text{K}$) is presented in figure 2. From this figure, we remark that in the absence of magnetic field ($\gamma = 0$), the binding energy decreases with the increase of the dot radius and approaches of the bulk case. When the temperature increases, the binding energy increases. The result shows that the behaviour of binding energy is purely temperature dependent for smaller dots.

In figure 3, we have plotted the variation of the binding energy of the donor impurity for CQD based on GaAs/AlGaAs in the presence of a magnetic field ($\gamma = 1$) for different values of the temperature. We notice that the binding energy increases with the increase of the temperature. This can be explained by the fact that the temperature and the magnetic field are confinements that add to the geometrical confinement and consequently the binding energy increases.

**Figure 2.** Variation of the binding energy as a function of $R$ and $H= 1a^*$ in the absence of a magnetic field ($\gamma = 0$) for different temperature value ($T=200\,\text{K}, 300\,\text{K}, 400\,\text{K}$)
Figure 3. Variation of the binding energy as a function of $R$ and $H = 1a^*$ in the present of a magnetic field ($\gamma = 1$) for different temperature values (T=200K, 300K, 400K).

In agreement with the previous explanation, we present the variation of the diamagnetic susceptibility of the donor impurity for different values of temperature (T= 200K, 300K, 400K) for two cases: in the absence of the magnetic field (see figure 4) and in the presence of magnetic field (see figure 5). In all cases, the absolute value of the diamagnetic susceptibility $|\chi_{dia}|$ increases with the increase of radius $R$ and decreases with increasing the temperature $T$ and the magnetic field. These results explain that in the presence of the magnetic field, the absolute value of the diamagnetic susceptibility remain constant for small quantum dots and decreases for large dots. So the absolute value of the diamagnetic susceptibility is dramatically dependent on the size of the cylindrical quantum dot and increases as the dot radius increases. Under a magnetic field, an additional confinement added to the geometrical confinement. So the absolute value of the diamagnetic susceptibility $|\chi_{dia}|$ decreases for nanostructure over a large range of QD dimensions.
Figure 4. Variation of the diamagnetic susceptibility $\chi_{\text{dia}}$ as a function of rayon R of CQD and $H=1a^*$ in the absence of a magnetic field ($\gamma = 0$), for different values of Temperature (T=200K, 300K, 400K)

![Graph showing the variation of diamagnetic susceptibility with rayon R for different temperatures without a magnetic field.]

Figure 5. Variation of the diamagnetic susceptibility $\chi_{\text{dia}}$ as a function of rayon R of CQD and $H=1a^*$ in the present of a magnetic field ($\gamma = 1$), for different values of Temperature (T=200K, 300K, 400K)

![Graph showing the variation of diamagnetic susceptibility with rayon R for different temperatures with a magnetic field.]

4. Conclusion
In this study, the temperature effect on the diamagnetic susceptibility and on the binding energy of a hydrogenic donor placed at the center in a cylindrical quantum dot (QD) in the presence of an uniform magnetic field are investigated. we notice that when with the the temperature or the magnetique field increases in the cylindrical quantum dot (CQD), the diamagnetic susceptibility in absolute value $|\chi_{\text{dia}}|$ decreases and the binding energy inceases. On the other hand, the effect of temperature is appreciable for larges CQD.

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