Form effect on the Diamagnetic Susceptibility of a magneto-donor in Quantum Dot

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Abstract: The diamagnetic susceptibility of a shallow donor confined to move in Quantum Dots ‘QD’ in the presence of a magnetic field is theoretically investigated. The numerical calculations are performed in the effective mass approximation, using a variational method. We describe the effect of the quantum confinement by an infinite deep potential. The form effect is studied for the Spherical Quantum Dot ‘SQD’ and Cylindrical Quantum Dot ‘CQD’. The results for these two forms of structures show that the diamagnetic susceptibility and the binding energy increase with the magnetic field. There are more pronounced for larger dot. We remark that for a zero magnetic field, the binding energy and the diamagnetic susceptibility are decreasing functions of the quantum dot radius.

1. Introduction

In the recent years, it became possible to fabricate high quality semiconductor quantum dots (QDs) with good electronic and optical properties due to the development of experimental crystal growth techniques [1-3]. These structural quantum dots have attracted a great deal of attention from academic and technological viewpoints [4-6]. The physical properties are improved by the reduction of the dimensional quantum confinement of carriers, they drastically changes the electronic structure in QDs from that of bulk semiconductors. In the past few years, several theoretical [7] and experimental [8] investigations have been reported on the behavior of shallow hydrogenic donor impurity in quantum dot. The effects of applied magnetic fields on the physical properties are given in the reference [9-11]. Recently, Ulas et al [12] have reported the study of electric field and geometrical effects on a shallow donors binding energy in a quantum well wire. They have obtained that the donor binding energy is sensitive to the interplay of the electric field and geometrical effects. Zounoubi et al [13] have studied the influence of magnetic fields on the binding energy and polarizability of a shallow donor impurity placed at the center of a cylindrical quantum dot (CQD). They have showed that the magnetic field increases the binding energy and strongly reduces the polarizability. For higher field strength and large dot, the magnetic field effects are predominant. Ulas et al [14] have also calculated electric field and geometrical effects on the self polarization in GaAs-(Ga-Al)As quantum well wires of square, rectangular and cylindrical cross-sections. They have found that the self-polarization effect outside of the center depends on both the geometrical form of the wire and the impurity position in the same structure. Several properties of the donors such as the polarizability [15] and diamagnetic susceptibility [16-19] are yet to be obtained experimentally. Recently, several theoretical works have been reported on the diamagnetic susceptibility of impurity in low dimensional systems. Peter et al [20] have computed and compared the susceptibility for a hydrogenic donor in a spherical confinement, harmonic oscillator-like and rectangular well-like potentials for a finite QDs. They observed a strong influence of the shape of confining potential and geometry of the dot on the
susceptibility. Rahmani et al [21] have studied the diamagnetic susceptibility of a confined donor in Ga1-xAlxAs-GaAs Inhomogenous Quantum Dot without a magnetic field. They found that the diamagnetic susceptibility depend strongly on the core and the shell radius and presents a minimum for a critical value of the ratio R1/ R2 depending on the value of the outer radius. Kilicarslan et al [22] have investigated the effects of the magnetic field and the dielectric screening on the diamagnetic susceptibility of a donor in a QW with anisotropic effective mass. Koksal et al [23] have studied the magnetic field effects on the diamagnetic susceptibility and binding energy of a hydrogenic impurity in a QWW by taking into account spatially dependent screening. They show that the diamagnetic susceptibility is more important for donors in QWW over a large range of wire dimensions. Kilcarslan et al [24] have studied the magnetic field effects on the diamagnetic susceptibility in a GaIn1-xNyAs1-y/GaAs QW and found that the diamagnetic susceptibility and binding energy of the magneto-donor in the GaIn1-xNyAs1-y/GaAs QW increases with Nitrogen mole fraction. El Ghazi et al [25] have studied the dependence of the binding energy as function of external magnetic field and donor’s position in GaN |(Ga,In)N | GaN spherical quantum dot–quantum well (SQDQW) Their results show that the magnetic field effect is more marked in large layer than in thin layer and it is more pronounced in the spherical layer center than in its extremities. A. Mmadi et al [26,27] have calculated the effects of an applied magnetic field on the diamagnetic susceptibility of a shallow donor confined to move in a spherical homogeneous Quantum Dots “HQD” and in Cylindrical Quantum Dot “CQD”.

The present paper is organized as follows: the model and the calculation method for calculating the ground-state binding energy and diamagnetic susceptibility of a shallow donor in QD are presented in Section2. The numerical results and discussions are shown for a Spherical QD of radius Rs and Cylindrical QD of radius Rc and length Hc in Section3.

2. Model and calculation

We consider a donor impurity located at the center of the spherical quantum dot “SQD” of radius Rs and the cylindrical quantum dot “CQD” with radius Rc and length Hc in the presence an applied a magnetic field $\mathbf{B}$ one along the z-direction.

2.1 Spherical Quantum Dot

The Hamiltonian that describes the problem of a hydrogenic impurity located in a spherical QD at the centre of the dot in the effective-mass approximation and in spherical coordinates can be expressed as [9]:

$$H = -\nabla^2 - \frac{2}{r} + \frac{1}{4} \gamma^2 r^2 \sin^2 \theta + V(r)$$

(1)

where the first term is the kinetic energy of the electron of the impurity, the second term correspond to the potential energy of the impurity the third and the fourth terms correspond to the effect of magnetic field. The last term $V(r)$ is the infinite confinement potential given by:

$$V(r) = \begin{cases} 0 & r < R_s \\ \infty & r \geq R_s \\ \end{cases}$$

(2)

We use the effective Bohr radius $\alpha^* = h^2 e^2 / m^* e^2$ and the effective Rydberg $R^* = m^* e^4 / 2 h^2 e^2$ as the units of length and energy. Furthermore, we introduce the dimensionless parameter $\gamma = \frac{\hbar \omega}{R^*}$ and
\( \omega_c = \frac{eB}{m^*c} \) characterizing the strength of the magnetic field and the effective cyclotron frequency respectively.

We use a variational method approach to determine the ground state binding energy; we adopt the wave function given by [9]:

\[
\psi_r(r) = \begin{cases} 
\sin \left( \frac{Kz}{R} \right) e^{-\lambda r} & \text{for } r \leq R, \\
0 & \text{for } r > R,
\end{cases}
\]

\( K = \frac{\pi}{R} \) and \( \lambda \) is a variational parameter. The exponential factor \( e^{-\lambda r} \) describes the Coulomb spatial interaction. The corresponding energy is obtained by minimization with respect to the variational parameter \( \lambda \):

The binding energy of the donor impurity located at the center of a Spherical Quantum Dot is given by

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

Where \( \langle H \rangle_{\text{min}} \) is the minimum of the expectation value of the Hamiltonian obtained by varying the variational parameter \( \lambda \).

### 2.2 Cylindrical Quantum Dot

In this section, we consider the case cylindrical quantum dot (CQD) with radius \( R \) and length \( H \), with a donor impurity placed at the center of the dot. In the effective mass approximation, the Hamiltonian can be written in cylindrical coordinates and reduced units as [26]:

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

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.

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

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 [14]:

\[
\psi(\rho, z) = \begin{cases} 
N J_\alpha \left( \theta_0 \frac{\rho}{R_c} \right) \cos \left( \frac{\pi z}{2} \right) e^{-\alpha \rho} \left[ e^{-\gamma L_z} \sin \left( \frac{Kz}{R} \right) \right] & \text{for } \rho \leq R \text{ and } |z| \leq \frac{H}{2}, \\
\infty & \text{for } \rho > R \text{ and } |z| > \frac{H}{2}.
\end{cases}
\]

where \( J_\alpha \) 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 variation parameters \( \alpha \) and \( \beta \). The binding energy of the donor impurity located at the center of a Cylindrical Quantum Dot is given by

\[
E_b = E_{Sub} - \langle H \rangle_{\text{min}}
\]
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 [27]:

$$\chi_{\text{dia}} = -\frac{e^2}{4\pi \varepsilon_0 c^2} \langle \psi^2 \rangle$$  \hfill (9)

The final results on the diamagnetic susceptibility are obtained by numerical minimization of the energy expression with respect to the parameters $\lambda$ for SQD and $\alpha$ and $\beta$ for CQD.

3. Numerical results and Discussion

(For the GaAs material, we have: the effective Bohr radius $a^* = 98.6$ $\text{Å}$, the effective Rydberg $R^* = 5.85$ MeV, the effective mass $m^* = 0.067$ me and finds dielectric = 12.5)

In this section, the diamagnetic susceptibility of a hydrogenic impurity confined in a quantum dot with and without applied magnetic field is calculated numerically. Using a variational procedure in the effective mass approximation. Numerical applications are for a typical GaAs SQD and CQD. The binding energy versus the quantum dot radius for different magnetic fields ($\gamma = 0, 0.5$ and $1$) is presented in Figure 1. From this figure, we remark that in the strong spatial confinement case ($R_s < 2a^*$) and ($R_c < 1.5a^*$), the binding energy is relatively insensitive to the magnetic field and is identical to the zero magnetic field case. This explains that the main contribution to the binding energy is the electron spatial confinement energy and that the electron spatial confinement prevails over the magnetic field confinement. For the week spatial confinement ($R_s > 2a^*$) and ($R_c > 1.5a^*$), the different magnetic field curves tend to deviate from each other and reach steady values as the dot radii increase. Also, we can see that without a magnetic field, the binding energy tends to the value of the bulk semiconductor ($E_b \rightarrow 1R*$), while for a given value of the magnetic field, the binding energy is larger than for the case without a magnetic field. The physical meaning of this is that increasing the strength of the magnetic field shrinks the electron wave function and decreases the cyclotron radius for the electron relative to the quantum radius and confines the electron closer to the on-center impurity.

Figure 1 Variation of donor binding energy as a function of $R_s$ radius of a SQD and as a function of
Rc radius and H = 3a* of a CQD for three values of magnetic field (γ = 0, 0.5 and 1)

We have reported in figure 2-a and figure 2-b the diamagnetic susceptibility \( \chi_{\text{dia}} \) of a donor as a function of the spherical radius Rs and as a function of the cylindrical radius Rc with different values of the lengths (Hc = 0.6a*, 1a*, 3a* and 20a*) for (γ = 0). We consider the case of a donor impurity placed at the center of this two structures. From figure 2-a, we can see that the diamagnetic susceptibility \( \chi_{\text{dia}} \) decreases as the radius Rs increases. We remark also that diamagnetic susceptibility decreases strongly and eventually converges to the bulk limit value (-1.1 a.u) [16, 18] for \( R_s \to \infty \). For figure 2-b, we remark that the diamagnetic susceptibility \( \chi_{\text{dia}} \) decreases when the radius Rc increases for each value H. Our results show that for strong axial confinement (Hc = 1a*) and weak radial confinement (Rc >> 1a*), the diamagnetic susceptibility \( \chi_{\text{dia}} \) decreases and tends to the quantum well value (-0.2a.u) [19]. Nevertheless, for weak axial confinement (Hc >> 1a*) and weak radial confinement (Rc > 1a*), we see that the diamagnetic susceptibility decreases with the increase of CQD length and approaches to the three dimensional value (-1.1a.u) which correspond to the bulk limit case (see Ref [16, 18]). It should be noted that the diamagnetic susceptibility \( \chi_{\text{dia}} \) is more sensitive for large dimensional in these two cases. Our results are in perfect agreement with previous calculations without the magnetic field.

![Graph](image1)

**Figure 2** Variations of the diamagnetic susceptibility \( \chi_{\text{dia}} \) as a function of Rs radius of a SQD : (a) and as a function of Rc radius and with several values of the length (H=0.6a*, 1a*, 3a* and 20a*) of a CQD: (b)

The diamagnetic susceptibility of a shallow donor as a function of a SQD and a CQD dimension obtained by using a variational method with an infinite barrier are presented in table 1 and table 2. From Table 1, we conclude that the diamagnetic susceptibility \( \chi_{\text{dia}} \) values decreases with increasing spherical radius. In the bulk limit \( \chi_{\text{dia}} \) should approach (-1.1a.u). We obtain \( \chi_{\text{dia}} = -1.1012 \) a.u for Rs = 11a*. As in table 2, It is easily observed that the variation of the diamagnetic susceptibility
$\chi_{\text{dia}}$ increases with cylindrical size and approaching the bulk value (-1.0807a.u) for $R_c=11a^*$ and $H_c=11a^*$. These two form of quantum dot gives good results of the diamagnetic susceptibility when the quantum dot size becomes very large, a comparison has been reported in Ref [28].

Table 1. Diamagnetic susceptibility of a Spherical Quantum Dot

| SQD   | RS = 1a$^*$ | RS = 3a$^*$ | RS = 5a$^*$ | RS = 7a$^*$ | RS = 9a$^*$ | RS = 11a$^*$ |
|-------|-------------|-------------|-------------|-------------|-------------|--------------|
| $\chi_{\text{dia}}$(a.u) | -0.0928 | -0.5408 | -0.9684 | -0.9684 | -1.0416 | -1.1012 |

Table 2. Diamagnetic susceptibility of a Cylindrical Quantum Dot

| CQD   | Rc = 1a$^*$ | Rc = 3a$^*$ | Rc = 5a$^*$ | Rc = 7a$^*$ | Rc = 9a$^*$ | Rc = 11a$^*$ |
|-------|-------------|-------------|-------------|-------------|-------------|--------------|
| $\chi_{\text{dia}}$(a.u) | -0.0827 | -0.4848 | -0.7955 | -0.9411 | -0.9869 | -1.0807 |

In order to investigate the magnetic field and the form effect, we display in figure 3-a and figure 3-b the diamagnetic susceptibility $\chi_{\text{dia}}$ as a function of the dot radius $R_s$ and $R_c$ of SQD and CQD respectively width several values of magnetic field ($\gamma = 0, 0.5$ and $1$). The donor is placed in the centre of the dot. There is a competition between the geometric confinement and the magnetic confinement. From figure 3-a, the magnetic field effect on the diamagnetic susceptibility is not remarkable for small dot ($R_s < 2a^*$), the magnetic field effect becomes important for large QD ($R_s \geq 2a^*$). Also as expected the diamagnetic susceptibility increases with magnetic field due to compression of the electron wave function with the magnetic field. It’s important to note that the diamagnetic susceptibility $\chi_{\text{dia}}$ decreases when the dot radius $R_s$ increases. For figure 3-b, the effects of the magnetic field on diamagnetic susceptibility $\chi_{\text{dia}}$ as a function of the radius $R_c$ for different values of the length $H_c$ ($H_c = 1a^*$ and $H_c = 3a^*$) has been plotted. We notice that for strong radial confinement ($R_c < 1.5a^*$), the magnetic field effect on the diamagnetic susceptibility is not remarkable. The diamagnetic susceptibility increases with the magnetic field. This increase is due to a shrinking of the charge distribution when an external magnetic field is applied. Furthermore, for given values of $R_c$ and $\gamma$, the diamagnetic susceptibility increases when the length of the dot decreases which reflects the increasing confinement. These results explain that in the presence of the magnetic field, the diamagnetic susceptibility $\chi_{\text{dia}}$ remain to be constant over a large dot [25, 32]. Also, the diamagnetic susceptibility are found to be almost identical for dot of spherical and cylindrical if the dot dimensions taken to be comparable.

Now, by comparing figure 4-a and figure 4-b, we plotted the variation of the diamagnetic susceptibility as a function of the magnetic field strength for fixed QD geometries. This figure reflects correctly the effect of the magnetic field, which confines more the electron and increases the diamagnetic susceptibility. From figure 4-a, we took three values of a spherical dot radius $R_s$ ($R_s = 1a^*$, $1.25a^*$ and $2a^*$). We notice that for quantum dots quite small geometrical dimensions ($R_s = 1a^*$ and $1.25a^*$), the diamagnetic susceptibility is relatively insensitive to the magnetic field and is identical to the zero magnetic field case. For the quantum dots which is the geometrical dimension wide enough ($R_s = 2a^*$), the diamagnetic susceptibility $\chi_{\text{dia}}$ increases when the magnetic field
increases and reaches a limit value when the magnetic field becomes very strong. For figure 4-b, we plot the variation of the donor diamagnetic susceptibility $\chi_{\text{dia}}$ for three different radius values of cylindrical quantum dot (Rc=1a*, 2a* and Rc = 3a*) and H = 3a. We can remark that the diamagnetic susceptibility $\chi_{\text{dia}}$ increases as CQD radius Rc decreases. The diamagnetic susceptibility is totally insensitive to the increase of the magnetic field for small radius confinement (Rc = 1a*). For large radius confinement case (Rc > 2a*), the variation of the diamagnetic susceptibility is much more pronounced due to the stronger confinement effect of the magnetic field. From the two forms of the dot, it is clearly seen that the diamagnetic susceptibility decrease as the QD radius increases or the magnetic field strength decreases. As observed that the magnetic field effect and geometry effect, influence directly on the diamagnetic susceptibility behavior.

Figure 3 Variations of the diamagnetic susceptibility $\chi_{\text{dia}}$ as a function of Rs radius of a SQD: (a) and as a function of Rc radius and (H = 1a* and H = 3a*) of a CQD: (b) for three values of magnetic field ($\gamma = 0$, 0.5 and 1)

Figure 4 Variation of the diamagnetic susceptibility $\chi_{\text{dia}}$ function of magnetic field with three
values RS (RS= 1a *, 1.25a * and 2a *) of a SQD: (a) and with three values radius (Rc=1a*, 2a* and 3a*) and Hc = 3a* of a CQD: (b)

4. Conclusion
In the present work, we have reported the form and magnetic field effects on the diamagnetic susceptibility of a hydrogenic donor placed in spherical and cylindrical quantum dot by using the effective mass approximation. The diamagnetic susceptibility is dramatically dependent on the size of the dot and increases as the radius of the dot decreases. Under a magnetic field, additional increases for diamagnetic susceptibility are presented for nanostructure over a large range of QD dimensions.

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