

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

S Janati.Edrissi¹, S M'Zred¹, Y Chrafi², K Rahmani², I Zorkani¹, A Mmadi¹ and A Jorio¹

¹Groupe des Nanomatériaux et Energies Renouvelables, L P S,
Faculté des Sciences Dhar Mehraz, BP 1796, Fès-Morocco

²Faculté polydisciplinaire-Beni Mellal-Morocco

E-mail: janati.edrissi.sanae@gmail.com

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 Ga_{1-x}Al_xAs-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. Kilcarslan 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. Koksai 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 Ga_xIn_{1-x}NyAs_{1-y}/GaAs QW and found that the diamagnetic susceptibility and binding energy of the magneto-donor in the Ga_xIn_{1-x}NyAs_{1-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”. They have found that the diamagnetic susceptibility increases with the magnetic field and is more important especially for larger structure of quantum dot.

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 R_s and Cylindrical QD of radius R_c and length H_c in Section3.

2. Model and calculation

We consider a donor impurity located at the center of the spherical quantum dot “SQD” of radius R_s and the cylindrical quantum dot “CQD” with radius R_c and length H_c in the presence an applied a magnetic field \vec{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]:

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

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:

$$V(r) = \begin{cases} 0 & r < R_s \\ \infty & r > R_s \end{cases} \quad (2)$$

We use the effective Bohr radius $a^* = \frac{\hbar^2 \epsilon_0}{m^* e^2}$ and the effective Rydberg $R^* = \frac{m^* e^4}{2\hbar^2 \epsilon_0^2}$ as the units of length and energy. Furthermore, we introduce the dimensionless parameter $\gamma = \frac{\hbar \omega_c}{R^*}$ 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]:

$$\psi_o(r) = \begin{cases} \psi = \frac{\sin(Kr)}{r} \exp(-\lambda r) & \text{for } r \leq R_s \\ 0 & \text{for } r > R_s \end{cases} \quad (3)$$

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

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

$$E_b = E_{Sub} - \langle H \rangle_{\min} \quad (4)$$

Where $\langle H \rangle_{\min}$ is the minimum of the expectation value of the Hamiltonian obtained by varying the variational parameter λ .

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]:

$$H = -\nabla^2 - \frac{2}{\sqrt{\rho^2 + z^2}} + \frac{\gamma^2}{4} \rho^2 + \gamma L_z + V(\rho, z) \quad (5)$$

Where ρ 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.

$$V(\rho, z) = \begin{cases} 0 & \text{for } \rho < R_c \text{ and } |z| < \frac{H_c}{2} \\ \infty & \text{for } \rho > R_c \text{ and } |z| > \frac{H_c}{2} \end{cases} \quad (6)$$

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]:

$$\psi(\rho, z) = \begin{cases} N J_0\left(\theta_0 \frac{\rho}{R}\right) \cos\left(\frac{\pi z}{H}\right) \exp\left(-\left(\frac{\rho^2}{8\alpha^2} + \frac{z^2}{8\beta^2}\right)\right) & \text{for } \rho \leq R \text{ and } |z| \leq \frac{H_c}{2} \\ 0 & \text{for } \rho > R \text{ and } |z| > \frac{H_c}{2} \end{cases} \quad (7)$$

where J_0 is the Bessel function of zero order; $\theta_0 = 2.40482$ is its first zero, α and β are variational parameters and N is the normalization constant. The corresponding energy is obtained by minimization with respect to the variation parameters α and β .

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

$$E_b = E_{Sub} - \langle H \rangle_{\min} \quad (8)$$

Where $\langle H \rangle_{\min}$ is the minimum of the expectation value of the Hamiltonian obtained by varying the variational parameters α and β .

The Schrodinger equation is solved variationally to find the ground state wave function, which has been used in the computation of diamagnetic susceptibility χ_{dia} of the hydrogenic donor given as [27]:

$$\chi_{dia} = -\frac{e^2}{6m^* \epsilon_0 c^2} \langle (\vec{r})^2 \rangle \quad (9)$$

The final results on the diamagnetic susceptibility are obtained by numerical minimization of the energy expression with respect to the parameters λ for SQD and α and β for CQD.

3. Numerical results and Discussion

(For the GaAs material, we have: the effective Bohr radius $a^* = 98.6 \text{ \AA}$, the effective Rydberg $R^* = 5.85 \text{ MeV}$, the effective mass $m^* = 0.067 m_e$ 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 weak 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 of 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.

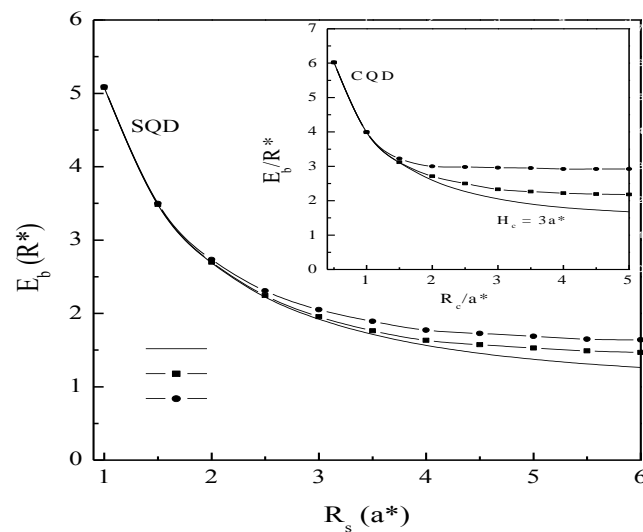


Figure.1 Variation of donor binding energy as a function of R_s radius of a SQD and as a function of R_c radius of a CQD.

R_c radius and $H = 3a^*$ of a CQD for three values of magnetic field ($\gamma = 0, 0.5$ and 1)

We have reported in figure2-a and figure2-b the diamagnetic susceptibility χ_{dia} of a donor as a function of the spherical radius R_s and as a function of the cylindrical radius R_c with different values of the lengths ($H_c = 0.6a^*, 1a^*, 3a^*$ and $20a^*$) for ($\gamma = 0$). 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 χ_{dia} decreases as the radius R_s increases. We remark also that diamagnetic susceptibility decreases strongly and eventually converges to the bulk limit value ($-1.1a.u$) [16, 18]

for ($R_s \rightarrow \infty$). For figure2-b, we remark that the diamagnetic susceptibility χ_{dia} decreases when the radius dot R_c increases for each value H . our results show that for strong axial confinement

($H_c = 1a^*$) and weak radial confinement ($R_c \gg 1a^*$), the diamagnetic susceptibility χ_{dia} decreases and tends to the quantum well value ($-0.2a.u$) [19]. Nevertheless, for weak axial confinement ($H_c \gg 1a^*$) and weak radial confinement ($R_c > 1a^*$), 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 χ_{dia} is more sensitive for large dimensional in these two cases. Our results are in perfect agreement with previous calculations without the magnetic field.

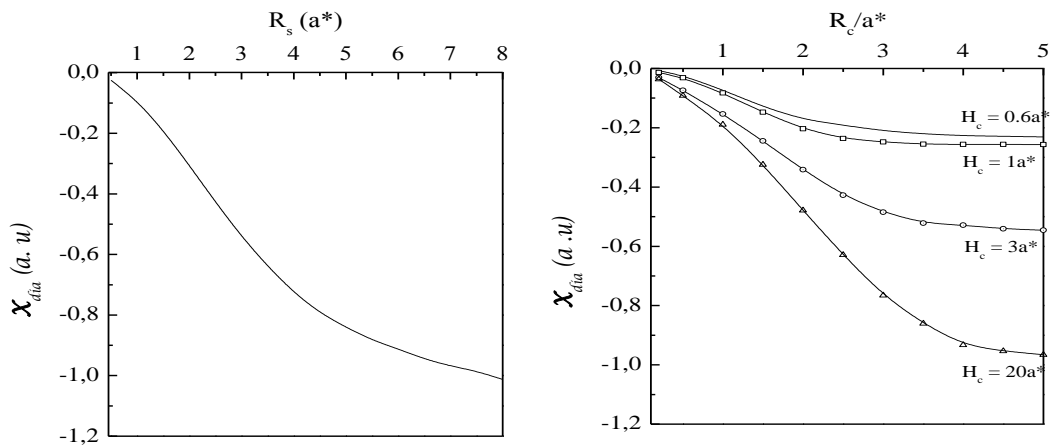


Figure.2 Variations of the diamagnetic susceptibility χ_{dia} as a function of R_s radius of a SQD : (a) and as a function of R_c radius and with several values of the length ($H = 0.6a^*, 1a^*, 3a^*$ and $20a^*$) of a CQD: (b)

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 table1 and table2. From

Table1, we conclude that the diamagnetic susceptibility χ_{dia} values decreases with increasing spherical radius. In the bulk limit χ_{dia} should approach ($-1.1a.u$). We obtain ($\chi_{dia} = -1.1012 a.u$) for $R_s = 11a^*$. As in table2, It is easily observed that the variation of the diamagnetic susceptibility

χ_{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].

Table1. Diamagnetic susceptibility of a Spherical Quantum Dot

SQD	RS =1a*	RS=3a*	RS=5a*	RS=7a*	RS=9a*	RS=11a*
Xdia(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*
	Hc=1a*	Hc=3a*	Hc=5a*	Hc=7a*	Hc= 9a*	Hc= 11a*
Xdia(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 figure3-a and figure3-b the diamagnetic susceptibility χ_{dia} as a function of the dot radius R_s and R_c of SQD and CQD respectively with 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 figure3-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 χ_{dia} decreases when the dot radius R_s increases. For figure3-b, the effects of the magnetic field on diamagnetic susceptibility χ_{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 γ , 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 χ_{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 figure4-a and figure4-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 figure4-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 χ_{dia} increases when the magnetic field

increases and reaches a limit value when the magnetic field becomes very strong. For figure4-b, we

plot the variation of the donor diamagnetic susceptibility χ_{dia} for three different radius values of cylindrical quantum dot ($R_c=1a^*$, $2a^*$ and $R_c = 3a^*$) and $H = 3a$. We can remark that the diamagnetic

susceptibility χ_{dia} increases as CQD radius R_c decreases. The diamagnetic susceptibility is totally insensitive to the increase of the magnetic field for small radius confinement ($R_c=1a^*$). For large radius confinement case ($R_c>2a^*$), 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.

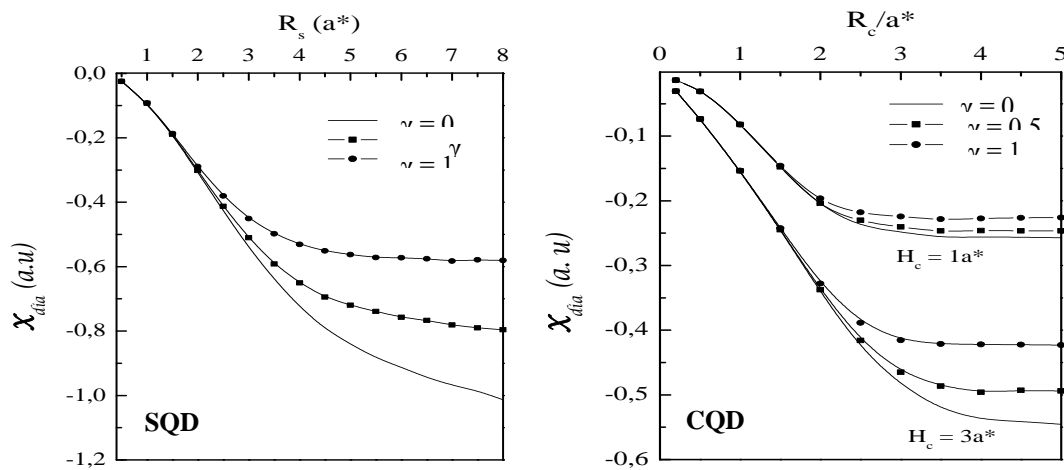


Figure.3 Variations of the diamagnetic susceptibility χ_{dia} as a function of R_s radius of a SQD: (a) and as a function of R_c radius and ($H = 1a^*$ and $H = 3a^*$) of a CQD: (b) for three values of magnetic field ($\gamma = 0, 0.5$ and 1)

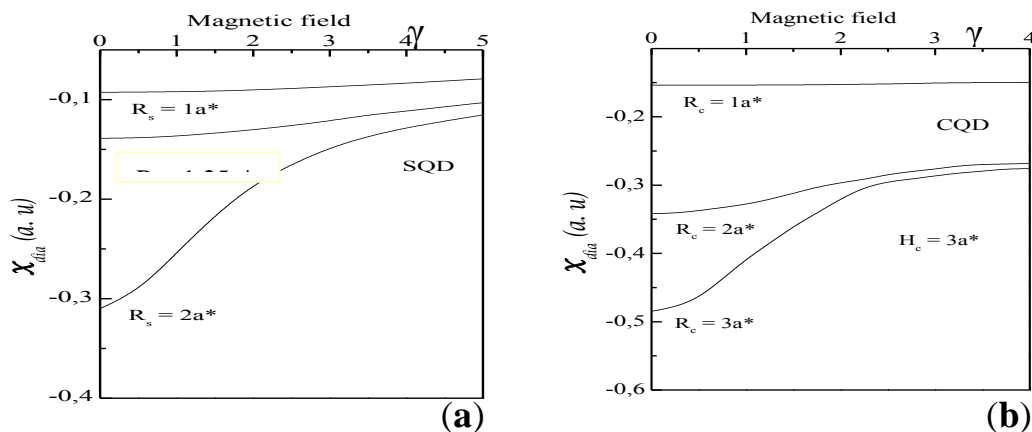


Figure.4 Variation of the diamagnetic susceptibility χ_{dia} function of magnetic field with three

values R_S ($R_S = 1a^*$, $1.25a^*$ and $2a^*$) of a SQD: (a) and with three values radius ($R_c = 1a^*$, $2a^*$ and $3a^*$) and $H_c = 3a^*$ 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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