Magnetic Field Effect on the Diamagnetic Susceptibility of Hydrogenic Donor in Cylindrical Quantum Dot

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The binding energy and diamagnetic susceptibility χ_{dia} are investigated for a shallow donor placed at the centre of a cylindrical quantum dot (CQD) in the presence of a magnetic field. We consider a cylinder of GaAs surrounded by $Al_xGa_{1-x}As$. Using the effective-mass approximation within a variational scheme, binding energy and diamagnetic susceptibility of donor are obtained as a function of the dot size and several values of the magnetic field strength. The result shows that the diamagnetic susceptibility decreases as the CQD radius increases or the magnetic field decreases. The magnetic field is appreciable especially for large CQD while for small CQD the geometrical confinement is predominant.

1. Introduction

With the recent progress in the last years of novel technologies in semiconductor growth, it has become possible to produce high quality many low-dimensional systems such as quantum wells (QW), Quantum Well Wires (QWWs) and Quantum Dots (QD) [1-4]. The low dimensional semiconductor hetero-structures exhibit novel phenomena and it has motivated an increasing interest in the studies of their optical and electronic properties [5,6]. The study of the hydrogenic impurities is one of the main important problems in semiconductor low-dimensional systems, because the presence of the impurity states in this nanostructure influences greatly both the electronic mobility and their optical properties [7-9]. Recently, Erdogan et al. [10] have studied the electric and magnetic field effects on the self-polarization in GaAs/AlAs cylindrical quantum well wires. They have found that the self-polarization decreases with increasing magnetic fields strength. Villamil et al. [11] have reported a calculation of the binding and transition energies for a shallow donor impurity in a cylindrical GaAs–GaAlAs QWWs as a function of the wire radius, the impurity position and an applied magnetic field. They have shown how the geometrical and magnetic confinements compete for the localization of the carrier wave function and their effects in determining the binding energy. Safwan et al. [12] studied the binding energy and stability of charged excitons in semiconductor cylindrical quantum dot. They showed that the negatively charged exciton has higher binding energy than the positively charged exciton when the QD half height is less than the effective Bohr radius (strong confinement regime). While for a large QD, the negatively charged exciton binding energy crosses down the positively charged exciton binding energy and becomes an unstable system. Zounoubi et al. [13] investigated the influence of magnetic field on the binding energy and polarizability of a shallow donor impurity placed at the center of a cylindrical quantum dot (CQD). They have found 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. The diamagnetic susceptibility has reported in Refs. [14,15]. Recently, the diamagnetic susceptibility of a hydrogenic donor placed in Si, Ge and GaAs quantum wells with infinite confinement potential have been reported [16-19]. It has been observed that the diamagnetic susceptibility of the donor in the anisotropic materials converges rapidly to the bulk limit as the well size increases. Rahmani et al. [14] have investigated the diamagnetic susceptibility of a confined donor in $Ga_{1-x}Al_xAs$-GaAs Inhomogenous Quantum Dot. They found that the binding energy and the diamagnetic susceptibility depend strongly on the core and the shell radius, the diamagnetic susceptibility presents a minimum for a critical value of the ratio R_1/ R_2 depending on the value of the outer radius. In previous paper, Mmadi et al. [15] have investigated the diamagnetic susceptibility of a magneto-donor Inhomogeneous Quantum Dots “IQD’’. We have found that the diamagnetic susceptibility increases

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with the magnetic field and is more pronounced for larger spherical layer. Arunachalam et al. [20] have studied the diamagnetic susceptibility in a strained InAs/InP quantum wire. Joseph Sharkey et al. [21] have reported a study on the magnetic field effects on the binding energy and diamagnetic susceptibility of a donor in a GaN/AlGaN quantum dot. They showed that the binding energy and the diamagnetic susceptibility increase with the magnetic field and are more pronounced for large dot. Kilcarslan et al. [22] 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 increases with Nitrogen mole fraction. 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. Recently, Safarpour et al. [24] have calculated the binding energy and diamagnetic susceptibility of hydrogenic donor impurity in a spherical quantum dot placed at the center of a cylindrical nano-wire. Their results show that both the binding energy and diamagnetic susceptibility decrease and reach a minimum value, and then increase as the nanowire radius increases. However, to the best of our knowledge, theoretical or experimental studies on the diamagnetic susceptibility of a shallow donor in a Cylindrical Quantum Dot have not been reported yet. In the present work, we use a variational method to calculate the hydrogenic donor binding energy and the diamagnetic susceptibility in a GaAs/$Ga_{1-x}Al_xAs$ CQD in presence of a magnetic field. This paper is organized as follows: in Sec. 2 we explain the Hamiltonian of hydrogenic impurity ground state in the presence of a magnetic field. We deduce the expression of the binding energy and the diamagnetic susceptibility. The numerical results and discussion are presented in Sec. 3.

2. General Formalism

We consider a cylinder of GaAs of radius R and a length H, surrounded by $Ga_{1-x}Al_xAs$, in the presence of a magnetic field applied along the z-direction, the z-direction is taken as the axis of the dot. In the effective mass approximation, the Hamiltonian is given by

$$H = \frac{1}{2m^*}\left[\vec{p} + \frac{e}{c}\vec{A}\right]^2 - \frac{e^2}{\varepsilon_0\left|\vec{r} - \vec{r}_0\right|} + V(\rho, z) \tag{1}$$

$$\left|\vec{r} - \vec{r}_0\right| = \sqrt{(\rho - \rho_0)^2 + (z - z_0)^2} \tag{2}$$

Where ε_0 is the dielectric constant, m^* is the effective electron mass and r_0 is the impurity position, measured from the center of the cylinder. The z-coordinate gives the relative separation of the electron from the donor impurity along the cylindrical quantum dot. $A(r)$ is the magnetic field potential and $V(\rho, z)$ is the confining potential given by [13]

$$V(\rho, z) = \begin{cases} 0 & for\ \rho < R\ and\ |z| < \dfrac{H}{2} \\ V_0 & for\ \rho > R\ and\ |z| > \dfrac{H}{2} \end{cases} \tag{3}$$

In the present paper, we suppose an infinite confinement potential and we assume a single donor impurity located at the center of the cylindrical quantum dot (i.e., $\rho_0 = 0$ and $z_0 = 0$). For a uniform magnetic field, we can write $A(r) = \frac{1}{2}(B \times r)$, where $B = B\hat{z}$. Choosing the symmetric gauge in the cylindrical coordinates, the magnetic field potential becomes $A = \frac{1}{2}B[0,0,\rho]$.

The Hamiltonian given in Eqn. (1) can be written in cylindrical coordinates and reduced units as

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

Where, the effective Rydberg $R^* = \frac{m^* e^4}{2\hbar^2\varepsilon_0^2}$ is the unit of energy and the effective Bohr radius $a^* = \frac{\hbar^2 \varepsilon_0}{m^* e^2}$ is the length unit. L_z is the z component of the angular momentum operator in units of $\hbar$, $\gamma = \frac{\hbar\omega_c}{2R^*}$ is a dimensionless measure of the magnetic field and $\omega_c = \frac{eB}{m^* c}$ is the effective cyclotron frequency. The trial wave function for the ground-state and energy of the system with the impurity is chosen as [13]

$$\psi(\rho,z)=\begin{cases} N\,J_0\left(\theta_0\,\dfrac{\rho}{R}\right)\cos\left(\dfrac{\pi z}{H}\right)\exp\left(-\left(\dfrac{\rho^2}{8\alpha^2}+\dfrac{z^2}{8\beta^2}\right)\right) & \text{for } \rho\le R \text{ and } |z|\le\dfrac{H}{2} \\ 0 & \text{for } \rho> R \text{ and } |z|>\dfrac{H}{2} \end{cases} \quad (5)$$

Where, J_0 is the Bessel function of zero order; $\theta_0 = 2.4048255577$ 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 variational parameters α and β.

$$\mathrm{E}=\min_{\alpha,\beta}\langle\psi(\rho,z)|H|\psi(\rho,z)\rangle \quad (6)$$

The binding energy E_b of donor is defined by:

$$\mathrm{E}_b=\mathrm{E}_{Sub}-\mathrm{E} \quad (7)$$

Where, E and E_{Sub} represent the state energy of an electron in CQD with and without the impurity, respectively.

The diamagnetic susceptibility χ_{dia} of the donor impurity in CQD, in atomic unit (a.u), is given by [25]

$$\chi_{dia}=-\frac{e^2}{6m^*\varepsilon_0 c^2}<(\vec{r})^2> \quad (8)$$

Where, c is the velocity of light and $<(\vec{r})^2>$ is the mean square distance of the electrons from the nucleus and given as

$$<r^2>=<\rho^2>+<z^2>=\left(\frac{I_3}{I_1}+\frac{J_3}{J_1}\right) \quad (9)$$

The final result on the diamagnetic susceptibility is obtained by numerical minimization of the energy expression with respect to the parameters α and β. The expression of the corresponding energy and the integral elements are given as

$$\mathrm{E}(\alpha,\beta,\gamma)=E_c+E_{coul}+E_m \quad (10)$$

$$E_c=\langle\psi|-\nabla^2|\psi\rangle=\left(\frac{\theta_0}{R}\right)^2+\frac{1}{2\alpha^2}-\frac{1}{2\alpha^2}\frac{\theta_0}{R}\frac{I_2}{I_1}-\frac{1}{16\alpha^4}\frac{I_3}{I_1}$$

$$+\left(\frac{\pi}{H}\right)^2+\frac{1}{4\beta^2}-\frac{\pi}{2H\beta^2}\frac{J_2}{J_1}-\frac{1}{16\beta^4}\frac{J_3}{J_1} \quad (11)$$

$$E_{coul}=\left\langle\psi\left|-\frac{2}{\sqrt{\rho^2+Z^2}}\right|\psi\right\rangle=-2\,\frac{\mathrm{M}_2}{\mathrm{M}_1} \quad (12)$$

$$E_m=\left\langle\psi\left|\frac{\gamma^2}{4}\rho^2+\gamma L_Z\right|\psi\right\rangle=\frac{\gamma^2}{4}\frac{I_3}{I_1} \quad (13)$$

Where the matrix element

$$\langle\psi|\gamma L_Z|\psi\rangle=0 \quad (14)$$

$$I_1=\int_0^R J_0^{\,2}\left(\theta_0\,\frac{\rho}{R}\right)\exp\left(-\left(\frac{\rho^2}{4\alpha^2}\right)\right)\rho\,d\rho \quad (15)$$

$$I_2=\int_0^R J_1\left(\theta_0\,\frac{\rho}{R}\right)J_0\left(\theta_0\,\frac{\rho}{R}\right)\exp\left(-\left(\frac{\rho^2}{4\alpha^2}\right)\right)\rho^2 d\rho \quad (16)$$

$$I_3=\int_0^R J_0^{\,2}\left(\theta_0\,\frac{\rho}{R}\right)\exp\left(-\left(\frac{\rho^2}{4\alpha^2}\right)\right)\rho^3 d\rho \quad (17)$$

$$J_1=\int_0^{H/2} Cos^2\left(\frac{\pi z}{H}\right)\exp\left(-\left(\frac{z^2}{4\beta^2}\right)\right)dz \quad (18)$$

$$J_2=\int_0^{H/2} Sin\left(\frac{\pi z}{H}\right)Cos\left(\frac{\pi z}{H}\right)\exp\left(-\left(\frac{z^2}{4\beta^2}\right)\right)z\,dz \quad (19)$$

$$J_3=\int_0^{H/2} Cos^2\left(\frac{\pi z}{H}\right)\exp\left(-\left(\frac{z^2}{4\beta^2}\right)\right)z^2 dz \quad (20)$$

$$M_1 = \int_0^R \int_0^{H/2} J_0^{\,2}\left(\theta_0 \frac{\rho}{R}\right) Cos^2\left(\frac{\pi z}{H}\right) \exp\left(-\left(\frac{\rho^2}{4\alpha^2}\right)\right) \exp\left(-\left(\frac{z^2}{4\beta^2}\right)\right) \rho d\rho dz \tag{21}$$

$$M_2 = \int_0^R \int_0^{H/2} \frac{\rho}{\sqrt{\rho^2 + z^2}} J_0^{\,2}\left(\theta_0 \frac{\rho}{R}\right) Cos^2\left(\frac{\pi z}{H}\right) \exp\left(-\left(\frac{\rho^2}{4\alpha^2}\right)\right) \exp\left(-\left(\frac{z^2}{4\beta^2}\right)\right) d\rho dz \tag{22}$$

3. Numerical Results and Discussion

We consider a cylindrical quantum dot made out of GaAs surrounded by $Ga_{1-x}Al_xAs$. In Fig.1, we plot the binding energy versus the cylindrical quantum dot radius for different cylindrical lengths (H = 0.1a*, 1a*, 3a* and 20a*) in the zero magnetic case (γ = 0). For a very small dot radius (R < 1a*, strong radial confinement), the binding energy diverge as R/a* → 0 in a several fashion for different cylindrical lengths. For a strong axial confinement (H < 1a*), the divergence is more prominent than in the weak axial confinement case (H > 1a*). The electron is squeezed in smaller volume than in the letter case. For weak radial confinement (R ≥ 3a*) and strong axial confinement (H < 1a*), the binding energy tends to the value of two dimensional hydrogen donor (E_b → 4R*) [26]. While for weak axial confinement (H >> 1a*) the binding energy approaches to the bulk case result, E_b → 1R, namely the Rydberg constant 1R* as confirmed by similar works in literature [13]. While in the case of finite height potential barrier, the binding energy increases with increasing radius of the dot, reaches a maximum value and finally decreases monotonically. We have reported in Fig. 2, the donor binding energy as a function of the dot radius for one value of length ($H = 3a^*$) and for several values of a magnetic field (γ = 0, 1, 3). We can see a competition between the magnetic field effect and the spatial confinement effect. For a very small dot radius (R < 1a*), the binding energy is relatively insensitive to the externally applied magnetic fields. In this region, the magnetic field has no effect on the ground state binding energy. For CQD radius R > 1a*, the curves tend to deviate from each other and reach steady values as the CQD radius increases for any γ values. While the CQD radius becomes very large (R >> 1a*), the ground state binding energy converges to the corresponding bulk values because the electron no longer interacts with the CQD boundary, so the impurity behaves like a free hydrogen atom.

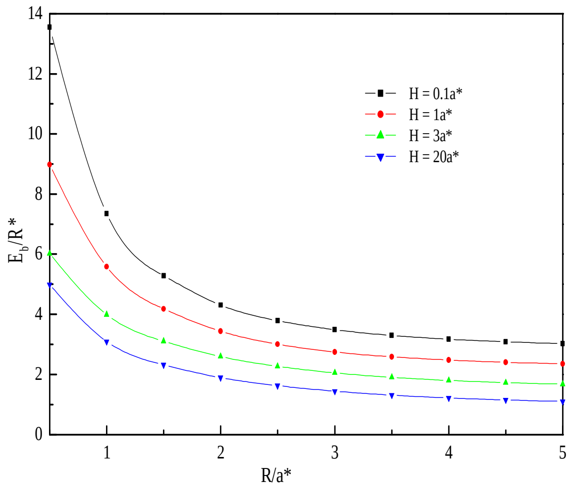

Fig.1: The binding energy as a function of the dot radius for several values of the CQD length (H = 0.1a*, 1a*, 3a* and 20a*).

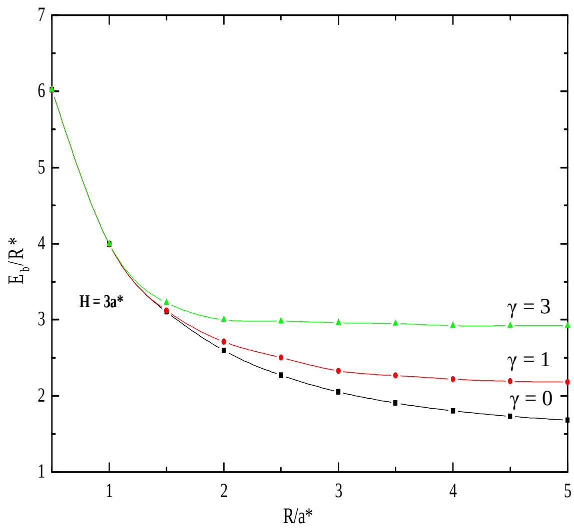

Fig.2: The binding energy as a function of the CQD radius for several values of the magnetic field γ (γ = 0, 1 and 3) with H = 3a*.

In Fig. 3, we plot the variation of the diamagnetic susceptibility χ_{dia} as a function of the CQD radius and for different values of the lengths (H = 1a*, 3a* and 20a*) and for γ = 0. For strong axial confinement (H = 1a*) and weak radial confinement (R >> 1a*), the diamagnetic susceptibility χ_{dia} decreases when the radius dot increases. We remark that the diamagnetic susceptibility χ_{dia} tends to two dimensional value -0.2a.u [19]. Nevertheless, for weak axial confinement (H > 1a*) and weak radial confinement (R > 1a*), we see that the diamagnetic susceptibility decreases with the increase of CQD length. It tends to the three dimensional value (-1.1a.u), which correspond to the bulk limit case (see Refs. [14,15,23]). Also the diamagnetic susceptibility χ_{dia} is more sensitive for large dimensions. We display in Fig. 4, the effect of the magnetic field on diamagnetic susceptibility χ_{dia} as a function of the radius R for different values of magnetic field (γ = 0, 1 and 3) and H = 3a*. For strong radial confinement (R < 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* and γ, the diamagnetic susceptibility increases when the length of the dot decreases. This reflects an increasing confinement. We present in Fig. 5 the variation of $\langle r^2 \rangle$ as a function of CQD radius R for several magnetic field values (γ = 0, 1 and 3) and (H = 1a* and 3a*). We can see that the mean value of $\langle r^2 \rangle$ increases when the CQD radius increases. The main reason for this behaviour is the spread out of electron wave function with increasing cylindrical quantum dot dimension. Also, we show that for two values (H = 1a* and 3a*), the field induced an additional geometric confinement, the electron wave function is more concentrated around the donor impurity and therefore $\langle r^2 \rangle$ decreases when the magnetic field γ increases. This result explains that in the presence of the magnetic field, the diamagnetic susceptibility χ_{dia} and $\langle r^2 \rangle$ remain constant over a large dot [15,23].

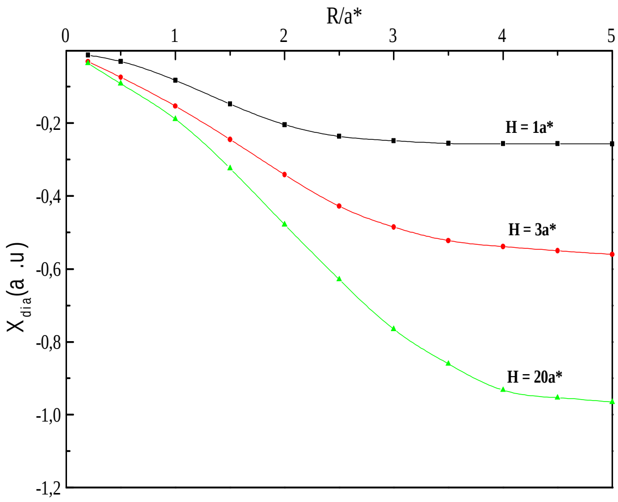

Fig.3: The variation of the diamagnetic susceptibility as function the CQD radius for three values of the length (H = 1a*, 3a* and 20a*.

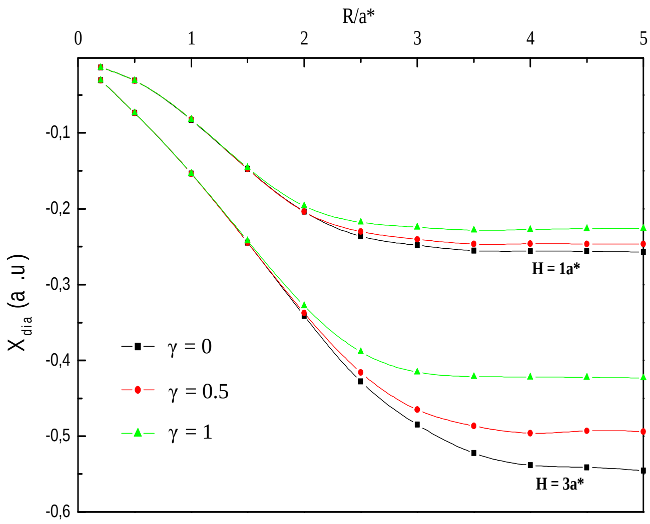

Fig.4: The variation of the diamagnetic susceptibility as function of the CQD radius for three values of the magnetic field γ (γ = 0, 1 and 3) with H = 1a* and H = 3a*.

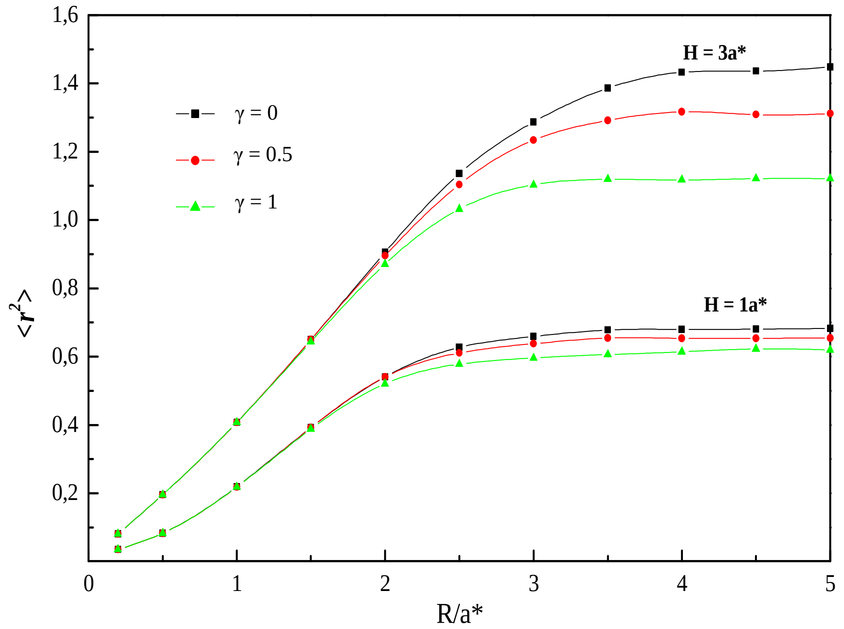

Fig.5: The variation of < r^2> as function of the CQD radius for several values of the magnetic field γ (γ = 0, 1 and 3) with H = 1a* and H = 3a*.

We present in Fig. 6, the diamagnetic susceptibility χ_{dia} as a function of the CQD length for two different radius (R = 1a* and 3a*). For small CQD R = 1a* (strong confinement regime) the magnetic field effect is not appreciable and the geometric confinement is predominate. While for large dot, R_2 = 3a* (weak confinement regime), the effect of the magnetic field on the susceptibility is more appreciable and the susceptibility increases with the magnetic field. We remark that the diamagnetic susceptibility χ_{dia} decreases as the CQD length H increases, it reflects the increasing confinement. Also in the absence of magnetic field, the χ_{dia} approaches to the three dimensional value ($\chi_{dia} \rightarrow$-1.1a.u) [14,15,23]. We give in Fig. 7, the variation of the donor diamagnetic susceptibility χ_{dia} as a function of the magnetic field for three different radius values of cylindrical quantum dot (R = 1a*, 2a*and R = 3a*) and H = 3a. We can see that χ_{dia} the diamagnetic susceptibility increases as CQD radius decreases. The diamagnetic susceptibility is totally insensitive to an increase of the magnetic field for small radius confinement (R = 1a*); for large radius confinement case (R > 2a*), the variation of the diamagnetic susceptibility is much more pronounced due to the stronger confinement effect of the magnetic field and the spatial confinement. It is clearly seen that the diamagnetic susceptibility decrease as the CQD radius increases or the magnetic field strength decreases.

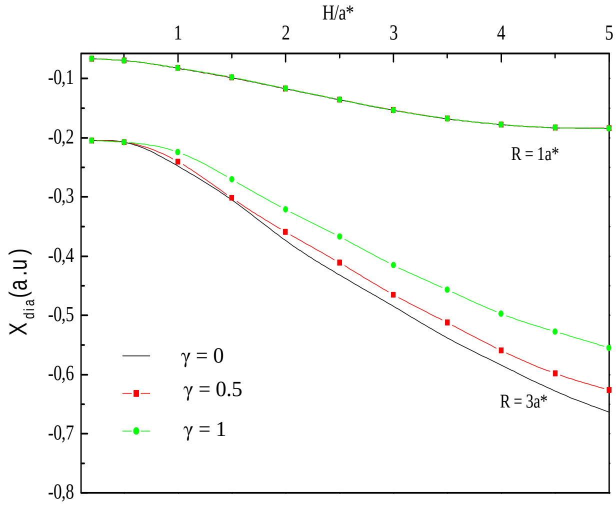

Fig.6: The variation of the diamagnetic susceptibility as function the length H for several values of the magnetic field (γ = 0, 0.5 and 1) with R = 1a* and R = 3a*.

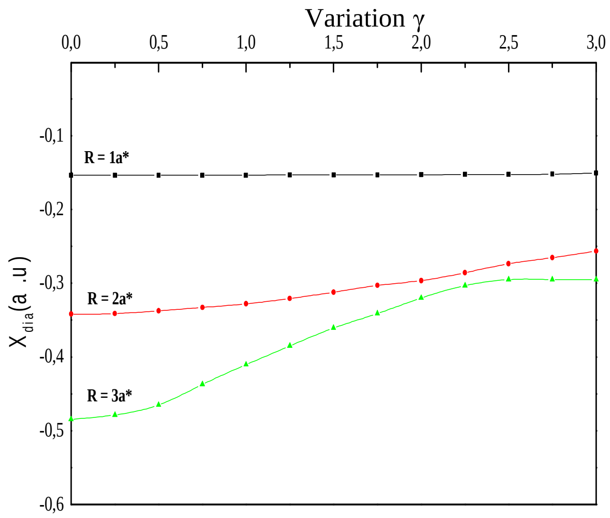

Fig.7: Variation of the diamagnetic susceptibility χ_{dia} function of magnetic field for three values radius (R = 1a*, R = 2a* and R = 3a*) for H = 3a*.

4. Conclusion

In this study, we have calculated the effects of a magnetic field on the diamagnetic susceptibility for ground state in an infinite cylindrical quantum dot. The calculations have been performed within the effective mass approximation by using the variational method. We have found that the diamagnetic susceptibility of the donor depends on the geometrical confinement and magnetic field. The magnetic field effect on the diamagnetic susceptibility is appreciable especially for large structures. Unfortunately, we could not compare our results as no explicit experimental data are available in the literature. The present model can be improved by including other relevant effects such as finite band offsets, which will be treated in a future work.

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