THE EFFECTS OF PRESSURE AND TEMPERATURE ON THE MAGNETIZATION OF A PARABOLIC QUANTUM DOT IN A MAGNETIC FIELD

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Received:14th November 2016 Revised: 11th December 2017 Accepted:12th March 2018
DOI: https://doi.org/10.22452/mjs.vol37no2.3

ABSTRACT In this work , we present a theoretical study of the magnetization of two-electron GaAs parabolic quantum dot (QD) under the combined effects of external pressure, temperature and magnetic field. First, we obtain the eigenenergies by solving the two electron quantum dot Hamiltonian using the exact diagonalization method. The obtained results show that the energy levels of the quantum dot depend strongly on the pressure and temperature. Next, we investigate the dependence of magnetization of a quantum dot as a function of external pressure, temperature, confining frequency and magnetic field. The singlet-triplet transitions in the ground state of the quantum dot spectra and the corresponding jumps in the magnetization curves have been shown .The comparison shows that our results are in very good agreement with the reported works.

PACS: 73.21.La, 65.80.-g

Keywords: Pressure; temperature; magnetization; quantum dot; magnetic field; exact diagonalization.

INTRODUCTION

Quantum dots (QDs), or artificial atoms, are the subject of interest research due to their physical properties and great potential device applications such as quantum dot lasers, solar cells, single electron transistors and quantum computers (Ashoori et al, 1993 ;Ciftja ,2013; Kastner , 1992 ; Burkard et al ,1999). The application of a magnetic field perpendicular to the dot plane will introduce an additional structure on the energy levels and correlation effects of the interacting electrons that are confined in a quantum dot. Different approaches were used to solve the two electrons QD Hamiltonian, including the effect of an applied magnetic field, to obtain the eigenenergies and eigenstates of the QD-system. Wagner et al. (1992) studied this interesting QD system and predicted the oscillations between spin-singlet (S) and spin-triplet (T) ground states.

Taut (1994) managed to obtain the exact analytical results for the energy spectrum of two interacting electrons through a coulomb potential, confined in a QD, just for particular values of the magnetic field strength. In references (Ciftja and Kumar , 2004 ; Ciftja and Golam Farouk , 2005) the authors solved the QD-Hamiltonian by variational method and obtained the ground state energies for various values of magnetic field(ω_c) and confined frequency(ω_0). In addition, they performed exact numerical diagonalization for the Helium QD-Hamiltonian and obtained the energy spectra for zero and finite values of magnetic field strength. Kandemir (2005) found the closed form solution for this QD Hamiltonian and the corresponding eigenstates for particular values of the magnetic field strength and confinement frequencies. Elsaid (2000 ; 2006) solved the QD-Hamiltonian by the dimensional expansion technique and obtained the energies of the two interacting electrons for any arbitrary ratio of coulomb to confinement energies and gave an explanation to the level crossings.

Maksym and Chakraborty (1990) used the diagonalization method to obtain the eigenenergies of interacting electrons in a magnetic field and show the transitions in the angular momentum of the ground states. They calculated the heat capacity curve for both interacting and non-interacting confined electrons in the QD presented in a magnetic field. The interacting model showed very different behavior from non-interacting electrons, and the oscillations in these magnetic and thermodynamic quantities like magnetization $(\mathcal{M})$ and heat capacity (C_v)were attributed to the spin singlet-triplet transitions in the ground state spectra of the quantum dot. De Groote, Hornos and Chaplik (1992) also calculated the magnetization, susceptibility and heat capacity of helium like confined QDs and obtained the additional structure in magnetization. In a detailed study, Nguyen and Peeters (2008) considered the QD in the presence of a single magnetic ion and applied magnetic field taking into account the electron-electron correlation in many electron quantum dot. They displayed the dependence of these thermal and magnetic quantities: $C_v, \mathcal{M}$ and χ on the strength of the magnetic field, confinement frequency, magnetic ion position and temperature. They observed that the cusps in the energy levels show up as peaks in the heat capacity and magnetization. Nammas et al. (2011) used the static fluctuation approximation (SFA) to study the thermodynamic properties of two dimensional GaAs/AlGaAs parabolic QD in a magnetic field.

Boyacioglu and Chatterjee (2012) studied the magnetic properties of a single quantum dot confined with a Gaussian potential model. They observed that the magnetization curve shows peaks structure at low temperature. In a recent work , Boda et al.,(2016) had considered the effect of Rashba spin-orbit interaction on the magnetic properties of a one-electron

Gaussian quantum dot in the presence of a magnetic field. Helle, Harju and Nieminen (2015) computed the magnetization of a rectangular QD in high magnetic field and the results showed the oscillation and smooth behavior in the magnetization curve for both, nteracting and non-interacting confined electrons, respectively.

In an experimental work , (Schwarz et al,2002), the magnetization of electrons in GaAs/AlGaAs semiconductor QD as function of applied magnetic field at low temperature 0.3 K had been measured. They had observed oscillations in the magnetization .To reproduce the experimental results of the magnetization, they found that the electron-electron interaction should be taken into account in the theoretical model of the QD magnetization. Furthermore, the density functional theory method (DFT) had been used to investigate the magnetization of a rectangular QD in the applied magnetic field (Rasanen et al.,2003). Climente et al. (2004) studied the effect of Coulomb interaction on the magnetization of quantum dot with one and two interacting electrons. The effects of pressure and temperature on the electronic and optical properties of a quantum dot presented in external magnetic and electric fields had been considered very recently by many authors (Rezaei and Kish , 2012) .

The authors presented a systematic study of the thermodynamic property , namely magnetization of two-electron system confined in parabolic potential in two-dimensional(2D) quantum dot (exemplified by GaAs).The system was treated using the quantum mechanical framework used for helium atom (two electron system) with non-interacting as well interacting electrons. The effects of pressure (P) and temperature (T) in the presence of magnetic field (in perpendicular direction to QD plane) on the magnetization are described through analysis and numerical solution. The effect of pressure and temperature we incorporated through dielectric constant and the effective electron mass. This procedure is an appropriate one as the experimental studies are interested in manipulating these (P,T) parameters to understand the dynamics of charge carriers in quantum dots. The present study is thus useful for validating experimental work aiming to characterize QD in magnetic field with respected to applied pressure and temperature variations. Schrodinger equation is solved for to theoretical study of the magnetization of two-electron GaAs parabolic quantum dot under the combined effects of external pressure , temperature and magnetic field. Energy eigenvalues are obtained by using the exact diagonalization method. The effects of external pressure , temperature and magnetic field are expressed by plotting some graphics.

The rest of this paper is organized as follows: section II presents the Hamiltonian theory and computation diagonalization technique of the interacting quantum helium atom. In section III, we show the numerical results of the magnetization from the mean energy expression. Conclusions are given in the final section .

THEORY

In this section we describe in detail the main two parts of the theory, namely: quantum dot Hamiltonian and exact diagonalization method .

Quantum dot Hamiltonian

The effective mass Hamiltonian for two interacting electrons confined in a QD by a parabolic potential in a uniform magnetic field $\vec{B} = B\,\hat{k}$ can be written in a separable form as:

$$\widehat{H} = \widehat{H}_{\mathrm{CM}} + \widehat{H}_{\mathrm{r}} \tag{1}$$

$$\widehat{H}_{\mathrm{CM}} = \frac{1}{2\mathrm{M}}\left[\vec{\mathrm{P}}_{\mathrm{R}} + \frac{\mathrm{Q}}{\mathrm{c}}\vec{\mathrm{A}}\left(\vec{\mathrm{R}}\right)\right]^2 + \frac{1}{2}\mathrm{M}\omega_0^2\mathrm{R}^2 \tag{2}$$

$$\widehat{H}_{\mathrm{r}} = \frac{1}{2\mu}\left[\vec{\mathrm{p}}_{\mathrm{r}} + \frac{\mathrm{q}}{\mathrm{c}}\vec{\mathrm{A}}(\vec{\mathrm{r}})\right]^2 + \frac{1}{2}\mu\omega_0^2\mathrm{r}^2 + \frac{\mathrm{e}^2}{\epsilon|\vec{\mathrm{r}}|} \tag{3}$$

Where ω_0, $\mu = \frac{m^*}{2}$ and ϵ are defined as the confining frequency, reduced mass and the dielectric constant for the GaAs medium, respectively. $\vec{R} = \frac{\vec{r_1}+\vec{r_2}}{2}$ and $\vec{r} = \vec{r_2} - \vec{r_1}$ are the center of mass and relative coordinates, respectively. $\omega_c = \frac{eB}{m^*}$ is the cyclotron frequency and $\mathbf{A} = \frac{1}{2}\mathbf{B} \times \mathbf{r}$ is the vector potential.

The corresponding energy of this Hamiltonian equation (1) is:

$$E_{total} = E_{CM} + E_r \tag{4}$$

The center of mass Hamiltonian given by equation (2) is a harmonic oscillator type with well-known eigenenergies:

$$E_{cm} = \mathrm{E}_{\mathrm{n_{cm}},\mathrm{m_{cm}}} = (2\mathrm{n_{cm}} + |\mathrm{m_{cm}}| + 1)\hbar\,\omega + \mathrm{m_{cm}}\frac{\hbar\omega_c}{2} \tag{5}$$

where n_{cm}, m_{cm} and $\omega = \sqrt{\frac{\omega_c^2}{4} + \omega_0^2}$ are the radial , angular quantum numbers and effective confining frequency, respectively.

However, the relative motion Hamiltonian part (H_r), given by equation (3) does not have an analytical solution for all ranges of ω_0 and ω_c. In this work, we applied the exact diagonalization method to solve the relative part of the Hamiltonian and obtaine the corresponding eigenenergies E_r.

Exact diagonalization method

For non-interacting case the relative Hamiltonian in equation (3) is a single particle problem with eigenstates $| n_r m_r >$ (Ciftja and Kumar , 2004 ; Ciftja and Golam Farouk , 2005) :

$$|n_r m_r\rangle = N_{n_r m_r} \frac{e^{i m_r \phi}}{\sqrt{2\pi}} (\alpha r)^{|m_r|} e^{-\alpha^2 r^2/2} L_{n_r}^{|m_r|}(\alpha^2 r^2) \quad (6)$$

where the functions $L_{n_r}^{|m_r|}(\alpha^2 r^2)$ are the standard associated Laguerre polynomials . We calculated the normalization constant $N_{n_r m_r}$ from the normalization condition of the basis, $< n_r m_r | n_r m_r >= 1$, which resulted in

$$N_{n_r m_r} = \sqrt{\frac{2 n_r! \alpha^2}{(n_r + |m_r|)!}} \quad (7)$$

We used α as a constant which has the dimensionality of an inverse length

$$\alpha = \sqrt{\frac{m\omega}{h}} \quad (8)$$

The eigenenergies of the QD Hamiltonian which are given by equation (4) consist of the sum of the energies for the center of mass Hamiltonian (E_{cm}) and the eigenenergies(E_r)which are obtained by direct diagonalization to the relative Hamiltonian part. For interacting case, we applied the exact diagonalization method to solve equation (3) and find the corresponding exact eigenenergies for arbitrary values of ω_c and ω_0.

We can write the matrix element of the relative Hamiltonian part using the basis $|n_r m_r>$as,

$$h_{nn'} = \langle n_r, m_r|\hat{H}_r|n'_r, m_r\rangle =< n_r m_r| \; -\frac{\hbar^2}{2\mu}\nabla^2 + \frac{1}{2}\; \mu\,\omega^2 r^2 \; |n'_r m_r > +$$

$$< n_r m_r| \; \frac{e^2}{\epsilon \vec{r}} \; | n'_r m_r >. \qquad (9)$$

The first term in the right side of equation (9) is diagonalized as,

$$[(2n + |m_z| + 1)\sqrt{(1+\frac{\gamma^2}{4})} - \frac{\gamma}{2}\,|\,m_z\,|\,]\,\delta_{nn'} \qquad (10)$$

Where the Coulomb matrix energy can be given as

$$\frac{\lambda}{\sqrt{2}}\sqrt{\frac{n'!n!}{(n'+|m_z|)!\,(n+|m_z|)!}} \times I_{nn'}\,|m_z\,| \qquad (11)$$

where $\gamma = \frac{\omega_c}{\omega_0}$ and $\lambda = \frac{\mathbf{e^2\alpha}}{\hbar\omega}$ are dimensionless parameters while $\omega^2 = 1 + \frac{\gamma^2}{4}$ is the effective confining frequency . By changing the coordinate transformation to t-variable by direct substitution of $r = \frac{\sqrt{t}}{\alpha}$ in the integration$I_{nn'} = I_{n_r n'_r}$, we can express the Coulomb energy matrix element into the integral form:

$$< n_r m_r| \; \frac{e^2}{\epsilon r} \; |n'_r m_r > \propto \; I_{nn'|m_z|} = \int_0^\infty dt \; t^{|m_z|} e^{-t} L_n^{|m_z|}(t) L_{n'}^{|m_z|}(t) \frac{1}{\sqrt{t}} \; . \qquad (12)$$

We evaluated the above Coulomb energy matrix element in a closed form by using the Laguerre relation given in the Appendix A (Nguyen and Das Sarma , 2011).

This closed form result of the Coulomb energy reduces greatly the computation time needed in the diagonalization process.

In our calculation, we used the basis $| \; n_r m_r >$ defined by equation (6) to diagonalize the relative QD Hamiltonian and obtain its corresponding eigenenergies E_r.

To include the effect of the pressure (P) and temperature (T) on the QD energy states and the magnetization we replace the dielectric constant ϵ with $\epsilon_r\ (P,T)$ and the effective mass m^* with $m(P,T)$ in the QD Hamiltonian as defined by Equations 2 and 3 ,where $\epsilon_r(P,T)$ and $m^*(P,T)$ are the pressure and temperature dependent dielectric constant and electron effective mass, respectively. These pressure and temperature dependent mass parameters should be included in the energy spectrum Eq.4 and the wave functions basis eq.6 of the Hamiltonian. For quantum dot made of GaAs the dependency of $\epsilon_r(P,T)$ and $m^*(P,T)$ are given in Appendix B (Rezaei and Kish , 2012) .

The pressure and temperature effective Rydberg ($R_y^*(P,T)$) is used as the energy unit and given as follows:

$$R_y^*(P,T) = \frac{e^2}{2\epsilon(P,T)a_B^*(P,T)} \tag{13}$$

where $a_B^*(P,T)$ is the effective Bohr radius and given as:

$$a_B^*(P,T) = \epsilon(P,T)\hbar^2/(m^*(P,T)e^2) \tag{14}$$

So the effective Rydberg can be written as:

$$R_y^*(P,T) = \frac{e^4 m^*(P,T)}{2\big(\epsilon(P,T)\big)^2\hbar^2} \tag{15}$$

The pressure and temperature values will be changed to study the effects on the ground state energy of the QD Hamiltonian in a zero ($\omega_c = 0$) and finite magnetic field (ω_c). Eventually, the ground state energies of the two electron-quantum dot system will be calculated as function of temperature (T), pressure (P), confining frequency (ω_0) and magnetic field cyclotron frequency (ω_c).The obtained numerical results are displayed in the next section.

RESULTS AND DISCUSSIONS

We present the effects of pressure, temperature , confining frequency and magnetic field cyclotron frequency on the magnetization of two interacting electrons in a quantum dot made from GaAs material (effective Rydberg R*$= 5.825\ meV$) in Figures 1 to 6 and Tables I . To achieve our aim, it is essential, as a first step, to investigate the dependence of the QD energy levels on the pressure and temperature. In Figure 1, we display the dependence of the QD energy states (m=0,1,2,3 and 4) on the magnetic field , ω_c, for pressure P=10Kbar and temperature T=0.0K. We found that the overall shape of the spectra of the QD remains the same while the eigenenergies are enhanced under the effect of external pressure. For zero magnetic field case , we have tested in Table 1 , the computed numerical results against the corresponding ones produced by Ciftja and Kumar (2004) . Furthermore, we also compared our energies calculated by exact diagonalization method ,in this case for finite magnetic field , against the energy results of analytical variational method (Figure 1 of Dybalski and Hawrylak (2005)) .The comparisons give excellent agreement between the energy spectra of two-electron QD Hamiltonian solved by different methods. The QD spectra shows transitions in the ground state angular momentum (m) as the magnetic field increases. For example , we observed the first transitions in the angular momentum of the ground state of the QD system , from m=0 to m=1 , occurs at $\omega_c \approx 0.8\, R^*$ while the second transition (from m=1 to m=2) occurs at $\omega_c \approx 1.2\, R^*$. These transitions show themselves as cusps in the presented QD-magnetization curves. Figure 2, displays the energies of the quantum dot state (m=0) against the magnetic field for pressure of values: P = 0, 10, 20 and 30 Kbar and Temperature T=0.0. The figure clearly shows an enhancement in the energy level as the pressure increases while the magnetic field is kept unchanged. Similarly, we have investigated , in Figure 3 ,the effect of temperature on the energy levels of the quantum dot by changing the temperature for a wide range : T=0 K, 150 K and 350 K for no external pressure , P= 0.0 Kbar . For fixed values of the magnetic field and pressure, the QD energy level decreases as the temperature increases. Next we show the dependence of the magnetization of the QD on the pressure, temperature and magnetic field. We calculated the magnetization (M) defined by: $M = -\frac{\partial\langle E\rangle}{\partial B}$, where $< E(\omega_0, \omega_c\,, P, T) >$ is the statistical average energy of the quantum dot system.

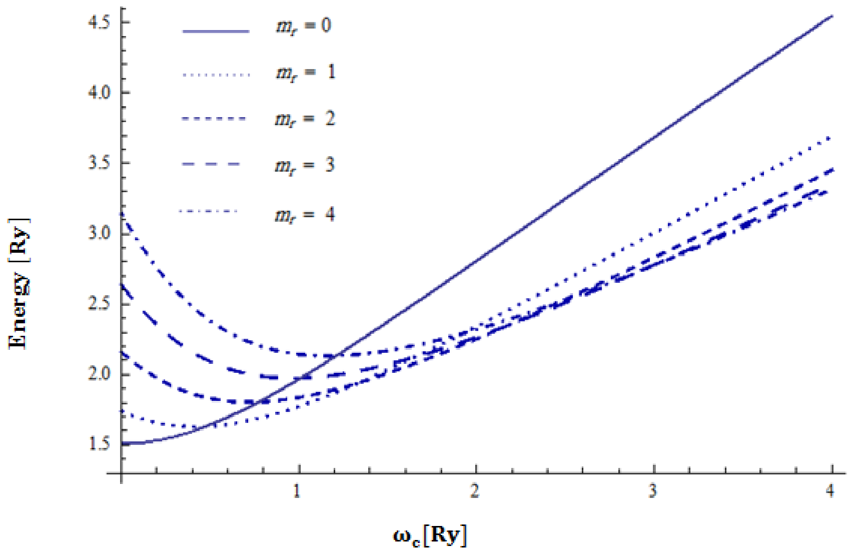

Figure 1: The computed energy spectra of quantum dot versus the strength of the magnetic field for $\omega_0 = 0.5R^*$, T=0K, P=10Kbar and angular momentum m = 0,1,2,3,4.

Table 1: The ground state energies of QD (in R^*) as a function of dimensionless coulomb coupling parameter $\boldsymbol{\lambda}$ obtained from exact diagonalization method (second column) compared with reported work (third column) , (Ciftja and Golam Faruk , 2005).

$\boldsymbol{\lambda}$	E (Present work)	E(Ciftja and Golam Faruk , 2005))
0	2.00000	2.00000
1	3.000969	3.00097
2	3.721433	3.72143
3	4.318718	4.31872
4	4.847800	4.84780
5	5.332238	5.33224
6	5.784291	5.78429
7	6.211285	6.21129
8	6.618042	6.61804
9	7.007949	7.00795
10	7.383507	7.38351

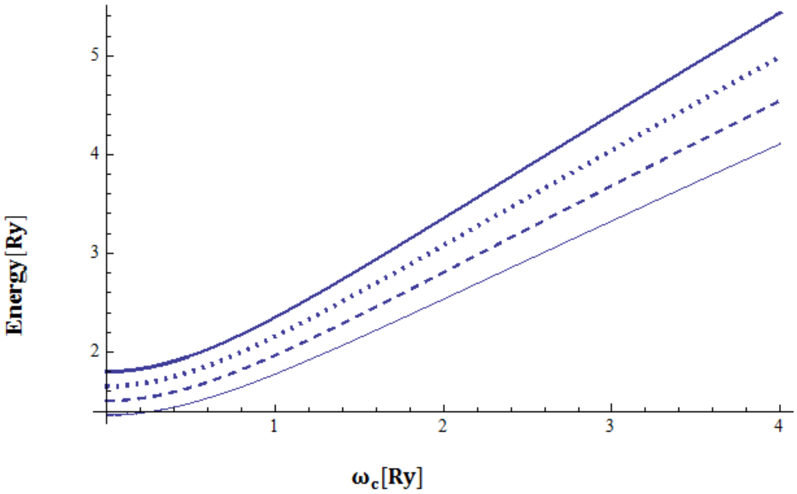

Figure 2: The computed energy spectra of quantum dot versus the strength of the magnetic field for $\omega_0 = 0.5R^*$, T=0K, m=0 and various pressures (P=0 Kbar ,solid; P=10Kbar ,dashed; P=20Kbar, dotted and P=30Kbar, thick).

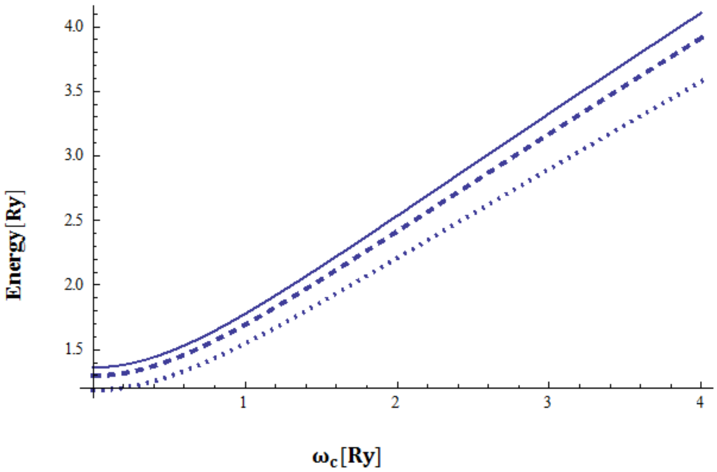

Figure 3: The energy of the quantum dot system versus the magnetic field strength for $\omega_0 = 0.5$ R* , P = 0 Kbar, m = 0 and various temperatures(T = 0 K, solid, T = 150 K , dashed and T = 350 K, dotted)

Figure 4 shows the effect of the pressure on the dependence of the magnetization on magnetic field . The magnetization curves are given for various values of pressure: P=0 kbar, 10 kbar , 20 kbar and 30kbar calculated at temperature T=.01 K and confining energy frequency $\omega_0 = 0.5\, R^*$. For example the magnetization changes approximately from $M/\mu_B =$

$-18\ (at\ P = 0.0\ Kbar\ )\ to\ {}^{M}/_{\mu_B} = -26\ (at\ P = 3\ Kbar)$ for $\omega_c = 4R^*$ .In the same manner , we show , in Figure 5 , the effect of temperature on the QD magnetization curve by changing the temperature ,T = 0.01K , 1K and 5 K for no external pressure (P=0.0 Kbar) and the same confining frequency , $\omega_c = 0.5R^*$. The magnetization curve shows again a significant temperature dependence. We can clearly see the great reduction in the height of magnetization jumps as the temperature increases. For T=5K the jumps disappear and the magnetization shows almost a smooth behavior curve . Furthermore, we study , in Figure 6 ,the effect of confining frequency ω_0 on the shape of the magnetization curve . We consider different values of confining frequencies: $\omega_0 = 0.5\ , 0.67\ and\ 0.8\ R^*$ keeping the temperature and the pressure parameters both are unchanged: P=0.0 kbar and T=0.01 K. The magnetization curves obviously show a significant confining frequency dependence. As we increase the confining frequency , ω_0 , the jumps or the peaks shift to the right. This means that more confining magnetic energy or high magnetic field strength field is needed to make the first transition in the angular momentum of QD ground state , for example : (m=0 to m=1 transition) .These transitions are studied intensively and that the origin of these transitions is found to be due to the effect of coulomb interaction energy in the QD Hamiltonian. These transitions in the angular momentum of the QD system correspond to the (S-T) transitions and manifest themselves as cusps in the magnetization curve of the QD, as we discussed previously.

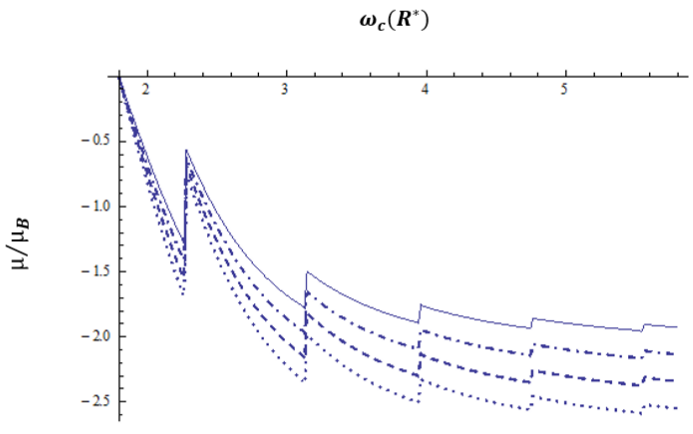

Figure 4: The behavior of the magnetization (${}^{M}/_{\mu_B}$) of the two electrons quantum dot as function of magnetic field strength for fixed value of confining frequency ($\omega_0 = 0.5$

R*) temperature T=0.01 K and various pressures (P=0 Kbar ,solid; P=10Kbar, dot-dashed; P=20Kbar , dashed and P=30Kbar ,dotted).

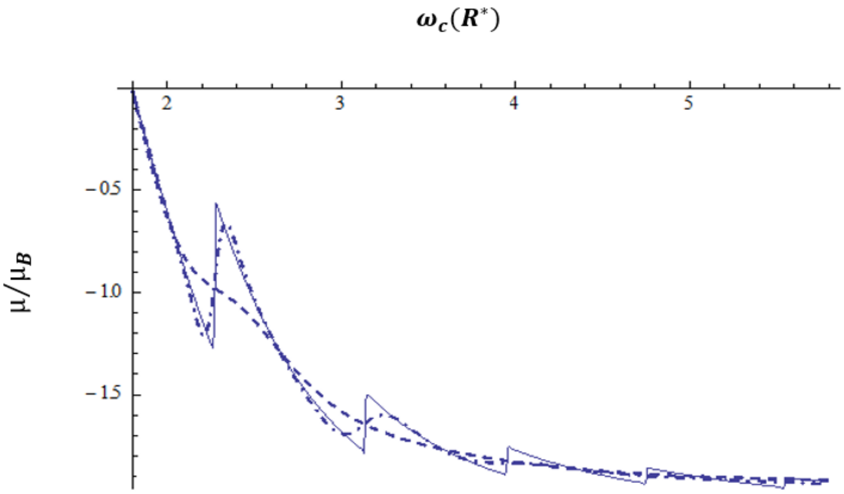

Figure 5: The magnetization (M/μ_B) of the quantum dot as function of magnetic field strength for fixed value of confining frequency (ω_0 = 0.5 R*) , pressure P=0 Kbar and various temperature (T=0.01K,solid; T=1K ,dot-dashed and T=5K ,dashed).

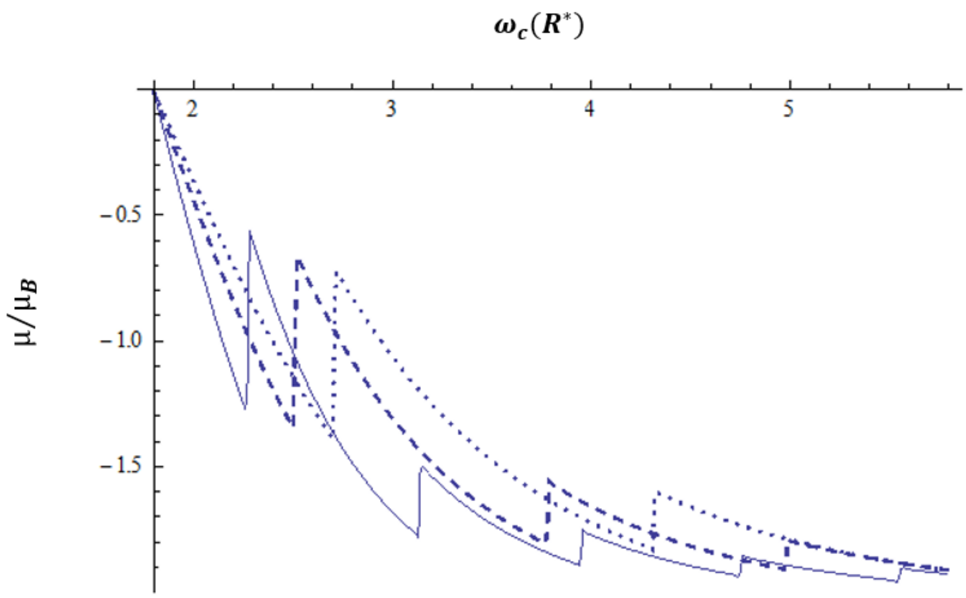

Figure 6: The dependence of the magnetization (M/μ_B) of the quantum dot on the magnetic field strength for fixed temperature (T=0.01K) , pressure (P=0 Kbar) and various confining frequencies (ω_0 = 0.5 R*, solid; ω_0 = 0.67 R*,dashed and ω_0 = 0.8 R*, dotted).

CONCLUSION

In conclusion, we have investigated the effects of external pressure, temperature and confining frequency on the magnetization curve of the QD as a function of magnetic field. The magnetization, as a thermodynamic quantity, shows a significant dependence on these quantum dot parameters .We apply the exact diagonalization method to solve the two electron-QD Hamiltonian. The comparison show that our results are in excellent agreement with other reported works.

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APPENDIX A: PROPERTIES OF THE LAGUERRE POLYNOMIALS

The following Laguerre relation was used to evaluate the Coulomb energy matrix element in a closed form:

$$\int_0^\infty t^{\alpha-1} e^{-pt} L_m^\lambda(at) L_n^\beta(bt) dt =$$

$$\frac{\Gamma(\alpha)(\lambda+1)_m(\beta+1)_n p^{-\alpha}}{m!n!} \sum_{j=0}^{m} \frac{(-m)_j(\alpha)_j}{(\lambda+1)_j\, j!} \left(\frac{a}{p}\right)^j \sum_{k=0}^{n} \frac{(-n)_k(\alpha+j)_k}{(\beta+1)_k\, k!} \left(\frac{b}{p}\right)^k \quad \text{(A 1)}$$

APPENDIX B: THE PRESSURE AND TEMPERATURE DEPENDENT DIELECTRIC CONSTANT AND ELECTRON EFFECTIVE MASS.

$$\epsilon_r\,(P,T) = \begin{cases} 12.74\exp(-1.73\times10^{-3}P)\exp[9.4\times10^{-5}(T-75.6)] \text{ for T} < 200 \text{ K} \\ 13.18\exp(-1.73\times10^{-3}P)\exp[20.4\times10^{-5}(T-300)] \text{ forT} \geq 200 \text{ K} \end{cases} \quad \text{(B 1)}$$

$$m^*(P,T) = \left[1 + 7.51\left(\frac{2}{E_g^\Gamma(P,T)} + \frac{1}{E_g^\Gamma(P,T)+0.341}\right)\right]^{-1} m_0 \quad \text{(B 2)}$$

$$E_g^\Gamma(P,T) = \left[1.519 - 5.405\times10^{-4}\frac{T^2}{T+204}\right] + bP + cP^2 \quad \text{(B 3)}$$

Where $m_0$is the free electron mass, $E_g^\Gamma(P,T)$ is the pressure and temperature dependent energy band gap for GaAs quantum dots at Γ point, b= 1.26× 10^{-1}eV $GPa^{-1}$and c = -3.77× 10^{-3}eV GPa^{-2}.