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ARTICLE

# Magnetization and Magnetic Susceptibility of GaAs Quantum Dot with Gaussian Confinement in Applied Magnetic Field

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**Abstract:** We present a theoretical study of the magnetization (M) and the magnetic susceptibility (χ) of single electron Gaussian quantum dot (GQD) presented in a magnetic field. We solve the Hamiltonian of this system including the spin by using exact diagonalization method. All the energy matrix elements are obtained in closed analytic form. We investigate the effects of temperature, magnetic field and confining potential depth on the behavior of magnetization and magnetic susceptibility of the quantum dot. Comparisons show that our results are in very good agreement with reported works.
**Keywords:** Gaussian quantum dot, Magnetic field, Exact diagonalization method, Magnetization, Magnetic susceptibility.
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## 1. Introduction

The study of quantum dot (QD) structures has received great attention in recent years due to their physical properties and great potential device applications, such as quantum dot lasers, solar cells, single electron transistors and quantum computers [1- 5]. The introduction of a magnetic field perpendicular to the dot plane introduces an additional structure on the energy levels and correlation effects of the interacting electrons confined in a quantum dot.

Different authors had solved the QD Hamiltonian with parabolic potentials by using analytical and various numerical methods [6-18]. The Gaussian potential has been proved to be an effective potential in many branches of physics. It has been solved approximately for a single particle problem by many authors [19-27]. The exact diagonalization and variational methods have been used to study the electronic, thermodynamic and magnetic properties of single and coupled QDs [28-35].

The purposes of this work are: first, to calculate the statistical energy <E> of a single electron confined in a Gaussian quantum dot (GQD) by solving the QD Hamiltonian using exact diagonalization method; second, the obtained statistical energy will be used to investigate the dependence of magnetization (M) and magnetic susceptibility (χ), as thermodynamic quantities, on magnetic field strength (B), temperature (T) and confining potential depth ($V_0$), taking into account the presence of the spin (S).

The structure of this paper is organized as follows: the Hamiltonian theory and computation method of a single electron in GQD are presented in section 2. In section 3, we show how to calculate magnetization and magnetic susceptibility from the mean energy expression. The final section is devoted to numerical results and discussion.

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## 2. Theory

The theory in this research consists mainly of three main parts: the two-dimensional (2D) Hamiltonian model, the exact diagonalization technique and the calculation of magnetic properties, such as statistical energy, magnetization and magnetic susceptibility.

**Quantum Dot Hamiltonian**

The Hamiltonian of a single electron system in an external magnetic field with the presence of Gaussian confinement potential is given as:

$$\hat{H} = \frac{1}{2m^*}\left(\vec{P} + \frac{e}{c}\vec{A}\right)^2 + V(\vec{\rho}) \tag{1}$$

where $\vec{\rho}$ refers to the position vector of an electron, $\vec{P}$ is the momentum operator, m* is the electron effective mass and $\vec{A}$ is the vector potential corresponding to the applied magnetic field $\vec{B}$ along z-direction including the spin Zeeman term. The magnetic field is given by $\vec{B}=\vec{\nabla}\times\vec{A}$ and $V(\vec{\rho})$ is the confining potential taken as Gaussian potential,

$$V(\rho) = -V_0 e^{-\frac{\rho^2}{2R^2}} \tag{2}$$

The Hamiltonian can be rewritten as:

$$\hat{H} = -\frac{\hbar^2}{2m^*}\nabla_\rho^2 + V(\rho) + \frac{1}{8}m^*\omega_c^2\rho^2 + \frac{1}{2}\hbar\omega_c(\hat{L}_z + g\hat{S}_z) \tag{3}$$

where $\hat{L}_z$ is the z component of the angular momentum of the electron, $\omega_c$ is the cyclotron frequency given by $\omega_c = eB/m^*$, where B is the strength of the applied magnetic field, R is the quantum dot radius, $V_0$ is the depth of the confining potential and g* is the effective Lande g-factor which equals -0.44 for GaAs.

**Exact Diagonalization Method**

The Gaussian potential term makes the analytical solution of this system not possible. We intend to solve the Hamiltonian by using the exact diagonalization method. The bases are taken to be Fock-Darwin states [21, 36], given as:

$$|nm_z\rangle = \frac{\alpha}{\sqrt{\pi}}\left(\frac{n!}{(n+|m_z|)!}\right)^{\frac{1}{2}}(\alpha\rho)^{|m_z|}L_n^{|m_z|}(\alpha^2\rho^2)e^{-\frac{1}{2}\alpha^2\rho^2}e^{im_z\phi}\chi(\sigma) \tag{4}$$

with

$$\alpha = \sqrt{\frac{m^*\omega}{\hbar}} \tag{5}$$

where n is the radial quantum number, $m_z$ is the azimuthal angular momentum quantum number, $L_n^{|m_z|}$ is the associated Laguerre polynomial and $\chi(\sigma)$ is the eigenstate of the spin operator $\hat{S}_z$.

The Hamiltonian can be rewritten as $\hat{H} = \hat{H}_0 + \hat{H}_1$; where

$$\hat{H}_0 = -\frac{\hbar^2}{2m^*}\nabla_\rho^2 + \frac{1}{2}m^*\omega^2\rho^2 + \frac{1}{2}\hbar\omega_c(\hat{L}_z + g\hat{S}_z) \tag{6}$$

$$\hat{H}_1 = -\frac{1}{2}m^*\omega_0^2\rho^2 - V_0 e^{-\frac{\rho^2}{2R^2}} \tag{7}$$

and $\omega^2$ is the effective frequency, defined as:

$$\omega^2 = \omega_0^2 + \frac{1}{4}\omega_c^2 \tag{8}$$

where $\hat{H}_0$ represents the harmonic oscillator Hamiltonian with well-known eigenstates $|nm_z\rangle$ and with energies of $E_n = (2n + |m_z| + 1)\hbar\omega + \frac{1}{2}\hbar\omega_c(m_z + gS_z)$.

We can write the matrix elements of the complete Hamiltonian $\hat{H}$ in terms of these bases $|nm_z\rangle$ using Eq. 4, as:

$$\langle n'm_z|\hat{H}|nm_z\rangle = \langle n'm_z|\hat{H}_0|nm_z\rangle + \langle n'm_z|\hat{H}_1|nm_z\rangle$$
$$= (2n + |m_z| + 1)\hbar\omega + \frac{1}{2}\hbar\omega_c(m_z + gS_z) + \langle n'm_z| - V_0 e^{-\frac{\rho^2}{2R^2}}|nm_z\rangle - \langle n'm_z|\frac{1}{2}m^*\omega_0^2\rho^2|nm_z\rangle \tag{9}$$

The matrix element for the Gaussian confinement potential $\langle n'm_z| - V_0 e^{-\frac{\rho^2}{2R^2}}|nm_z\rangle$ can be evaluated in a closed form by using the following Laguerre relation [16]:

$$\int_0^\infty t^{\alpha-1}e^{-pt}L_m^\lambda(at)L_n^\beta(bt)dt = \frac{\Gamma(\alpha)(\lambda+1)_m(\beta+1)_n p^{-\alpha}}{m!n!}\sum_{j=0}^m \frac{(-m)_j(\alpha)_j}{(\lambda+1)_j\, j!}\left(\frac{a}{p}\right)^j \sum_{k=0}^n \frac{(-n)_k(\alpha+j)_k}{(\beta+1)_k\, k!}\left(\frac{b}{p}\right)^k \tag{10}$$

This closed form reduces significantly the computation time needed in the diagonalization process.

**Statistical Energy, Magnetization and Magnetic Susceptibility**

We have used computed energies of the GQD system as essential data to calculate the statistical average energy as:

$$\langle \mathrm{E}\left(T,B,R,V_o\right)\rangle = \frac{\sum_{\alpha=1}^{N} \mathrm{E}_\alpha e^{-\frac{\mathrm{E}_\alpha}{k_B T}}}{\sum_{\alpha=1}^{N} e^{-\frac{\mathrm{E}_\alpha}{k_B T}}} \quad (11)$$

which describes the mean thermal energy of the electron.

The magnetization of the GQD system is evaluated as the magnetic field partial derivative of the mean energy of the GQD.

$$\mathrm{M}\left(T,B,R,V_o\right) = \frac{-\partial\langle \mathrm{E}(\mathrm{T,B,R,V_0})\rangle}{\partial \mathrm{B}} \quad (12)$$

The magnetic susceptibility of the GQD system is evaluated as the second magnetic field derivative of the mean energy of the DQD.

$$\chi\left(T,B,R,V_o\right) = -\frac{\partial^2 < E(\mathrm{T,B,R,V_0}) >}{\partial^2 B} \quad (13)$$

## 3. Results and Discussion

We present our computed results for the energy spectra by solving the single electron GQD Hamiltonain using numerical diagonalization method and Fock-Darwin bases. The material parameter for GaAs medium is taken to be $m^* = 0.067m_0$; the effective Rydberg of $R^* = 5.83$meV and Bohr radius of $a^* = 9.8$ nm are used as energy and length, respectively. The energy spectra, $E_n$, are essential input data to calculate magnetization and magnetic susceptibility. Diagrams were used to illustrate the results.

### Quantum Dot Energy Spectra

First, we calculate the ground state energy of the QD for fixed potential height ($V_0$) and different QD radii, as displayed in Fig. 1.

We show in Fig. 2 the ground state and few excited state energies of the Gaussian QD *versus* the magnetic field B. The figure shows clearly the effects of the Zeeman and the spin terms on each particular state. As the magnetic field increases, the spin and Zeeman terms show significant energy contribution effects. These results are in full agreement with the previous published results of Boyacioglu and Chatterjee [38].

Next, we found the average thermal energy of the ground state of the QD as in Fig. 3. This figure describes the average thermal energy $\langle E\rangle$ *versus* the magnetic field for GQD, taking into account the effect of the electron spin term.

Fig. 3 shows that at low temperature of 5mK, the energy decreases as the magnetic field increases, because at low temperatures, the thermal energy contribution is small, so the negative energy contribution due to the spin term ($\omega_c g^* \hat{S}_z$) is significant and reduces the statistical energy; this behavior continues up to B≈4 T, then the energy starts increasing as the magnetic field increases. As the temperature increases, from 5mK to 10 and 20 K, the ground state energy curve of the QD shows a great enhancement. This behavior is due to the significant increment in the thermal energy contribution.

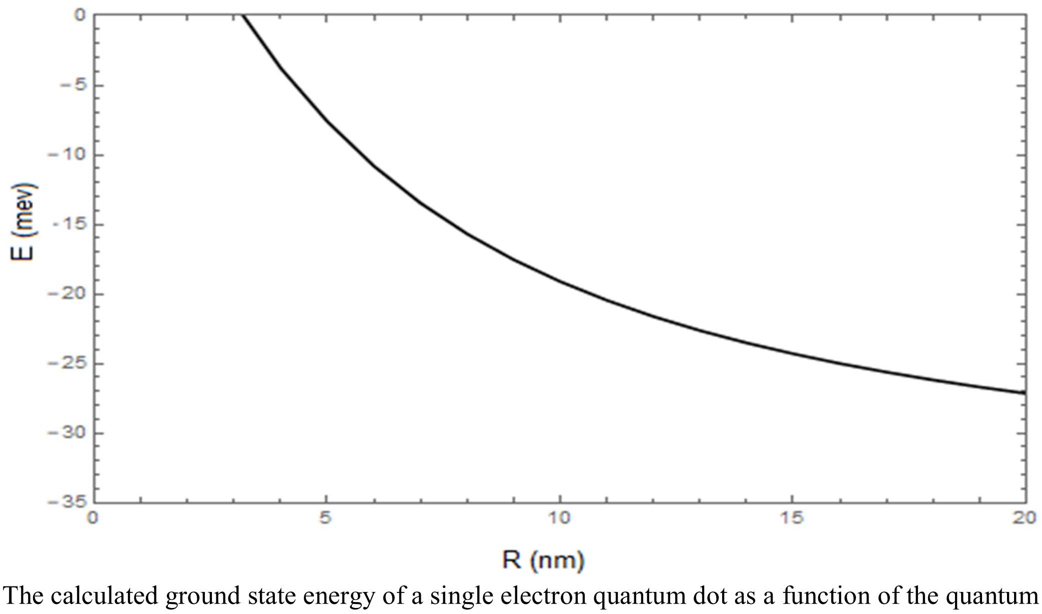


FIG. 1. The calculated ground state energy of a single electron quantum dot as a function of the quantum dot size R at zero magnetic field B = 0 and $V_0 = 36.7$meV.

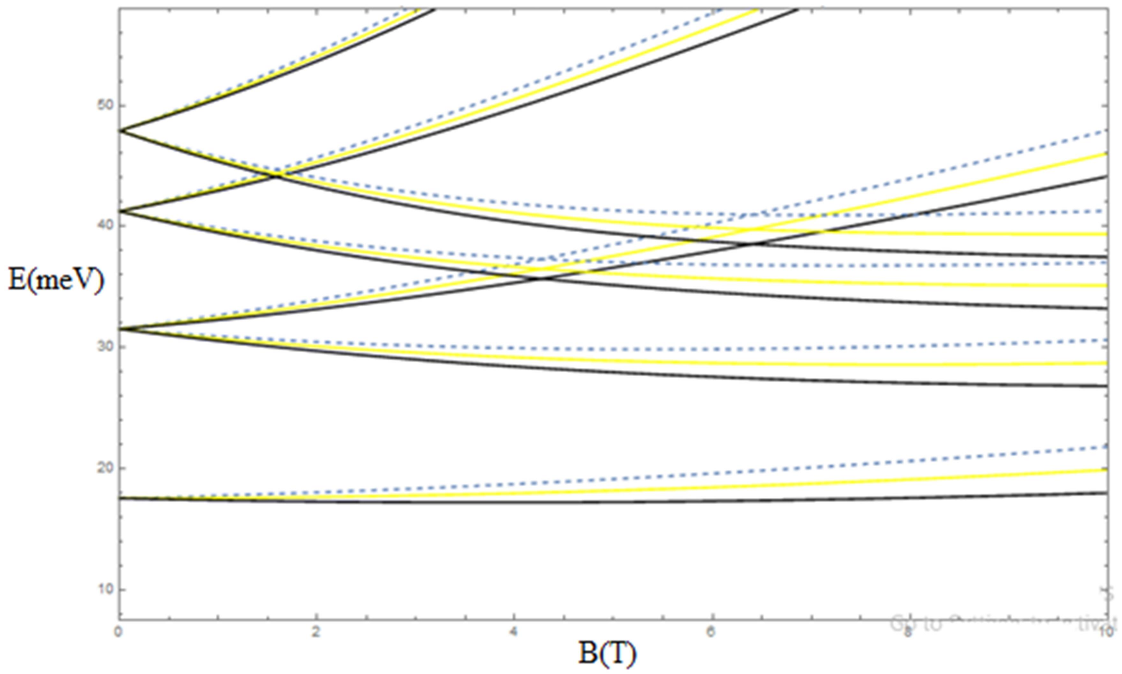


FIG. 2. Computed ground and first few exited energy states of one electron GQD *versus* the magnetic field at $V_0$ = 36.7 meV and R = 10 nm. The dashed curve is for S = −1/2 and the solid curve is for S = 1/2.

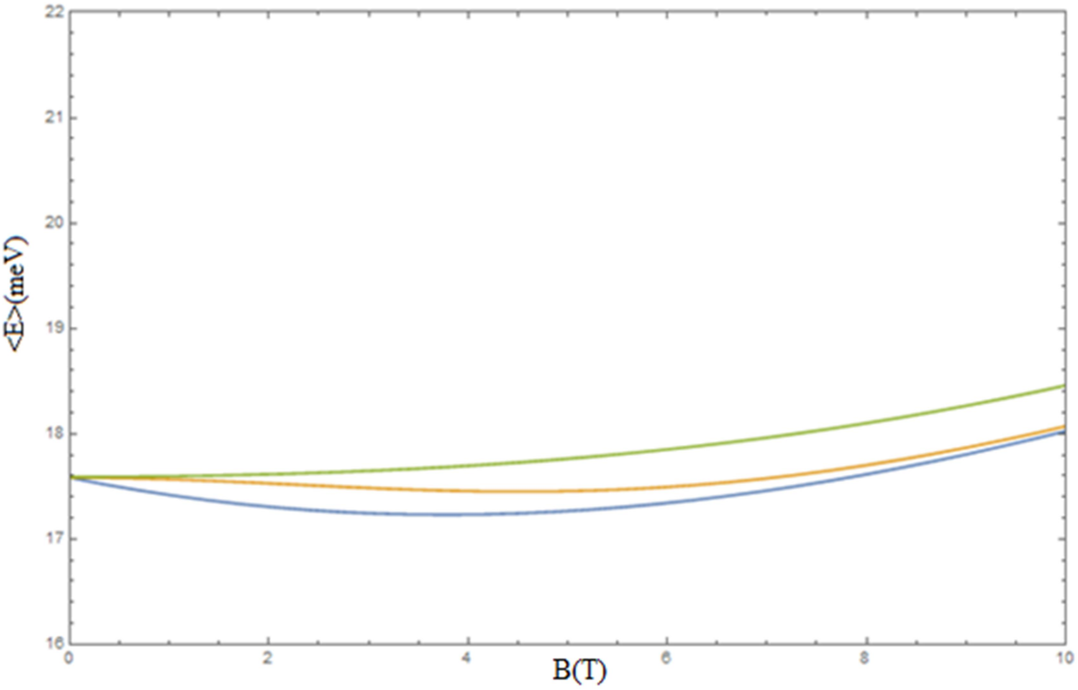


FIG. 3. The average thermal energy *versus* the strength of the magnetic field B at $V_0$ = 36.7meV, R = 10nm, g* = −0.44 and T = 5 mK, 10 and 20 K, from bottom to top.

In Fig. 4, we show the dependence of the convergence of our GQD energy spectra on the temperature by plotting the average energy *versus* the temperature at constant B = 2T for R = 10nm and $V_0$ = 36.7 meV and various numbers of bases (n) used in the exact diagonalization process. It is clear from the figure that, to reach numerical stability, we need more bases as the temperature increases.To achieve very good numerical stability calculations, we raised the number of bases to more than 90, at high temperature, as shown. This behavior is also supported by the results of a recent work reported by Nammas [34].

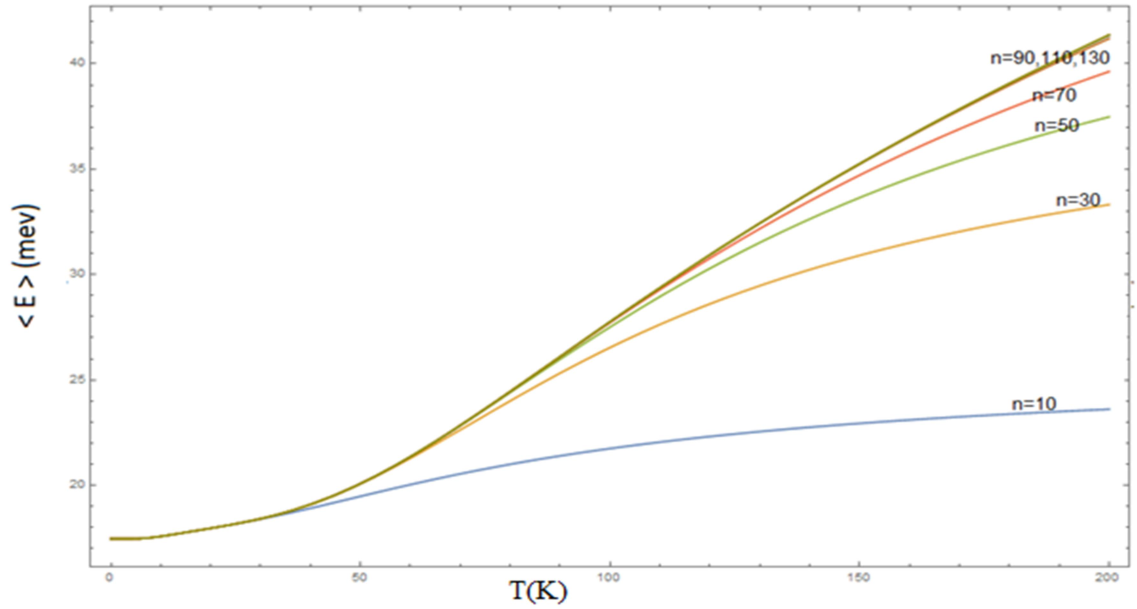


FIG. 4. Average thermal energy<E> against temperature T at $V_0$ = 36.7 meV, R = 10nm, g* = −0.44, B = 2T and n = 10, 30, 50, 70, 90, 110 and 130.

**Magnetization**

In this section, we will present and discuss the computed results for the behavior of magnetization (M) as a function of QD physical parameters of a single electron QD confined by a Gaussian potential. Magnetization was calculated by using the computed eigenenergies of a confined electron in a QD, as essential input data.

In Fig. 5, we present the dependence of M on B for fixed values of the confinement depth $V_0$ and quantum dot radius R, at different temperatures, T.

By focusing on the results obtained in the figure, we observe that at low temperatures (T=5mK, 5K and 10 K), magnetization M has the following behavior: magnetization increases as the magnetic field B increases, reaching a peak value, then it starts decreasing. As the temperature increases, the peak value in the magnetization curve decreases and the curve becomes flat. For example, at high temperatures of T=20K and 30K, the thermal energy ($E_{th} = k_B T$) becomes very significant and in this case, it affects greatly the average energy behavior of the system, as shown in Fig. 3. This leads to a linear decrease in the magnetization curve against the magnetic field.

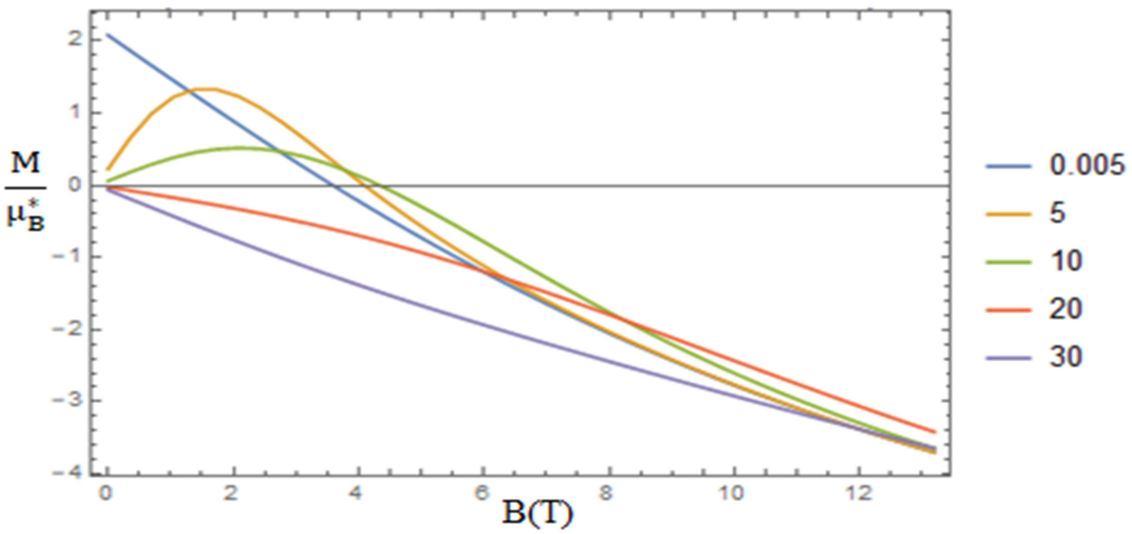


FIG. 5. Magnetization, per effective Bohr magneton $\frac{M}{\mu_B^*}$, gainst the strength of the magnetic field B at $V_0$ = 36.7 meV, R = 10 nm and T = 0.005, 5,10, 20 and 30K.

Fig. 6 shows the effect of the confining potential depth $V_0$ on the variation of the magnetization curve. As the potential depth $V_0$ increases, magnetization increases. This behavior of magnetization is due to the negative energy contribution of the Gaussian potential ($-V_0 e^{-\rho^2/2R^2}$) to the statistical energy $\langle E\rangle$ of the QD. The reduction in the statistical energy leads to an enhancement in magnetization, where $M\left(T,B,R,V_o\right)=\frac{-\partial\langle E(T,B,R,V_0)\rangle}{\partial B}$.

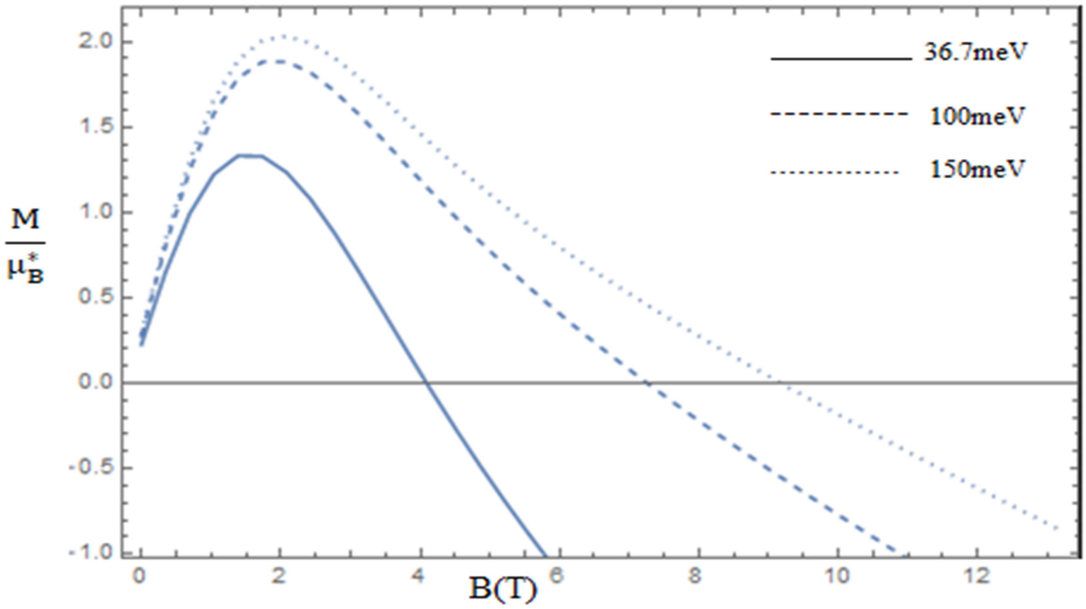


FIG. 6. Magnetization, per effective Bohr magneton $\frac{M}{\mu_B^*}$, *versus* the strength of the magnetic field B at $V_0$=36.7, 100 and 150 meV, R=10 nm and T= 5K.

**Magnetic Susceptibility**

This section is devoted for the variation of magnetic susceptibility $\chi$ as a function of magnetic field B, temperature T, quantum dot radius R and confining potential depth $V_0$, of a single electron QD confined by a Gaussian potential. The magnetic susceptibility of the GQD system is evaluated as the second magnetic field derivative of the mean energy of the GQD, as given in Eq. (13); $\chi\left(T,B,R,V_o\right)=-\frac{\partial^2<E(T,B,R,V_0)>}{\partial^2 B}$.

In Fig. 7, we present the dependence of magnetic susceptibility on magnetic field B for fixed values of confining potential depth $V_0$ = 36.7meV and quantum dot radius R = 10nm, at different temperatures T = 5mK, 5, 10 and 20K. The figure shows clearly a great change in the behavior of the magnetic susceptibility curves, at each temperature, as we increase the magnetic field strength B. At low temperatures ($T = 5$ mK and 5 K), it is found that at particular values of magnetic field strength, magnetic susceptibility ($\chi$) flips its sign from positive ($\chi > 0$) to negative ($\chi < 0$); equivalent to a phase change in the QD-media from paramagnetic to diamagnetic. However, at higher temperatures (T = 10K, 20K), it is observed that the sign of the magnetic susceptibility of the system is negative ($\chi < 0$) for the entire magnetic field range.

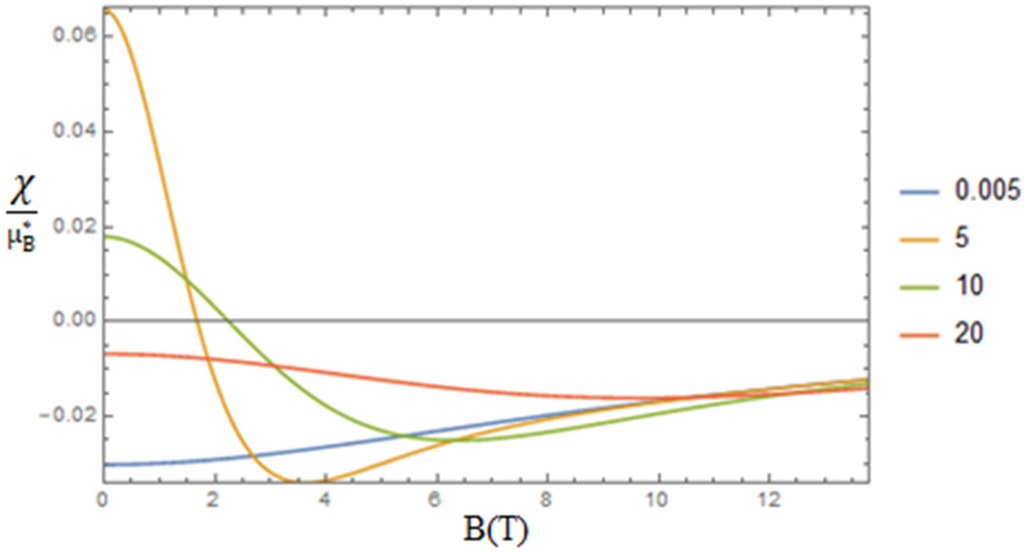


FIG. 7. Magnetic susceptibility, per effective Bohr magneton $\frac{\chi}{\mu_B^*}$, *versus* the strength of the magnetic field B at $V_0$ = 36.7meV, R = 10 nm and T = 0.005, 5, 10 and 20K.

## Conclusion

The exact diagonalization method has been used to solve the QD Hamiltonian and calculate eigenenergies' spectra, magnetization (M) and magnetic susceptibility $(\chi)$ of a single GaAs quantum dot with Gaussian confinement, as a function of the magnetic field strength (B), QD radius (R), confining potential ($V_0$) and temperature (T). In this work, we have shown the dependence of the energy on the QD radius (R). Next, we have calculated the statistical energy $\langle E \rangle$, taking into account the presence of the spin (S). The QD-energy results are displayed against the physical parameters of the QD: magnetic field strength (B), QD radius (R), temperature (T) and confining potential ($V_0$). In addition, we have studied the dependence of magnetization and magnetic susceptibility of the system on the external magnetic field, temperature and confining potential of the GQD. It is found that at certain values of $T$ and $V_0$, the QD-system has a magnetic phase change from diamagnetic to paramagnetic.

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