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ARTICLE

Pressure and Temperature Effects on the Magnetic Properties of Donor Impurities in a GaAs/AlGaAs Quantum Heterostructure Subjected to a Magnetic Field

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Abstract: The exact diagonalization method has been used to solve the effective-mass Hamiltonian of a single electron confined parabolically in the GaAs/AlGaAs quantum heterostructure, in the presence of a donor impurity and under the effect of an applied uniform magnetic field. The donor impurity is located at distance (d) along the growth direction which is perpendicular to the motion of the electron in a two-dimensional heterostructure layer. We have investigated the dependence of the magnetization (M) and magnetic susceptibility (χ) of a GaAs/AlGaAs quantum heterostructure nanomaterial on the magnetic field strength (ω_c), confining frequency (ω_o), donor impurity position (d), pressure (P) and temperature (T).

Keywords: Exact diagonalization, Donor impurity, Magnetic field, Magnetization, Magnetic susceptibility, Pressure and temperature.

1. Introduction

The recent physical and technological research on nanosystems (low-dimension systems), such as quantum well (QW), quantum well wire (QWW) and quantum dot (QD) in theoretical and applied physics, play significant roles in the present quantum electronic nanodevices [1, 2]. The electrical, optical and transport properties of the heterostructures QW, QWW and QD are very sensitive to adding external electrical field, magnetic field and to different parameters, like pressure, temperature, and shallow donor impurities near the heterostructure surface [3, 4]. The study of quantum dots is motivated by their applications in solar cells, quantum computers, single electron transistors and lasers [5].

Furthermore, the donor impurity effects on the properties of the low-dimensional semiconductor heterostructure have been among the interesting problems to study in low-dimensional semiconductors, where adding the donor impurity atoms to low-dimension systems changes the effective charge and mass of them [6]. In addition, the most interesting phenomenon is to investigate the effects of temperature and pressure on the donor impurity binding energy in reduced dimensions [7], where the energy gap of the heterostructure changes because of the binding energy of the impurity and the Columbic interaction between the system charge carriers and the donor impurity [8, 9]. The donor impurity binding energy was investigated for all heterostructure systems, where it depends on the dimensionality of the system, the impurity position, the presence of magnetic or electrical fields, pressure and temperature [1, 10-12].

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Different methods have been used to solve the system's Hamiltonian with the presence of the donor impurity, like variational and analytical methods under the presence of electric or magnetic fields for different shapes and donor impurity locations [13-18].

The dependence of the photoionization of impurities in infinite-barrier quantum wells on the photon energy had been calculated as a function of quantum well width [19]. In addition, the thermodynamic properties of quantum dots in a magnetic field, such as magnetization, magnetic susceptibility and specific heat, had been computed. For Helium-like confined quantum dots, the thermodynamic properties show sharp peak structure in the susceptibility and the specific heat curves [20]. The pressure and temperature dependence of the diamagnetic susceptibility and the binding energy of the donor impurity had been shown analytically, where the diamagnetic susceptibility increases as the pressure increases and decreases as the temperature increases [21]. Peter in Ref. [22] used the variation method to show the behavior of the binding energy levels of shallow hydrogenic impurities in a parabolic quantum dot with pressure. He found that the ionization energy is purely pressure-dependent. In addition, the binding energy of hydrogenic impurities, in a spherical quantum dot, was calculated using the variational and perturbation approaches as a function of pressure, QD size and impurity position. It was found that the pressure effect is enhancing the binding energy [23]. Using exact diagonalization method, including the pressure and temperature effects, the two electrons QD problem had been solved, where the magnetization and magnetic susceptibility of confined electrons in parabolic quantum dot were investigated in both experimental and theoretical studies [24, 25]. Recently, the electronic, thermodynamic and magnetic properties of two electrons confined in a single quantum dot and coupled quantum dots (CQD) had been also solved [26-34].

The purpose of this work is to investigate the combined effects of pressure, temperature and impurity position on the magnetic properties of GaAs/AlGaAs heterostructure material. The magnetization and magnetic susceptibility of a confined electron presented in a magnetic field are computed and displayed as function of the Hamiltonian system physical parameters. The structure of this paper is organized as follows: First, the Hamiltonian theory, as well as the computation diagonalization technique of a single electron in GAs/AlGaAs heterostructure in the presence of donor impurity located at a finite distance along the growth (z-axis) are discussed. Magnetization and magnetic susceptibility expressions and pressure and temperature material parameters relations used in the present calculations are given in Section 2. The numerical results and discussion are given in Section 3. Final section is devoted to the conclusion.

2. Theory

This section presents the main parts of the donor impurity formalization: i) The effective-mass Hamiltonian (EM) of donor impurities in quantum heterostructure, ii) The exact diagonalization method, iii) The magnetization and the magnetic susceptibility and iv) The effects of pressure and temperature.

A quantum heterostructure is a two-dimensional (2D) system where electrons are confined in the x-y plane with parabolic confinement potential of the form, $\frac{1}{2}m^*\omega_0^2\rho^2$ with confining strength ω_o and bound to off-plane donor impurity located at the z axis. The impurity position vector is (0, 0, d), where d is the distance from the two –dimensional heterostructure plane to the impurity center. A pictorial view of the electron in the xy-plane interacting with the donor impurity at the z axis is given by Alfonso *et al.* in Ref. [35]. This system is subjected to a uniform external magnetic field of strength B directed along the z direction. The magnetic field is given by $\mathbf{B}=\nabla\times\boldsymbol{A}$, where $A=\frac{B}{2}(-y,x)$ is the vector potential.

The Hamiltonian operator of the donor impurity, in effective Bohr radius (a^*) and Rydberg (R^*) units, is given as, [32, 35]:

$$\hat{H}=-\left(\rho^{-1/2}\frac{\partial^2}{\partial\rho^2}\rho^{1/2}+\frac{1}{\rho^2}\left(\frac{\partial^2}{\partial\phi^2}+\frac{1}{4}\right)\right)+\frac{1}{4}\omega^2\rho^2-i\frac{\omega_c}{2}\frac{\partial}{\partial\phi}-\frac{2}{|\boldsymbol{\rho}-\mathbf{d}|} \quad (1)$$

The given Hamiltonian ($\hat{H}$) in Eq.1, given in terms of ρ and φ variables, can be separated into two parts as:

$$\hat{H}=\hat{H}_\perp+V(\rho) \quad (2)$$

where:

$$\hat{H}_{\perp} = -\left(\rho^{-1/2}\frac{\partial^2}{\partial\rho^2}\rho^{1/2} + \frac{1}{\rho^2}\left(\frac{\partial^2}{\partial\phi^2}+\frac{1}{4}\right)\right) + \frac{1}{4}\omega^2\rho^2 - i\frac{\omega_c}{2}\frac{\partial}{\partial\phi} \quad (3)$$

and

$$V(\rho) = -\frac{2}{|\boldsymbol{\rho}-\mathbf{d}|} = -\frac{2}{\sqrt{\rho^2+d^2}}, \quad (4)$$

where the terms in brackets are due to the kinetic energy operator, the second term is the effective parabolic confining term, the third term is the z-component of the angular momentum and the last term is the attractive Coulomb-type energy. The part $\hat{H}_{\perp}$ is the harmonic oscillator Hamiltonian which has an analytical well-known solution, as shown later in Eqs. 5-7 [32, 35]. The effective confinement frequency ω in $\hat{H}_{\perp}$-Hamiltonian is a combination of the magnetic field cyclotron frequency ω_c and parabolic confining frequency ω_o, given as: $\omega^2 = \omega_0^2 + \frac{\omega_c^2}{4}$. The potential $V(\rho)$ represents the Coulomb interaction between the electron in the GaAs layer and the donor impurity ion, located at distance d along the z-direction in AlGaAs barrier.

Initially, the donor impurity Hamiltonian given by Eq. (1) will be solved using the exact diagonalization technique, to obtain the eigenenergies as an essential step to study the electronic and magnetic properties of the heterostructure.

If there is no impurity, the Hamiltonian ($\hat{H}_{\perp}$), in Eq. (1) reduces to harmonic oscillator-type with a well-known eigenstate |n, m> and eigenenergies ($E_{n,m}$). The harmonic oscillator bases (|n, m> $= \psi_{n,m}(\rho,\varphi)$) will be used to diagonalize the full Hamiltonian and to obtain the ground state energy of the impurity system.

The bases wave functions are, [32, 35]:

$$|n,m> = \psi_{n,m}(\rho,\varphi) = \frac{1}{\sqrt{2\pi}}R_{n,m}(\rho)e^{im\varphi} \quad (5)$$

where,

$$R_{n,m}(\rho) = e^{-\frac{1}{2}\rho^2\alpha^2}\rho^{|m|}\alpha^{|m|}\sqrt{\frac{2\alpha^2 n!}{(n+|m|)!}}L_n^{|m|}(\rho^2\alpha^2) \quad (6)$$

and the corresponding eigenenergies:

$$E_{n,m} = (2n+|m|+1)\hbar\omega, \quad (7)$$

where $L_n^{|m|}(\rho^2\alpha^2)$ is the standard associated Laguerre polynomials used in Ref. [35] and α is an inverse length dimension constant which is given by:

$$\alpha = \sqrt{\frac{m^*\omega}{\hbar}} \quad (8)$$

These harmonic oscillator bases $|n,m>$ will be used to calculate the energy matrix elements of the full donor impurity Hamiltonian in Eq. (1), $\langle R_{n,m}(\rho)|\hat{H}|R_{\acute{n},m}(\rho)\rangle$.

The magnetic properties, such as magnetization (M) the magnetic susceptibility (χ) of the donor impurity in a heterostructure, are calculated from the computed energies of the donor impurity system.

The magnetization of the donor impurity in a heterostructure is evaluated as the magnetic field derivative of the energy of the donor impurity [26, 28].

$$M = -\frac{\partial E(\omega_c,\omega_o,d)}{\partial B} \quad (9)$$

The magnetic susceptibility is evaluated as the magnetic field derivative of the magnetization of the donor impurity in a heterostructure as [26, 28]:

$$\chi = \frac{\partial M}{\partial B} \quad (10)$$

or

$$\chi = -\frac{\partial^2 E(\omega_c,\omega_o,d)}{\partial B^2} \quad (11)$$

We investigated the dependence of the computed magnetic properties, M and χ, of the donor impurity in a heterostructure on the system's physical parameters: magnetic field ω_c, confining frequency ω_o and impurity position d.

The effective Bohr radius and Rydberg constant will be defined in terms of pressure and temperature, to study their effects on M and χ of the donor impurity in a heterostructure.

The effective Bohr radius, $a_B^*(P,T)$, is given as, [12, 27, 32]:

$$a_B^*(P,T) = \frac{\epsilon(P,T)\hbar^2}{m^*(P,T)e^2} \quad (12)$$

The effective Rydberg constant can be written as, [12, 27, 32]:

$$R_y^*(P,T) = \frac{e^4 m^*(P,T)}{2(\epsilon(P,T))^2\hbar^2} \quad (13)$$

The effects of the pressure and the temperature on the energy, magnetization and susceptibility of the ground state will be studied using the effective mass approximation method (EMA).

The material parameters, such as: electron effective mass, $m^*(P,T)$ and dielectric constant $\epsilon_r(P,T)$, are now used in the impurity Hamiltonian as shown below:

$$\hat{H}(\rho) = \frac{1}{2m^*(P,T)}\left[\vec{p}(\rho) + \frac{e}{c}\vec{A}(\rho)\right]^2 + \frac{1}{2}m^*(P,T)\omega_0^2\rho^2 - \frac{e^2}{\epsilon_r(P,T)\sqrt{\rho^2+d^2}} \quad (14)$$

For quantum heterostructure made of GaAs, the dielectric constant $\epsilon_r(P,T)$ and the electron effective mass $m^*(P,T)$ are presented by [12, 27, 32]:

$$\epsilon_r(P,T) = \begin{cases} 12.74\exp(-1.73\times10^{-3}P)\exp[9.4\times10^{-5}(T-75.6)] & \text{for } T < 200\text{ K} \\ 13.18\exp(-1.73\times10^{-3}P)\exp[20.4\times10^{-5}(T-300)] & \text{for } T \geq 200\text{ K} \end{cases} \quad (15)$$

$$m^*(P,T) = \left[1 + 7.51\times\left(\frac{2}{E_g^{\Gamma}(P,T)} + \frac{1}{E_g^{\Gamma}(P,T)+0.341}\right)\right]^{-1} m_0 \quad (16)$$

$$E_g^{\Gamma}(P,T) = \left[1.519 - 5.405\times10^{-4}\frac{T^2}{T+204}\right] + bP + cP^2 \quad (17)$$

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 heterostructure at Γ point, b = 1.26×10^{-1} eV GPa^{-1} and c = -3.77$\times10^{-3}$ eV GPa^{-2}.

For heterostructure systems made from GaAs, the numerical values of the material parameters are: effective Rydberg $R^* = 5.926\, meV$, dielectric constant $\epsilon = 12.4$ and the effective mass of an electron $m^* = 0.067\, m_e$ at ambient zero temperature and pressure.

3. Results and Discussion

Initially, we will show the donor impurity energy dependence. The ground state eigenenergy (where m = 0) for the donor impurity of GaAs/AlGaAs heterostructure is computed as a function of the magnetic field strength ω_c, impurity located at the origin (d=0) and for two specific values of the confinement frequency strength, $\omega_0 = 5.412\, R^*$ and $\omega_0 = 3.044\, R^*$.

First, we will verify the convergency of the computed eigenstates. Fig. 1 shows the computed ground state energies (E) of the donor impurity against the number of basis (n) from 1 up to 38 for $\omega_0 = 3.044\, R^*$, impurity distance $0.5\, a^*$ and magnetic field strength $\omega_c = 2\, R^*$. The figure shows a very good numerical stability in the computed energies.

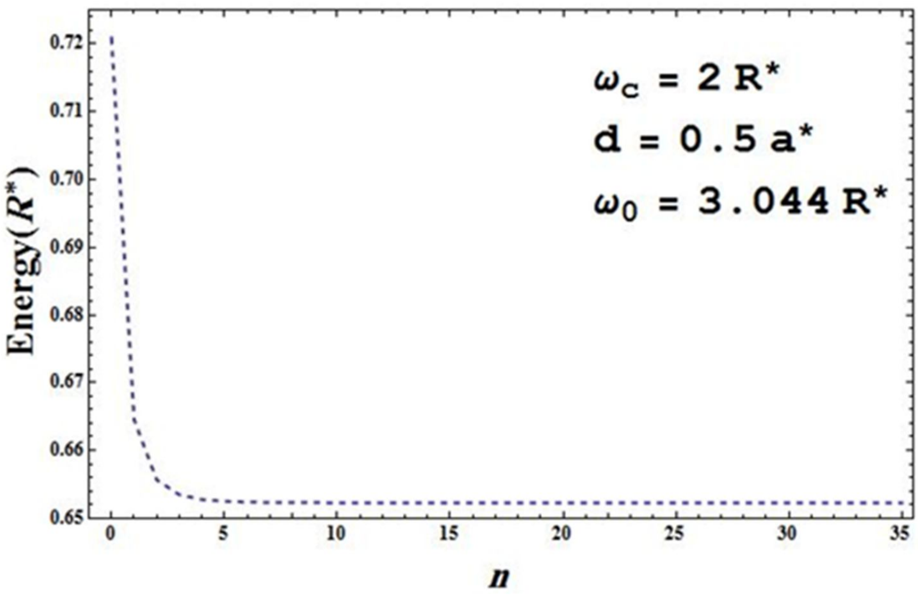

FIG. 1. The ground state energy of the quantum heterostructure for fixed values of magnetic field strength (ω_c) = 2 $R^*$and parabolic confinment strength $\omega_0 = 3.044R^*$ against the number of basis (n) for donor impurity at (d = 0.5 a^*).

The ground-state eigenenergies (E) for two specific values of confinement frequency ($\omega_0 = 3.044$ R*, dashed line and $\omega_0 = 5.412$ R^*, *solid line*) are computed as a function of the magnetic strength ω_c and for impurity distance d = 0.5 a^*, as shown in Fig. 2. We can clearly notice that as the magnetic field strength ω_c increases, the energy also increases. Moreover, the curves of energies of higher parabolic confinement effect, $\omega_0 = 5.412$ R^*, have larger values than those for $\omega_0 = 3.044$ R*. This is because the parabolic effective frequency ($\omega^2 = \omega_0^2 + \frac{\omega_c^2}{4}$) increases also as ω_0 increases, which leads to the enhancement of the electron energy due to the parabolic confinement term of the donor impurity Hamiltonian, $\frac{1}{4}\omega^2\rho^2$.

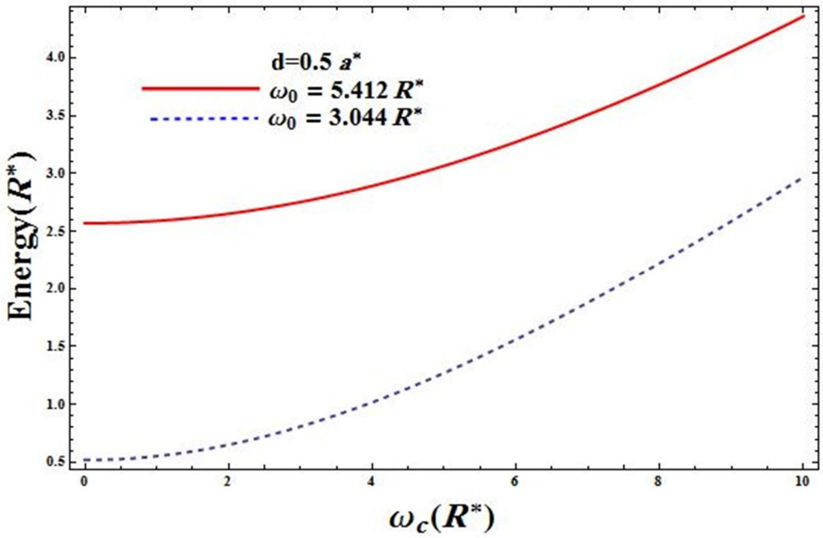

FIG. 2. The variation of the ground state energy against the magnetic field strength ω_c for $\omega_0 = 3.044$ R*(dashed line), $\omega_0 = 5.412$ R^* (solid line) and d = 0.5 a^*.

We have also studied the temperature and pressure effects on the magnetization and the magnetic susceptibility. The plots of the magnetic quantities are shown as a function of the magnetic field strength. The results for M of GaAs/AlGaAs quantum heterostructure doped with donor impurity at d = 0.5a^* are presented in Fig. 3. The curve of M against ω_c is calculated at $\omega_0 = 3.044$ R^*, d = 0.5a^*, at various temperatures ($T = 5K, 100K, 200K$) and a fixed value of P = 10 kbar. It is clear that the ground state magnetization curves decline as ω_c increases. The material parameters m^* *and* ϵ_r are pressure- and temperature-dependent: effective mass $m^*(P,T)$ and dielectric constant $\epsilon_r(P,T)$. For a fixed value of P, m^* decreases and ϵ_r increases as the temperature increases, which leads to the increase in the values of $|M|$.

Fig. 4 displays the dependence of the magnetic susceptibility (χ) on the temperature for a fixed value of P = 10 kbar, $d = 0.5$ a^* and $\omega_0 = 3.044$ R^*. The plots clearly show that the absolute value of the magnetic susceptibility $|\chi|$, at a fixed value of temperature, enhances as the cyclotron frequency, ω_c, increases. However, the curves show a small decrease in $|\chi|$-values as the temperature increases, for particular values of magnetic strength. Moreover, we can notice that the sign of χ is negative ($\chi < 0$), which indicates that the material is of a diamagnetic type.

The effect of the pressure on the donor magnetization as a function of the magnetic field strength is studied in Fig. 5. The values of M are computed at fixed temperature T = 20 K, $\omega_0 = 3.044$ R*, impurity position d = 0.5a^* and various pressures: P = 0, 10 and 20 kbar. The magnetization plots, at various pressure values, decline as ω_c increases. Furthermore, for a fixed value of T, m^* increases and ϵ_r decreases as the pressure increases, which leads to the decrease in the values of $|M|$.

Fig. 6 displays the variation of the magnetic susceptibility as a function of the magnetic field strength at T = 20K, $\omega_0 = 3.044R^*$ and different pressure values: (0, 10 and 20 kbar).

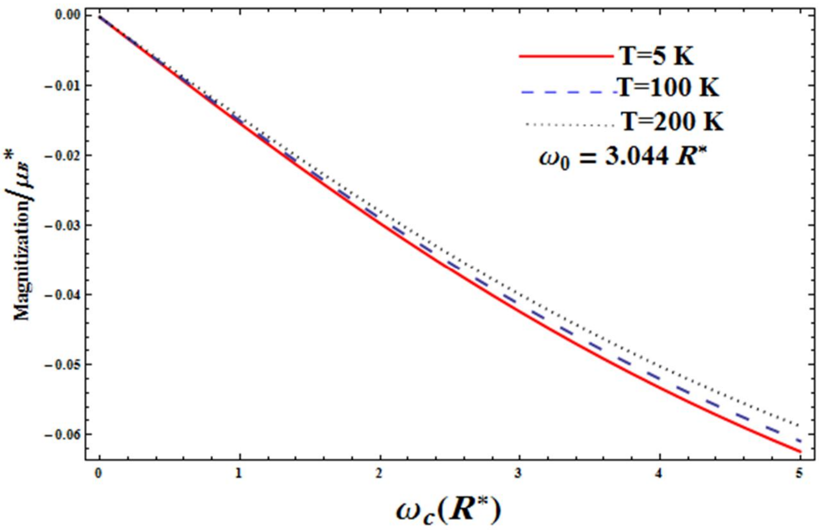

FIG. 3. The magnetization for d = $0.5a^*$ and $\omega_0 = 3.044\ R^*$ at constant pressure (P = 10 kbar) as a function of ω_c for three temperatures (5K, 100K and 200K).

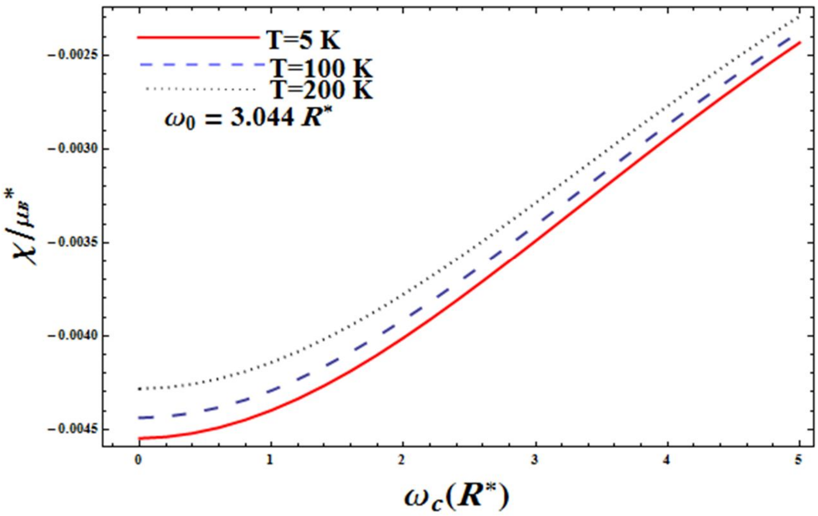

FIG. 4. The magnetic susceptibility for d = $0.5a^*$ at constant pressure (P = 10 kbar) as a function of ω_c for three temperatures (5K, 100K and 200K); for $\omega_0 = 3.044\ R^*$.

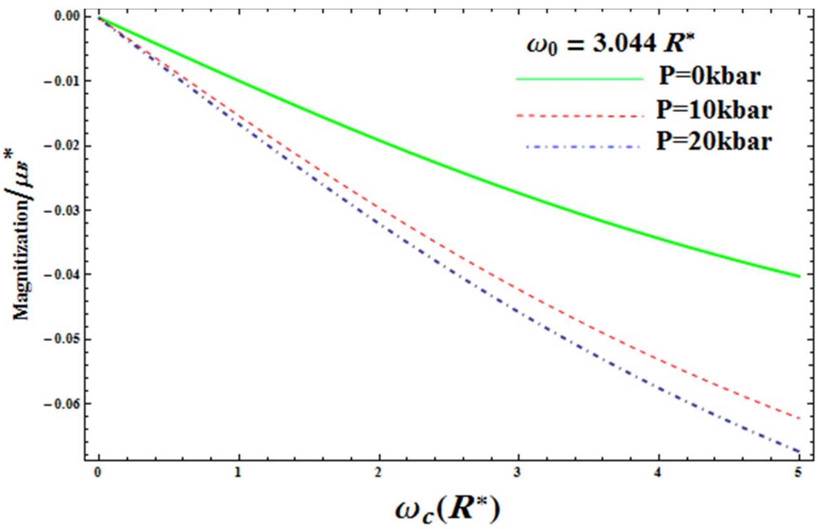

FIG. 5. The magnetization for d = $0.5a^*$ against ω_c at a fixed temperature (20K) for three pressure values (0, 10 and 20 kbar); for $\omega_0 = 3.044\ R^*$.

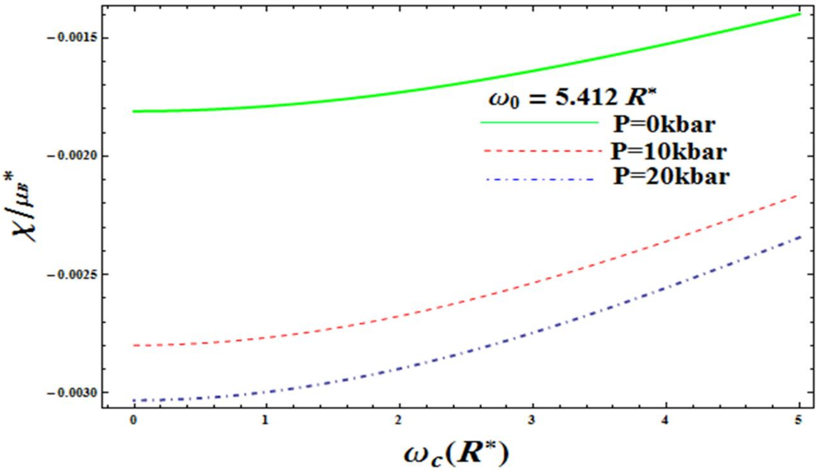

FIG. 6. The magnetic susceptibility for d = $0.5a^*$and $\omega_0 = 3.044\ R^*b$ against ω_c at a fixed temperature (20 K) for three pressure values (0, 10 and 20 kbar).

Furthermore, we have investigated, in Figs. 7a and 7b, the effects of varying the impurity position, d, on the magnetic susceptibility, χ, against the cyclotron frequency,ω_c, for d = 0.1 a^* and d = 0.5 a^*, calculated at various confinements: $\omega_0 = 3.044\ R^*$ and $\omega_0 = 5.412\ R^*$, respectively. The plots show that the absolute value of susceptibility, $|\chi|$ enhances as we increase the donor impurity position, d, which is located along the z-axis, perpendicular to the plane of the heterostructure. This result is attributed to the reduction in the attractive Coulomb energy, $-\frac{2}{\sqrt{\rho^2+d^2}}$, between the electron confined in the heterostructure plane and the impurity located at distance, d, along the z-direction.

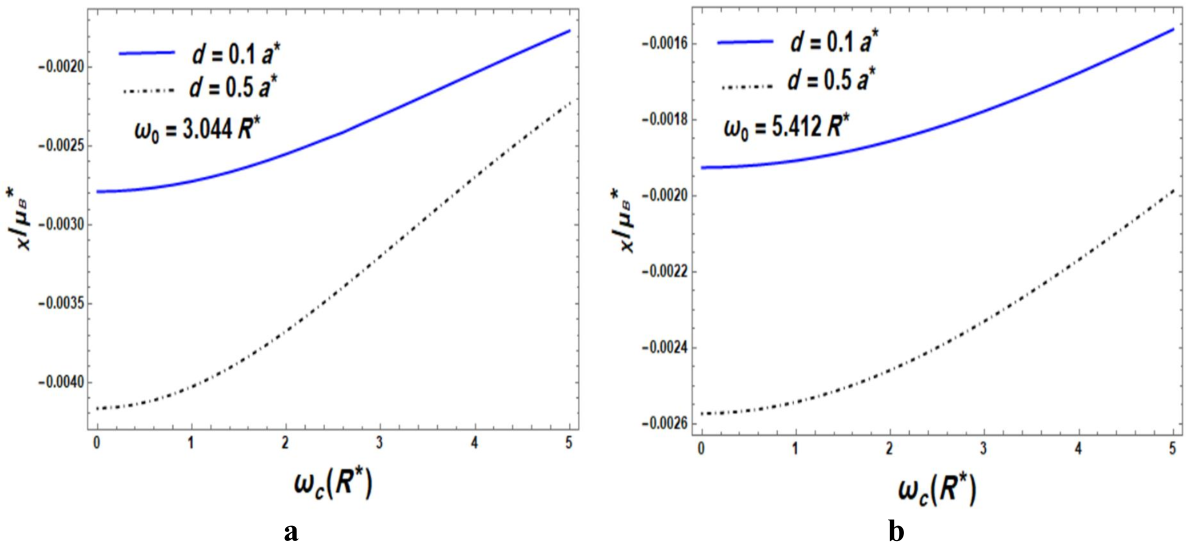

FIG. 7. The dependence of the magnetic susceptibility on the position impurity (d) for a) $\omega_0 = 3.044\ R^*$ and b) $\omega_0 = 5.412\ R^*$.

Conclusion

In conclusion, the effective-mass (EM) Hamiltonian of donor impurity in GaAs/AlGaAs heterostructure had been solved using the exact diagonalization method. The effect of temperature and pressure on magnetization (M) and magnetic susceptibility (χ) had been investigated. The curves of the magnetic properties had been plotted as functions of magnetic field strength, parabolic confinement, impurity position, temperature and pressure. The results show that, at a fixed value of P, the values of $|M|$ and $|\chi|$ increase as the temperature increases. In contrast, at a fixed value of T, the values of $|M|$ and $|\chi|$ decrease as the pressure increases.

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