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The influence of off-centre donor impurity on the tuning of the quantum ring magnetic susceptibility

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ABSTRACT

The 1/N expansion method has been used to investigate the problem of an electron moving in a two-dimensional semiconductor quantum ring with an off-center impurity. The energy spectra, magnetization, and magnetic susceptibility have been calculated as a function of the magnetic field, impurity position, temperature, and quantum ring parameters. Interesting energy-level crossings attributed to QR confinement manifest themselves as low-temperature oscillations in the magnetization and magnetic susceptibility curves. On the contrary, the presence of impurity at the QR center eliminates these level crossings. This work shows that changing the impurity position can manipulate the magnetic field value correspondence to these diamagnetic-paramagnetic phase transitions.

1. Introduction

As a result of nanostructure fabrication methods, carriers can be confined in all spatial dimensions, resulting in fully quantized spectra for quantum dots (QDs). A quantum ring (QR) was created using the same techniques, and the carriers within it were bound by the ring's walls [1]. The QR research area has received much attention due to its applications, such as photonic detectors and quantum computing [2].

Many theoretical and experimental studies of the electronic, thermal, magnetic, and optical properties of QRs have recently been published [3–14]. For example, the presence of a magnetic field can influence the electronic structure of carriers confined in a low-dimensional system. This topic has attracted the interest of researchers [15–20]. Furthermore, doped impurities are also crucial in changing the properties of nanomaterials [21–34].

Various techniques have been used to solve the reduced-dimensional Hamiltonian, including the magnetic field effect. The authors of Ref [35] used a variational method to study the energy spectra and the magnetization of a two-electron quantum dot. Their results show that the magnetization oscillates due to the presence of a Coulomb potential. The effect of dimensionality on the ground state energy of a quantum dot system was investigated using the 1/N expansion method [36]. Furthermore, the numerical diagonalization method was used to determine the magnetic properties of the quantum dot in the presence of a magnetic field [37]. At a low temperature (0.3 K), Schwarz et al. experimentally studied the magnetization of a quantum ring, which exhibits oscillation behavior [38].

This work investigates the effect of an off-center impurity on the QR properties. We shall calculate the energy spectra, binding energy (BE), magnetization, and magnetic susceptibility of an off-center donor impurity in a quantum ring system under the presence of an external magnetic field. We shall use the shifted 1/N expansion technique to solve the quantum ring Hamiltonian.

2. Theory

2.1. Model and formulation

In this work, we considered a 2D-GaAs QR subjected to a magnetic field perpendicular to the QR plane. The confinement along the growth direction (z-axis) is much stronger, so we don't consider any excitation in that direction.

The confinement potential of the quantum ring is given by, $V(r) = \frac{a_1}{r^2} + a_2 r^2 - V_0$. The first term in the confinement potential represents the repulsive term, the second one is a harmonic oscillator-type potential that constrains the electron to the ring, and the final term is $V_0 = 2\sqrt{a_1 a_2}$, the confinement potential has a minimum at $R_0 = \sqrt[4]{a_1/a_2}$, with R_0 is the average radius of the ring. The potential $V(r)$, for r near R_0, can be simplified by parabolic form $\frac{1}{2}m^*\omega_0^2(r-R_0)^2$, where $\omega_0 =$

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$\sqrt{8a_2/m^*}$ describes the strength of the transverse confinement, m^* is the effective mass of the electron in the material.

Moreover, we can control the shape of the confinement potential because the width and the radius of the quantum ring can be adjusted independently by a suitable choice of a_1 and a_2 [39].

The Hamiltonian of a two-dimensional QR system in the presence of off-center donor impurity can be expressed as follows:

$$\widehat{H} = \frac{\hbar}{2m*}\left(\mathrm{P}+\frac{\mathrm{e}}{\mathrm{c}}\mathrm{A}\right)^2 + \frac{1}{2}m^*\omega_0^2(r-R_0)^2 + \frac{1}{2}g^*\mu_B B\sigma_z - \frac{\alpha\, e^2}{\in\ |\,\mathrm{r}-\rho\,|} \quad (1)$$

where P (r) indicates the 2D momentum (position) operator of an electron with effective mass m* and charge e, A represents the vector potential associated with the magnetic field B applied perpendicular to the QR plane, ω_0 is the confinement strength and R_0 is the main radius of the QR. The applied magnetic field, $B = \nabla \times A$ in the z-direction, introduces a Zeeman splitting given by $\frac{1}{2}g^*\mu_B B\sigma_z$, where $g^*, \mu_B,\ \sigma_z$ are the Lande g factor, Bohr magneton, and the Pauli matrix, respectively.

The confinement frequency is inversely proportional to the width of the ring, as ω_0 increases, the ring becomes narrower.

The last term in the Hamiltonian is due to the presence of the donor impurity, where $\in$ is the dielectric constant and ρ is the impurity position vector.

Using the symmetric gage for vector potential, $A = \frac{\mathrm{B}}{2}$ (-y, x, 0), and the impurity location depicted in Fig. 1(a), the Hamiltonian of the system can be shown as follows:

$$\widehat{H} = \frac{-\hbar^2}{2m*}\nabla^2 + \frac{1}{2}m*\omega_0^2(r-R_0)^2 + \frac{1}{8}\mathrm{m}*\omega_c^2 r^2 + \frac{1}{2}\,\hbar\,\omega_c\,(\mathrm{L_z}+g*S_z) - \frac{\alpha\, e^2}{\in\ \sqrt{r^2+d^2}} \quad (2)$$

$\omega_c = \frac{eB}{m^*}$ is the cyclotron frequency, L_z is the z-component of the orbital angular momentum with eigenvalues $m_l\hbar$ where $m_l = 0, \pm1, \pm2,$ and d represent the distance between the impurity and the ring center.

A flat QR can be obtained by droplet molecular-beam epitaxy technique [40], where the impurity is located in the AlGaAs layer to avoid electron-impurity collision.

The shifted 1/N expansion approach was utilized to compute the system spectra, and the obtained energies were then used to determine the system properties.

The 1/N method is efficient in the case of a spherical symmetric Hamiltonian, and it gives accurate results [41]. As a starting point, using the N-dimensional radial Schrodinger equation written as:

$$\left[-\frac{\hbar}{2\,m^*}\left(\frac{d^2}{dr^2} + \frac{N-1}{r}\frac{d}{dr}\right) + \frac{l(l+N-2)}{r^2} + V(r)\right]\psi(r) = E\,\psi(r) \quad (3)$$

Where,

$$V(r) = \frac{1}{2}m^*\omega_0^2(r-R_0)^2 + \frac{1}{8}\mathrm{m}^*\omega_c^2 r^2 + \frac{1}{2}\omega_c\,(\mathrm{m_l}+g^*S) - \frac{\alpha\, e^2}{\in\sqrt{r^2+d^2}} \quad (4)$$

For further details, refer to previously published work [42,43].

2.2. Binding energy and magnetic properties

Binding energy $(B.E)$ can be defined as the difference in ground-state energy E_G between the absence and presence of the impurity,

$$B.E = E_{G_{\alpha=0}} - E_{G_{\alpha=1}} \quad (5)$$

Initially, the energy spectra have been used to calculate the statistical average energy as,

$$\langle E\rangle = \frac{\sum_j^{N_{max}} \mathrm{E}_j\, e^{-E_j/k_BT}}{\sum_j^{N_{max}} e^{-E_j/k_BT}} \quad (6)$$

Where the summation is taken over all the energy spectra of the system.

The magnetization (the magnetic susceptibility) can be obtained by finding the first (second) derivative of the average energy of the QR system with respect to B, mathematically,

$$M(T,\omega_0,B,R_0,\ d) = -\frac{\partial\langle E\rangle}{\partial \mathrm{B}} \quad (7)$$

$$\chi(T,\omega_0,B,R_0,\ d) = -\frac{\partial^2\langle E\rangle}{\partial \mathrm{B}^2} \quad (8)$$

3. Result and discussion

The previous theory is valid for any material type, but in this work, we have considered QR made from, for which the material parameters are given by: $m^* = 0.067m_e,\ \in = 12.4,\ \mathrm{g}^* = -0.44$.

3.1. Energy spectra

The energy spectra of a single electron confined in GaAs QR as a function of the magnetic field are displayed in Fig. 2. Fig. 2(a) displays the well-known Fock-Darwin levels in case ($R_0 = 0$)and without impurity ($\alpha = 0$), which matches the parabolic quantum dot spectra provided

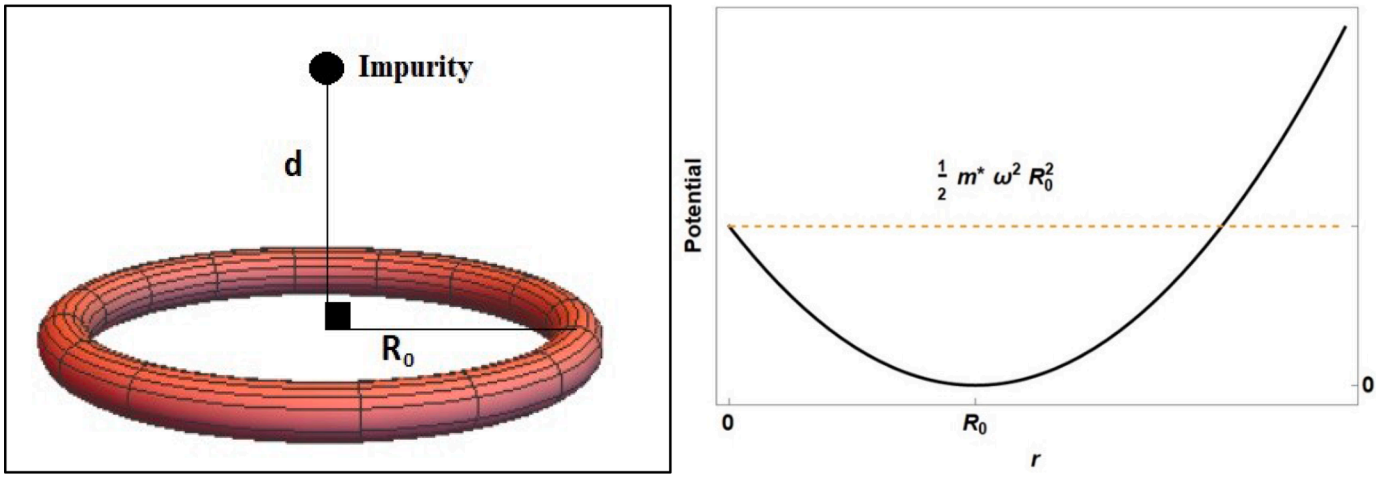

Fig. 1. (a) the QR scheme in the presence of the off-center impurity. (b) The parabolic confinement potential of QR as a function of radial position r.

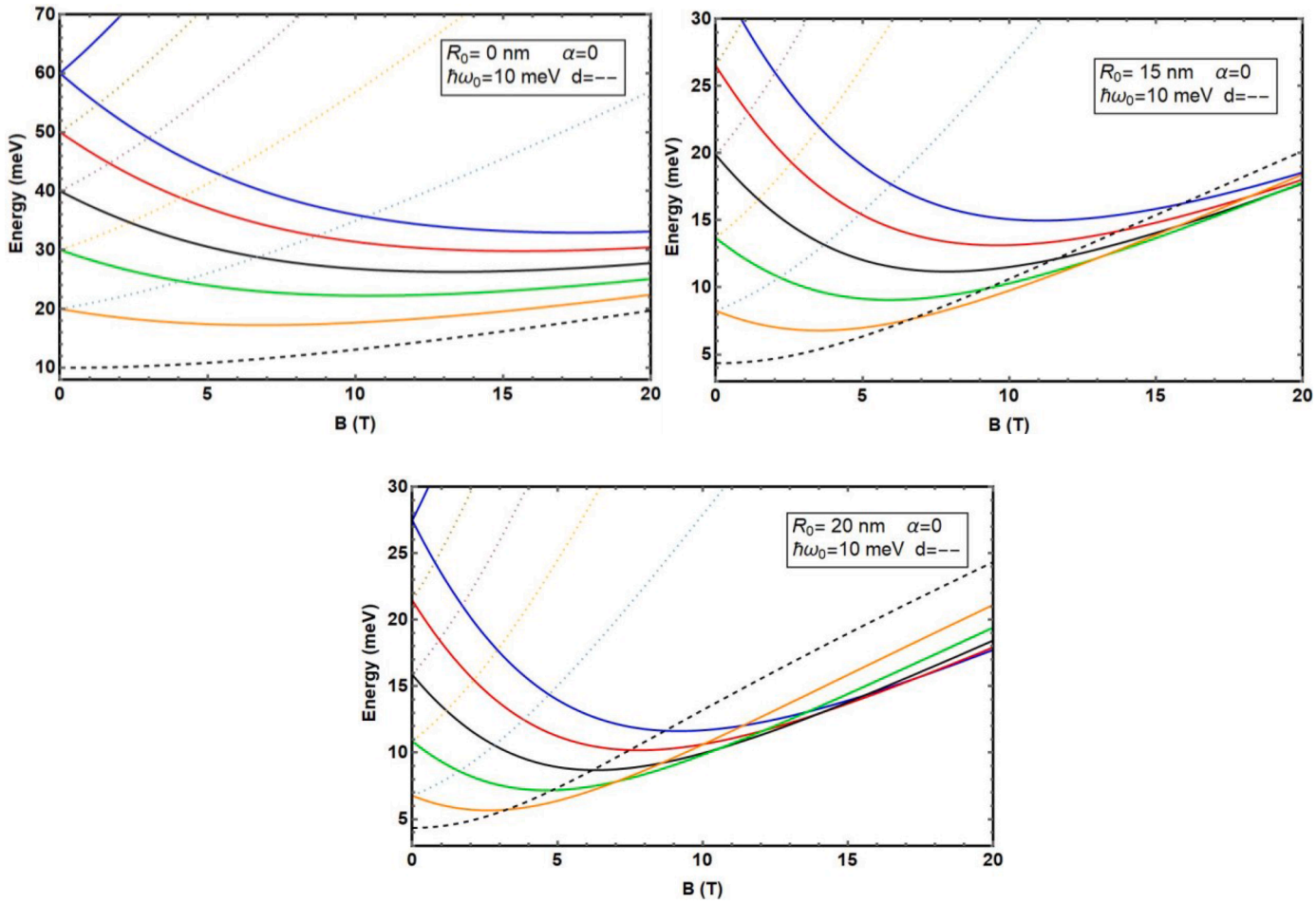

Fig. 2. Energy spectra as a function of the applied magnetic field in the absence of the impurity at $\hbar\omega_0 = 10$ *meV* and various values of R_0: (a) $R_0 = 0$ *nm*, (b) $R_0 = 15$ *nm* and (a) $R_0 = 20$ *nm*.

by $(n + |m| + 1)\hbar\omega - \hbar\, m\, \omega_c/2$, where $\omega = \sqrt{\omega_0^2 + \omega_c^2/4}$ and the spin term was neglected. Fig. 2(b) shows the system spectra in the case of $R_0 = 15$ *nm*, we can observe interesting level crossings; consequently, $m = 0$ will no longer be the ground state as the magnetic field increases, which is consistent with the experimental results of Ref [44].

Fig. 2(c) shows the system spectra in the case of $R_0 = 20$ *nm* and $\hbar\omega_0 = 10$ *meV*. In this figure, we can notice fascinating level crossings shifting to lower magnetic field strength; consequently, $m = 0$ will no longer be the ground state as the magnetic field increases.

Fig. 3(a) shows the influence of impurity on the QR spectra. We can see a considerable shift in the ground state $m = 0$, without level crossings, due to electron-impurity coulomb interaction. In Fig. 3(b) and (c), the off-center impurity case has been studied for $d = 12$ nm and $d = 20$ nm; we can notice that as d increases, the electron-impurity coulomb interaction decreases, so the level crossings shift to lower magnetic field strength.

3.2. Binding energy

The impurity binding energy is studied in Fig. 4 as a function of the quantum ring radius (R_0)and the impurity distance (d). In Fig. 4(a), the BE is plotted for $B = 6$T, $\hbar\omega_0 = 7$ *meV* and different values of d: (0,5,10) nm. From this figure, we can conclude that as the radius of the ring increases, the electron-impurity repulsion coulomb interaction decreases, so the BE curves decline. Moreover, we can notice the decrease in the BE curves as d increases due to reducing the electron-impurity repulsion coulomb interaction. In Fig. 4(b), the BE is plotted for $\hbar\omega_0 = 7$ *meV* , $B = 0$ T and two values of the radius, $R = 0$ nm (quantum dot case) and $R = 15$ nm. This figure shows the decline in BE curves as d increases because of the decrease in the electron-impurity repulsion coulomb interaction. It can be noticed that the values of BE in the $R = 0$ nm case are higher than in the $R = 15$ nm case. This is because, in the case of $R = 0$ nm, the impurity is centrally above the electron, increasing the attraction between them, so the BE values decrease.

3.3. Statistical energy

The statistical average energy has been plotted as a function of temperature in Fig. 5. The curves show that at low temperatures ($T < 10K$), the electron has a small probability of being in the higher states. As a result, $\langle E \rangle$ approaches the same value regardless of the increase in the levels taken by Eq. (6). For relatively higher temperatures, we can conclude that, after examining the convergence up to a temperature of 20 K, it is considered sufficient to deal with the value of N_{max} up to 40 since all the observations in this work are within the range ($T < 40\ K$).

We have plotted in Fig. 6 the average statistical energy as a function of magnetic field strength. In two cases: the presence and absence of the donor impurity for $\omega_0 = 10$meV, $T = 0.5$ K, and various values of R_0 and d. We found that in the absence of the donor impurity ($\alpha = 0$), the curve of average statistical energy is smooth as it has no crossing in the energy levels when $R_0 = 0$. In contrast, in the case of $R_0 = 15$ *nm*, cusps appear in the curve due to the crossing of the energy levels. In the presence of the donor impurity ($\alpha = 1$), we have displayed the curves of the average statistical energy for two values of d, $d = 20nm$, and $d =$

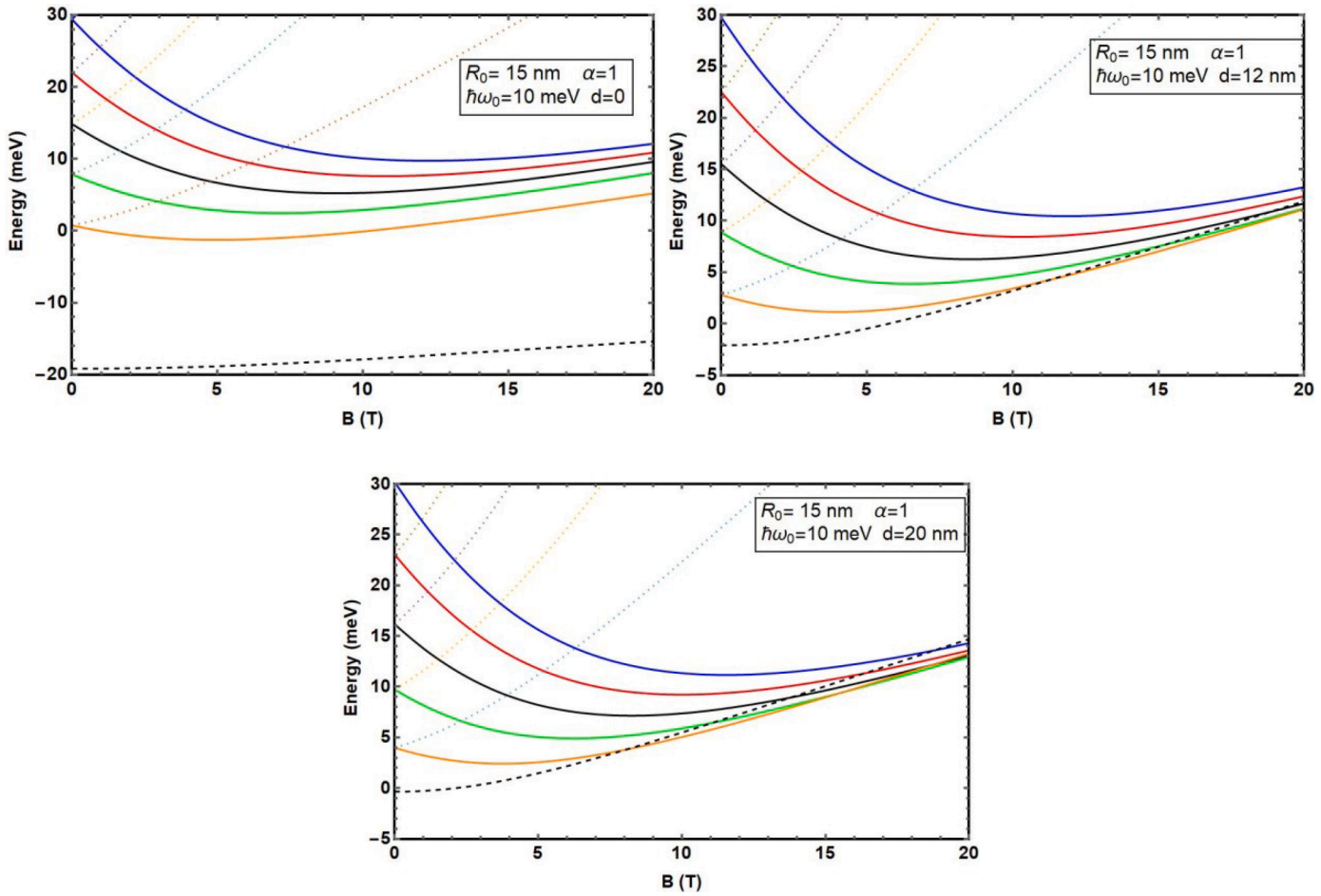

Fig. 3. Energy spectra as a function of the applied magnetic field for $\alpha = 1$ at $\hbar\omega_0 = 10\ meV$, $R_0 = 15\ nm$ and various values of d : (a) $d = 0\ nm$, (b) $d = 12\ nm$, and (a) $d = 20$ nm.

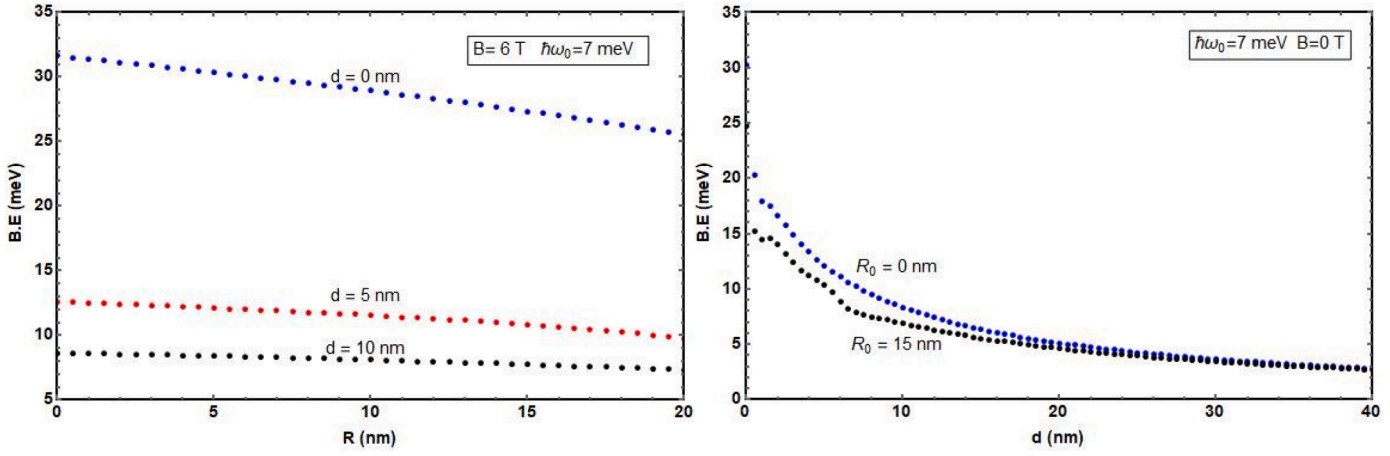

Fig. 4. Impurity Binding energy for $\omega_0 = 7\ meV$, as a function of (a,) impurity position d, (b) quantum ring radius R.

50*nm*. For both curves, we can notice the cusps in the curves. The cusps in average statistical energy curves manifest themselves in the magnetic properties' curves.

3.4. Magnetization and magnetic susceptibility

In Fig. 7, we have investigated the dependence of the magnetic properties (*M and* χ) on the magnetic field, at ω_0= 10meV, $T = 0.5$ K and $R_0 = 15nm$, for both cases: $\alpha = 0$ and $\alpha = 1$ and for different values of d. In Fig. 7(a), the cusps in the magnetization curves resulting from energy levels crossings can be noticed clearly. These cusps in the magnetic susceptibility curve can be seen in Fig. 7(b). In addition, we can notice in both figures, Fig. 7(a) and (b), that as d increases, the electron-impurity coulomb interaction decreases, so the levels crossing shifts to lower magnetic field strength. As a result, the cusps in the magnetic properties curves move to lower B values.

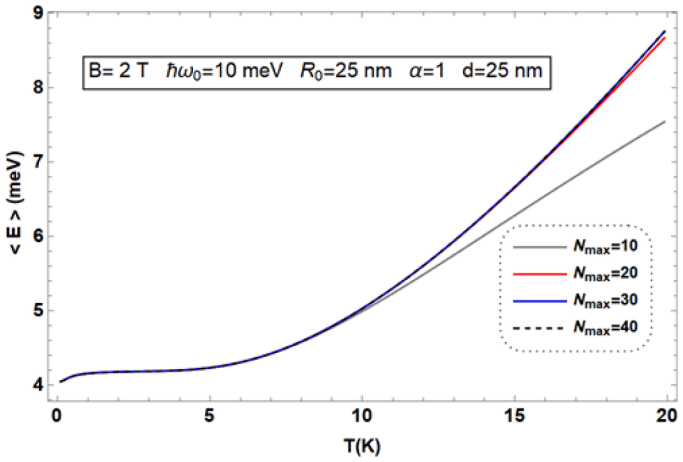

Fig. 5. $\langle E \rangle$ vs. T for different numbers of states (N_{max}).

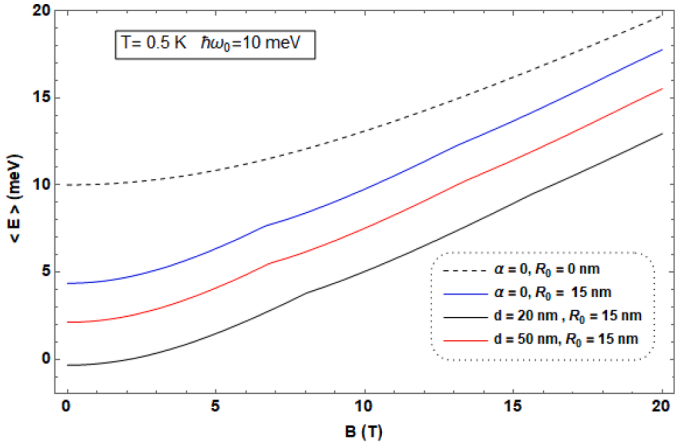

Fig. 6. $\langle E \rangle$ vs. B for fixed confinement strength and various values of α, R_0 *and d*..

The contour plots of the magnetic susceptibility have been demonstrated in Fig. 8. At $T = 1K$. The plot shows a diamagnetic-paramagnetic transition occurs at $B \approx 6.2T$ $(7.6\ T)$ in the absence (presence) of the impurity. For higher temperatures, the transition occurs at the lower magnetic field due to the spectral line shape of the magnetic susceptibility. The present result is in agreement with a published work [45].

To show the effect of the impurity position on the susceptibility, the contour plot for χ, as a function of the magnetic field and off-center impurity position, is given in Fig. 9. The figure shows the significant effect of the impurity position in manipulating the dia-paramagnetic phase transition. In the case of the on-center impurity, the ground state energy shifts to a lower value, lifting the level crossings, which enhances the diamagnetic behavior of the material for all ranges of the magnetic field. On the other hand, as the impurity is moved away, the shift in the ground state decreases gradually. as a result, the transition point moves to a lower magnetic field value. Eventually, it converges to the magnetic field value $(B \approx 6.2T)$, the transition point in the absence of impurity, as previously mentioned.

4. Conclusion

In this work, we consider the Hamiltonian of a single electron moving in a two-dimensional (2D) quantum ring, taking into account the presence of an off-center impurity. We have used the shifted 1/N expansion method to solve the QR Hamiltonian and find the energy spectra as a function of the system parameters. In addition, the computed eigenvalues are used to calculate the statistical average energy, binding energy, magnetization, and magnetic susceptibility as a function of confinement strength, ring average radius, impurity location, and temperature. It has been shown that the QR nanostructure generates ground-state transitions due to its geometric heterostructure, resulting in oscillatory magnetic behavior. Furthermore, the results show that energy level crossings depend on the QR radius and impurity location, attributed to the attraction-coulomb interaction between the confined electron and the donor impurity.

Moreover, the results explain the dependence of the binding energy on the quantum ring radius, impurity position, and the applied magnetic field. We have found that the binding energy for the quantum dot $(R_0 = 0)$ is more enhanced than the quantum ring.

The crossings of the energy levels manifest themselves as oscillations in the magnetic properties of the QR system. We can conclude that the magnetization and the magnetic susceptibility peak positions depend on the QR radius and impurity location. As a result, changing the impurity position can manipulate the magnetic field value correspondence to these diamagnetic-paramagnetic phase transitions.

CRediT authorship contribution statement

Ayham Shaer: Conceptualization, Software, Writing – original draft, Visualization. **Eshtiaq Hjaz:** Investigation, Writing – original draft, Writing – review & editing. **Mohammad K. Elsaid:** Conceptualization, Methodology, Supervision.

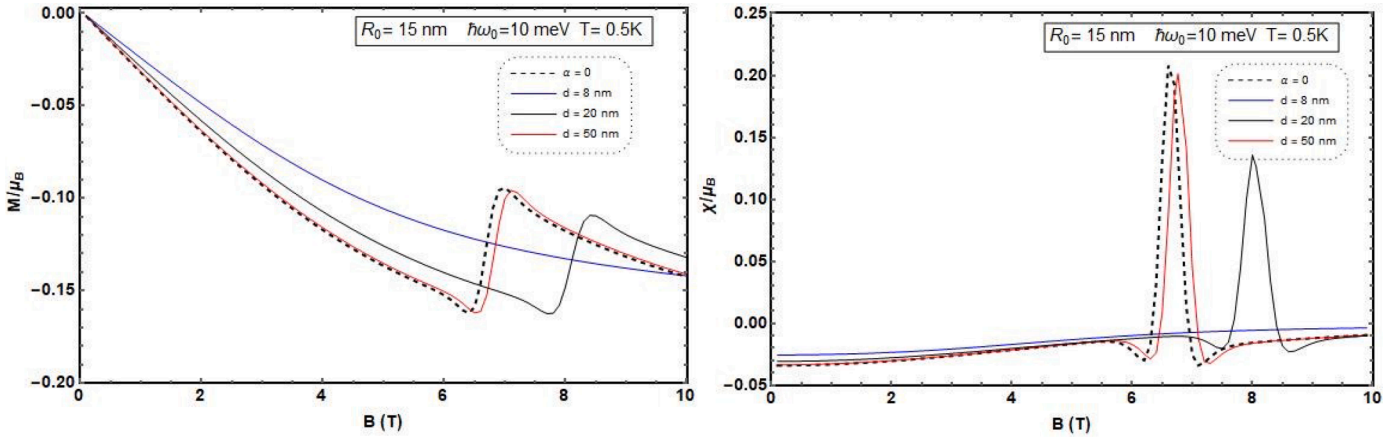

Fig. 7. The magnetic properties curve as a function of magnetic field strength for $\hbar\omega_0 = 10$meV, $T = 0.5$ K and $R_0 = 15nm$:(a) magnetization as a function of B, (b) magnetic susceptibility as a function of B.

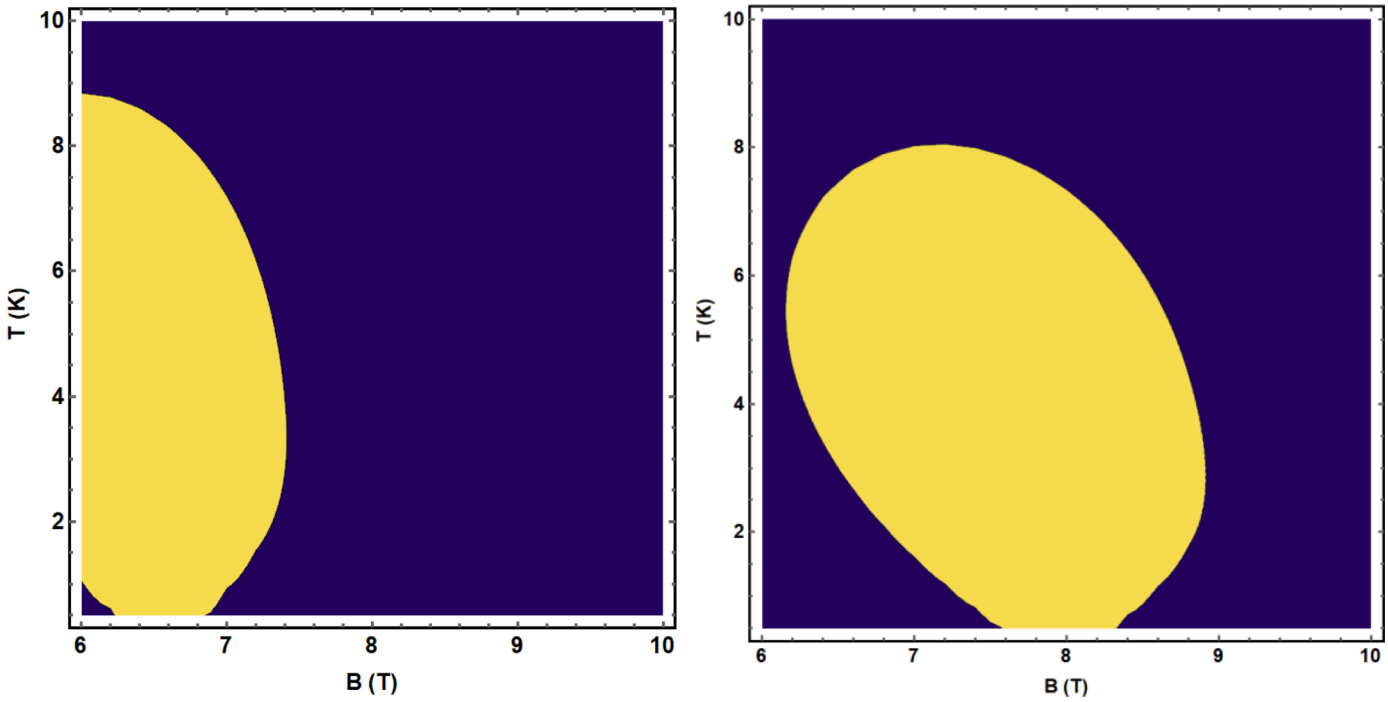

Fig. 8. (a) χ as a function of B and T for $R_0 = 15\ nm$, $\hbar\omega_0 = 10\ meV$ (a) in the absence of impurity (b) $d = 20$ nm.

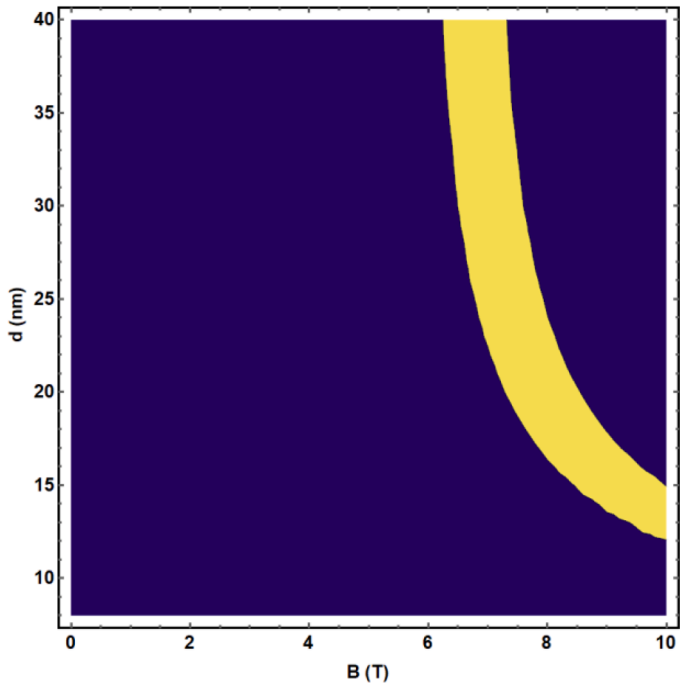

Fig. 9. χ as a B and d for $R_0 = 15\ nm$, $\hbar\omega_0 = 10\ meV$ *and* $T = 1\ K$.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

No data was used for the research described in the article.

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