

# The Effect of Magnetic Field on the Thermodynamic Properties of Three-Dimensional GaAs Quantum Dot

M. M. Al Shorman<sup>1</sup>

<sup>1</sup> Department of Applied Physics, Tafila Technical University, Tafila, Jordan

Correspondence: M. M. Al Shorman, Department of Applied Physics, Tafila Technical University, Tafila, 66110 Jordan.

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## Abstract

The problem of parabolically single three-dimensional semiconductor GaAs quantum dot in the presence of an external magnetic field and including the spin of the electron is studied using canonical formalism. The energy spectrum is obtained as a function of temperature and magnetic field. It is observed that the system tends to absorb the largest amount of heat at critical values of the magnetic field which depends on the temperature. A schottky-like anomaly in heat capacity is observed at low temperature, while at high temperature it converges rapidly and saturates. It was also found that the entropy is inversely proportional to the magnetic field strength, also entropy showed exciting behavior at low temperature, a shoulder is observed which becomes curvier when the magnetic field decreases. However, at high temperature, entropy increases monotonically with temperature and becomes essentially independent of the magnetic field. The substantial effect of magnetic field on the magnetic properties of quantum dot is observed at low temperature. It is shown that, magnetization increases significantly at low temperature and shows strong dependence on magnetic field, while its magnitude increases as the temperature increases and reduces to zero regardless the value of magnetic field strength. In addition, at low temperature susceptibility peaks and is found to be paramagnetic and at high temperature the diamagnetic state is found to be a favored state of the system and susceptibility becomes completely independent of magnetic field. It is also shown that for a fixed value of temperature, susceptibility increases rapidly with magnetic field and beyond a critical value of magnetic field, the increase becomes much slower, susceptibility exhibits a crossing behavior, and magnetization shows a significant drop as the magnetic field increases. So far, no study has been made in literature on the effect of magnetic field on the thermal and magnetic properties of three-dimensional quantum dot.

**Keywords:** quantum dot, heat capacity, entropy, magnetization, susceptibility

## 1. Introduction

In the last few years, the growing interest in the development of nanoscience and one of the latest applications of nanotechnology has led to the manufacture of a distinctive type of semiconductor called quantum dots (A. A. Shukri et al., 2019; Kouwenhoven, 2001). They might be manufactured on semiconducting material chips with the aid of electrostatic confinement of a two-dimensional electron gas. Quantum dot could be a tiny semiconductor region, where the electrons are confined into a tiny low size (~100 nm) exhibiting a discrete spectrum of energy levels, usually it contains a few controllable numbers of electrons starting from one electron to many thousand (Kastner, 1993). The discrete, quantized energy levels of quantum dots relate them more closely to atoms than bulk materials and have resulted in quantum dots being nicknamed 'artificial atoms', since the potential of the nucleus is replaced by the confinement potential. In Addition, size, shape and number of confined electrons can be manipulated precisely. These QDs can be viewed as tiny semiconductor devices where the expectations of quantum mechanics can be investigated decisively, so that the impacts of quantum mechanics show up obviously (Chakraborty, 1999; Sichert et al., 2015). Few-electron QD attracted the interest of both experimental and theoretical researchers because their spectrum is expected to be extraordinarily rich because the single-electron confinement energy, the cyclotron energy for modest fields and the electron-electron interaction energy can all be of comparable significance (typically a few meV), and they scale differently as far as one varies dot parameters. However, the energy spectrum is also likely to be strongly depends on the number of confined electrons (e.g.  $N < 20$ ) (Read et al., 1989; Jacak et al., 1998; Johnson, 1995). Due to their exceptionally tunable properties, QD

technology continues to expand, the research is striving to bring their benefits to more and more technologically applied fields such as solar cells, transistors, LEDs, medical imaging and quantum computing (Banyai et al., 1993; Reimann et al., 2002; Kouwenhoven et al., 2001; Alhassid, 2000).

The vast majority of hypothetical investigations concentrated on the energy spectra of few-electron quantum dots and utilized numerical and computational methods to construct new precisely solvable many-body models in higher dimensions and explore novel correlations, for example, Hartree-Fock approximation (HF) (Pfannkuche et al., 1993), Density Functional Theory (DFT) (Jiang- et al., 2003), the exact methods like Exact Diagonalisation (ED) (Ezaki et al., 1998), Quantum Montecarlo (QM) (Williamson et al., 2002) and static fluctuation approximation method (Nmmas et al., 2011). The consequences of these computations demonstrated that there is a particular parameter for every quantum dot. There have been several investigations in the last few years of the quantum thermodynamics characteristics of quantum dots, because of the enormous potential for future technological applications. Haddad *et al.* (Haddad *et al.*, 2017) calculated the thermal properties analytically for one electron confined in three-dimensional parabolic quantum dot. Nmmas *et al.* (Nmmas et al., 2011) found the numerical results for heat capacity and magnetization. They observed sharp peaks in heat capacity due to the crossing of the lowest level with a higher level and magnetization has a monotonic diamagnetism and exhibits sharp jumps. Thermal and magnetic properties of cylindrical quantum dot with asymmetric confinement have been investigated using canonical formalism in the presence of external electric and magnetic fields (Gumber et al., 2015). They demonstrated that, thermal and magnetic properties do not depend on the electric field, but they are very sensitive to the temperature interaction with the magnetic field and dot size. It was found that there are transitional regions of the magnetic field and temperature, after which there is no significant change in heat capacity and magnetization, such that heat capacity saturates and magnetization reaches a constant value. Also, the paramagnetic state is found to be a preferred state of the system. Boyacioglu and chatreeg (<sup>1</sup>Boyacioglu et al., 2012) studied the total magnetization and susceptibility of GaAs quantum dot with Gaussian confinement including the spin Zeeman effect. They observed the paramagnetic behavior at low magnetic field and low temperature, while at high magnetic field and high temperature the system is in a diamagnetic state. Gumber *et al.* (Gumber et al., 2016) investigated thermal and magnetic properties of InSb Rashba quantum dot. It is noted that the effect of Rashba spin-orbit interaction is significant on magnetization, heat capacity and susceptibility only at low values of magnetic field, its sharpness the peak observed in heat capacity, it shifts it to the lowest temperature value. Recently, heat capacity and entropy have been calculated in a closed form, for two electrons with parabolic interaction confined in parabolic quantum dot in the presence of external magnetic field (Al Shorman et al., 2018). Canonical formalism had been used to calculate thermal and magnetic properties of one electron confined in two-dimensional Gaussian quantum dot (<sup>2,3</sup>Boyacioglu et al., 2012). The specific heat was obtained by solving Schrodinger's equation analytically for two electrons confined in a parabolic quantum dot, considering both the harmonic interaction between the electrons and the Dresselhaus spin-orbit interaction (DSOI) (Kumar et al., 2016). It is noted that heat DSOI has intangible effect on heat capacity at low magnetic field even at finite temperature. While at high magnetic field DSOI decreases the heat capacity and a peak is observed due to transition from Fock-Darwin state to landau-state. In the present paper, thermal and magnetic properties are calculated analytically as a function of temperature and magnetic field for one electron confined in three-dimensional quantum dot (3DQD) in the presence of the spin Zeeman effect.

The paper is organized as follows, in Section 2 the mathematical formalism for the system is presented. Analysis and discussion of the thermal and magnetic properties obtained for GaAs QD are summarized in Section 3. In Section 4, the paper ends with important conclusions and observations.

### 1.1 Model and Formulation

The beginning stage for computing the thermodynamic functions is the calculation of the energy spectrum of two electrons in a 3DQD. This can be accomplished by solving the Schrodinger wave-equation analytically. The effective Hamiltonian of a system of one electron moving in a 3D parabolic QD and subjected to a uniform magnetic field is given by

$$\hat{H} = \frac{1}{2m^*} (\vec{p} + e\vec{A}(\vec{r}))^2 + \frac{1}{2} m^* \omega_0^2 r^2, \quad (1)$$

where,  $\vec{p}$  is the corresponding momentum operator,  $\vec{r}$  refers to the position vector of an electron in three dimensions,  $m^*$  is the electron effective mass (to include the effect of the host semiconductor material),  $\omega_0$  is the confinement frequency of the parabolic potential and  $\vec{A}$  is the vector potential corresponding to the magnetic field  $\vec{B}$  which has been applied in the z direction. The vector potential corresponding to a uniform magnetic field may be

written as  $\vec{A} = \frac{1}{2}(B\hat{z} \times \vec{r})$ , choosing the gauge such that  $\vec{A}$  divergence-less and including the spin-Zeeman term, one can write Eq. (1) as

$$\hat{H} = \frac{\hat{p}^2}{2m^*} + \frac{1}{2}m^*\omega_0^2r^2 + \frac{eB}{2m^*}\hat{L}_z + \frac{e^2B^2}{8m^*}(x^2 + y^2) + \frac{1}{2}g^*\hbar\omega_c\hat{S}_z, \quad (2)$$

where  $\omega_c$  is the bare electron cyclotron frequency given by  $\omega_c = eB/m^*$ ,  $g^* = -0.44$ , is the effective Lande factor for GaAs QD and  $\hat{L}_z$  is the z-component of the angular momentum of the electron. The third terms in Eq. (2) is associated with paramagnetism, the fourth one with diamagnetism. Before addressing the role of these separate contributions in a QD, let us first estimate their relative magnitude. With  $\langle x^2 + y^2 \rangle \approx a_0^2$ , where  $a_0$  denotes the Bohr radius, and  $\langle \hat{L}_z \rangle \approx \hbar$ , the ratio of the paramagnetic and diamagnetic terms is given by

$$\hat{H} = \frac{\frac{e^2B^2}{8m^*}\langle x^2 + y^2 \rangle}{\frac{eB}{2m^*}\langle \hat{L}_z \rangle} = \frac{eB^2a_0^2}{4\hbar B} = 10^{-6} B/T. \quad (3)$$

Therefore, while electrons remain bound to a QD, for fields that can be achieved in the laboratory ( $B = 1T$ ), the diamagnetic term is negligible as compared to the paramagnetic term. Retaining only the paramagnetic contribution, the Hamiltonian for an electron moving in a parabolic confining potential in the presence of a constant magnetic field then takes the form,

$$\hat{H} = \hat{H}_0 + \frac{eB}{2m^*}\hat{L}_z + \frac{1}{2}\hbar\omega_c g^* \hat{S}_z, \quad \hat{H}_0 = \frac{\hat{p}^2}{2m^*} + \frac{1}{2}m^*\omega_0^2r^2 \quad (4)$$

Since  $[\hat{H}_0, \hat{L}_z] = 0$  and  $[\hat{H}_0, \hat{S}_z] = 0$ , eigenstates of unperturbed Hamiltonian,  $\hat{H}_0$ , defined by  $\Psi_{nlms}$ , remain eigenstates of  $\hat{H}$ , with eigenvalues (Stechle, 1966; Greiner, 1989),

$$E_{nlms} = \hbar\omega_0 \left( 2n + l + \frac{3}{2} \right) + \frac{1}{2}\hbar\omega_c g^* s + \frac{1}{2}\hbar\omega_c m \quad (5)$$

where  $n \geq 0$ , is the radial quantum number,  $l \geq 0$ , is the angular momentum quantum number,  $m = 0, \pm 1, \pm 2, \dots$ , is the magnetic quantum number and  $s = \pm 1/2$ , is the eigenvalues of the spin operator  $\hat{S}_z$ . In the present work, we are interested in the dependence of thermal and magnetic properties on the temperature and magnetic field. The partition function can be calculated exactly and is given by (Landau et al., 1975; Greiner et al., 1995)

$$Z = \frac{\left( 1 + \text{Cosh}\left[\frac{g^*\hbar\omega_c}{2k_B T}\right] + \text{Sinh}\left[\frac{g^*\hbar\omega_c}{2k_B T}\right] \right) \left( \text{Cosh}\left[\frac{\hbar(2\omega_0 + 2\omega_c - g^*\omega_c)}{4k_B T}\right] + \text{Sinh}\left[\frac{\hbar(2\omega_0 + 2\omega_c - g^*\omega_c)}{4k_B T}\right] \right)}{\left( \text{Cosh}\left[\frac{\hbar\omega_0}{k_B T}\right] - \text{Cosh}\left[\frac{\hbar\omega_c}{2k_B T}\right] + \text{Sinh}\left[\frac{\hbar\omega_0}{k_B T}\right] - \text{Sinh}\left[\frac{\hbar\omega_c}{2k_B T}\right] \right) \left( -1 + \text{Cosh}\left[\frac{\hbar\omega_0}{k_B T} + \frac{\hbar\omega_c}{2k_B T}\right] + \text{Sinh}\left[\frac{\hbar\omega_0}{k_B T} + \frac{\hbar\omega_c}{2k_B T}\right] \right)} \quad (6)$$

Now, it is straightforward to use the partition function through which, thermal and magnetic properties of the system can be calculated, i.e., mean internal energy  $\bar{\epsilon} = k_B T^2 (\partial \ln Z / \partial T)$ , heat capacity  $C = \partial \bar{\epsilon} / \partial T$ , Helmholtz free energy  $F = -k_B T (\ln Z)$ , is employed to obtain the entropy  $S = -\partial F / \partial T$ , magnetization  $M = -\partial \bar{\epsilon} / \partial B$  and susceptibility  $\chi = \partial M / \partial B$ . We do not give a closed form expression for these properties, because they are too long. However, we shall demonstrate their behavior graphically.

In the next section, we examine the behavior of mean energy, heat capacity, entropy, magnetization and susceptibility of 3D parabolic GaAs QD as a function of temperature and magnetic field and present the results with related discussions.

## 2. Results and Discussion

In this work, we present the results for one electron confined in a three-dimensional parabolic quantum dot made from GaAs semiconductor material with  $m^* = 0.067m_e$  and confinement potential  $\hbar\omega_0 = 30\text{meV}$ . In Figure 1,

the mean energy has been plotted as a function of temperature at three different values of magnetic field. It is clear that, the mean energy enhances as the temperature increases at a fixed value of the magnetic field. However, the behavior of mean energy at low temperatures is qualitatively different. For example, at low temperature, the effect of the magnetic field on the mean energy is obvious, and mean energy develops a curvy behavior. This curvy behavior becomes more and more pronounced as the magnetic field decreases. However, at high temperature, i.e.,  $T > 55\text{K}$ , the mean energy increases monotonically with temperature and becomes independent of the magnetic field and finally converges to a straight line. This indicates a peak in heat capacity; this reminds us to enter a mixed phase of liquid-gas.

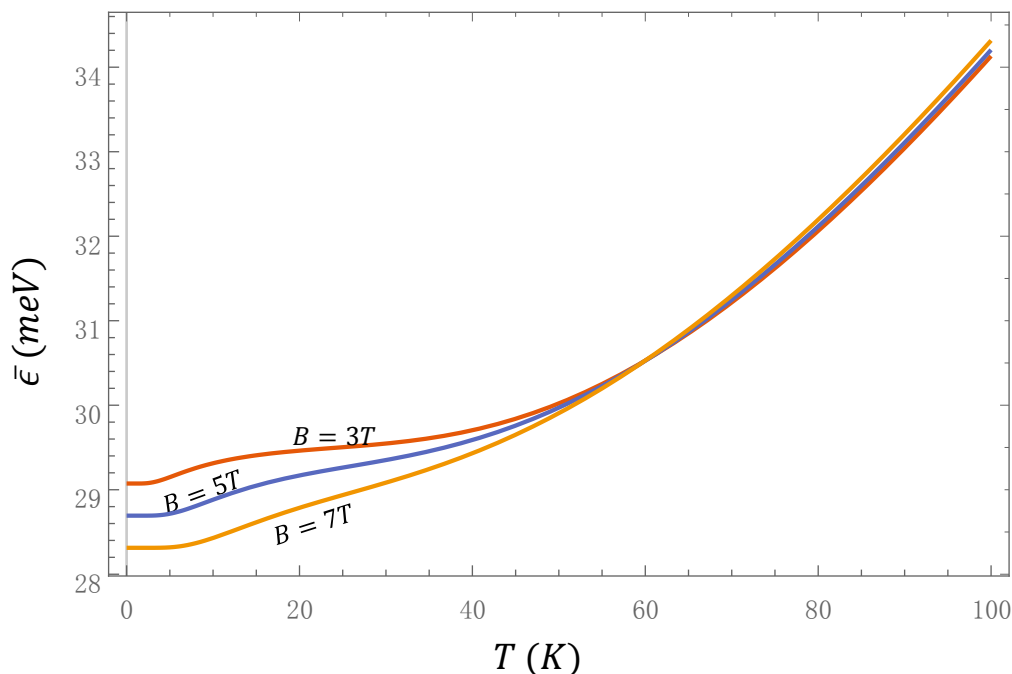


Figure 1. The average thermal energy ( $\bar{\epsilon}$ ) vs. temperature ( $T$ ) of 3D parabolic GaAs quantum dot for  $B=3, 5$  and  $7$  Tesla

A variation of the mean energy with respect to the magnetic field is presented in Figure 2 for different values of temperatures. The figure shows a significant energy enhancement when the magnetic field increases. Also, it is noted that for a fixed value of magnetic field, the mean energy increases as the temperature increases, i.e., the slope of the curve strongly depends on the temperature. For example, the smaller the slope of the curves corresponds to larger temperature. Furthermore, as the magnetic field increased the electron strongly confined in the QD, resulting in an increase in the magnetic energy, and in effect the energy levels. This affirms the fact that the confinement effects are appreciable for strong magnetic field.

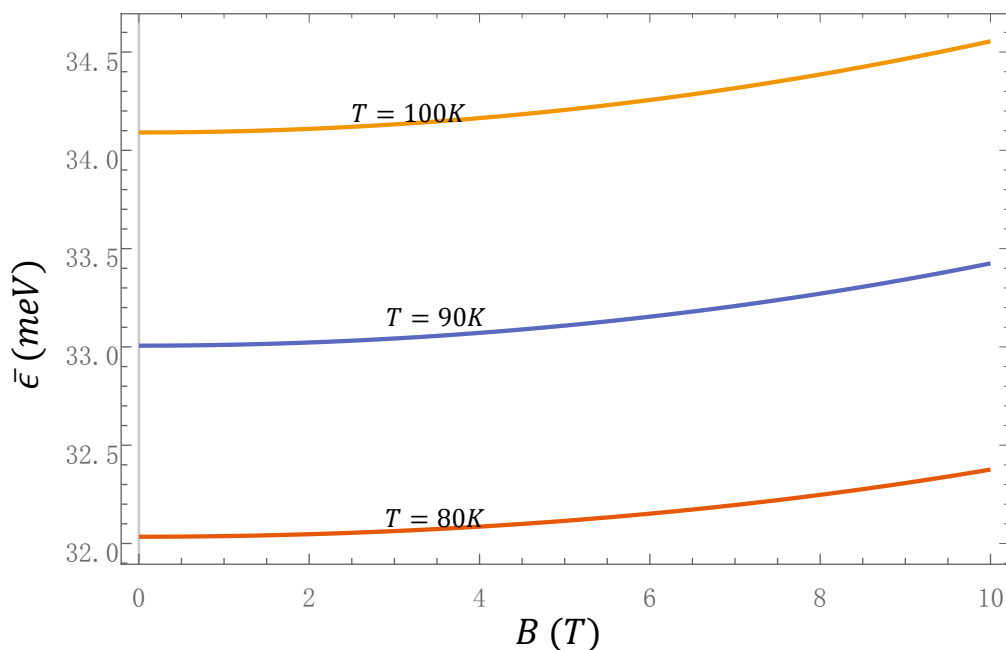


Figure 2. The average thermal energy ( $\bar{\epsilon}$ ) vs. magnetic field (T) of 3D GaAs QD for  $T=80, 90$  and  $10K$

The dependence of heat capacity on temperature is presented in Figure 3. It is noted that at low temperature heat capacity shows a peak structure related to the electron's spin, and when the magnetic field increases, this peak shifts to the right and becomes wider in width. Also, it is observed that at  $B=10T$ , peak turns into a shoulder. In fact, this peak structure reminds us of the Schottky anomaly of the heat capacity for the two-level systems at low temperatures. However, as the temperature continues to rise, the specific heat reaches saturation with value  $1.5K_B$ .

In Figure 4, we have shown the variation of heat capacity with magnetic field at three different values of temperature. From the figure we conclude that, heat capacity peaks at specific values of the magnetic field related to maximum accessible states for electron of energy  $k_B T$  and then drops very rapidly to zero, more quickly at a low temperature like  $1K$ . It was also observed that, peak width increases at high temperature values like  $10K$  and becomes broader and never comes to zero. This situation can be clarified as follows. Using known parameter values of QD we are expected to obtain a specific discrete energy spectrum. The QD environment will be able to excite the system thermally and the excitement will be maximum at certain values of the temperature at which the system can absorb the maximum energy from the medium, only at specific values of the magnetic field. At other values of the magnetic field, the system will absorb a very little energy available in the QD environment, causing the heat capacity to decrease very rapidly and then reduces to zero.

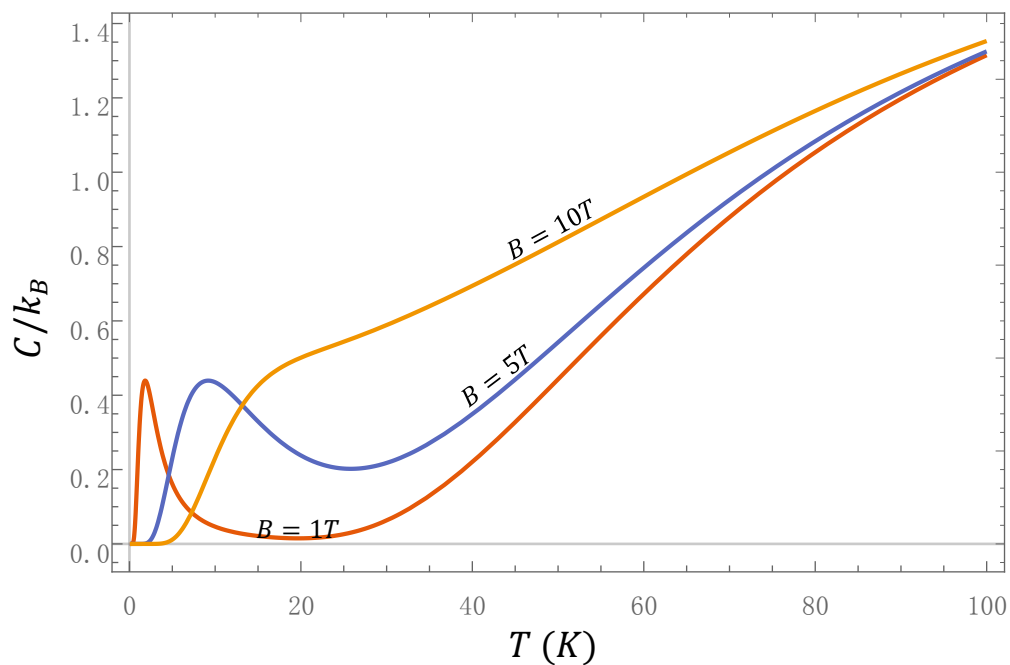


Figure 3. Heat capacity ( $C/k_B$ ) vs. temperature ( $T$ ) of 3D parabolic GaAs QD for  $B=1, 5$  and  $10$  Tesla

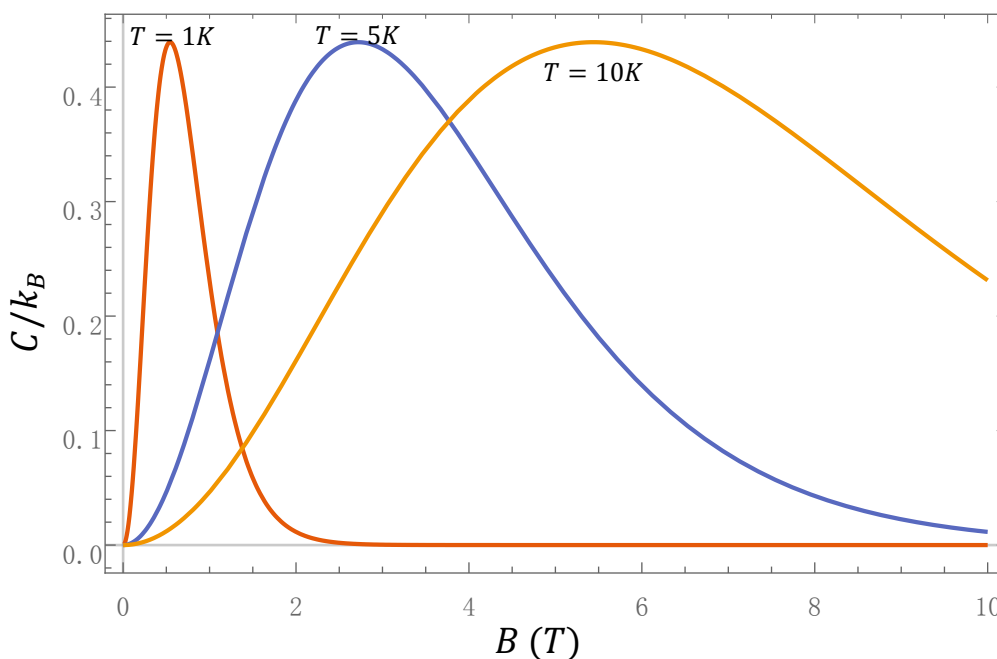


Figure 4. Heat capacity ( $C/k_B$ ) vs. magnetic field ( $B$ ) of 3D parabolic GaAs QD for  $T=1, 5$  and  $10$  K

Entropy is a measure of the random activity in a system. The dependence of the entropy upon the temperature is shown in Figure 5 for three different values of magnetic field. As expected, entropy increases as the temperature increases. However, at high temperatures, the entropy changes almost linearly with temperature; while at low temperature, a shoulder was observed and as the magnetic field decreases, it becomes more and broader. The behavior of  $S-T$  is consistent with the  $C-T$  behavior at low temperature at  $B=1T$ . The increase of entropy with temperature is due to the enhanced heat energy of the electrons that bring more and more disturbance in the form of random motion.

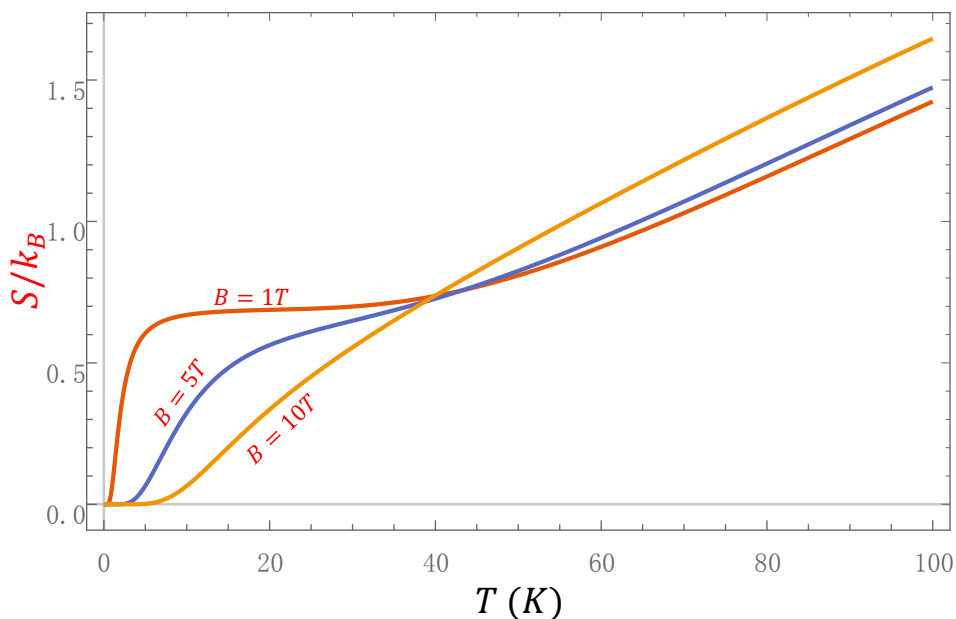


Figure 5. Entropy ( $S/k_B$ ) vs. temperature ( $T$ ) of 3D parabolic GaAs QD for  $B=1, 5$  and  $10$  Tesla

In Figure 6 we plot entropy as a function of magnetic field at three different values of temperature. It was demonstrated that entropy is inversely proportional to the magnetic field. This behavior can be understood as follow, by increasing the magnetic field, the movement of the electron becomes constrained to Landau-type levels, then disorder decreases and consequently entropy reduces to zero. It is, however, more important to note that at  $T=1, 5K$ , the system is in perfect order at  $B=2, 8T$  respectively. While at  $T=10K$ , entropy decreases but never comes to zero, this is due to a competition between thermal energy and magnetic confinement for high values of temperatures and magnetic field.

We now begin to study the magnetic properties of the system. The physical quantity responsible for how the system responds to the magnetic field is magnetization. Figure 7 shows the relationship between magnetization and temperature at three different values of the magnetic field. Magnetization at very low temperatures increase rapidly and depends heavily on the magnetic field, while at high temperatures, magnetization becomes independent of both temperature and magnetic field then it reduces to zero value.

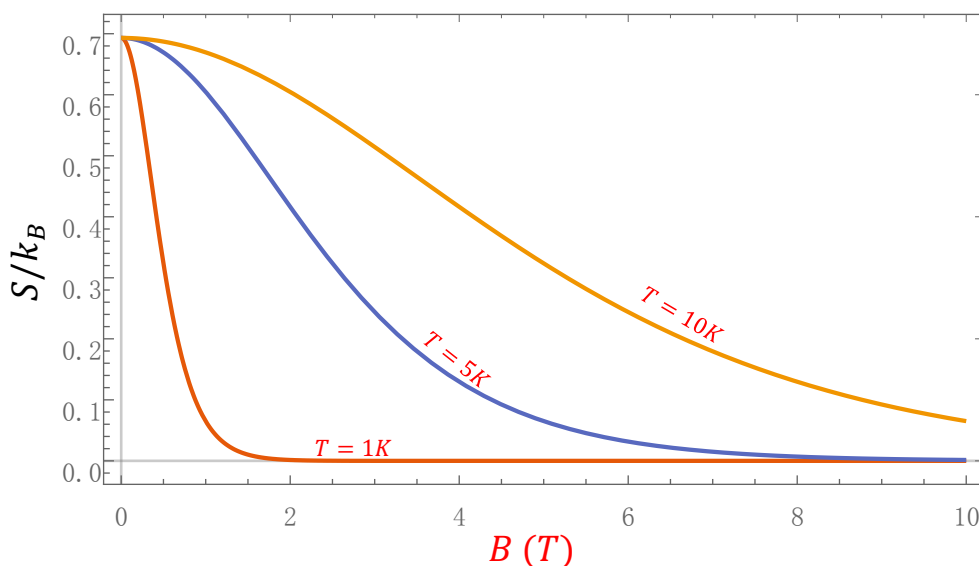


Figure 6. Entropy ( $S/k_B$ ) vs. magnetic field ( $B$ ) of 3D parabolic GaAs QD for  $T=1, 5$  and  $10$  K

Another important magnetic property has been studied is the susceptibility. We have shown in Figure 8 the variation of the susceptibility as a function of temperature for three different values of the magnetic field. At very low temperature, susceptibility is found to be paramagnetic, the effect of magnetic field is appreciable, while at high temperature it becomes diamagnetic due to randomization of the electron's spin also it does not depend on the value of the magnetic field. It is clearly evident that the system prefers to be in a diamagnetic state for large range of temperature regardless of the value of magnetic field. Also, at a critical value of temperature, susceptibility changes abruptly and positive peak is observed after which susceptibility falls sharply and starts decreasing and with further increase in temperature susceptibility approaches zero value.

The magnetic field dependence of the magnetization is presented in Figure 9. It is noticeable that the magnitude of magnetization increases by increasing the magnetic field regardless of the temperature value. Also, one can see a linear relation of magnetization at low values of magnetic field, but at high values of magnetic field the behavior may be quite significant. What we want to say here is that magnetization is diamagnetic this is evident from signature of the curves. The decrease in magnetization can be summarized as follows. The occupation of a state of higher angular momentum becomes strongly favorable for the system and this leads a decrease in magnetization.

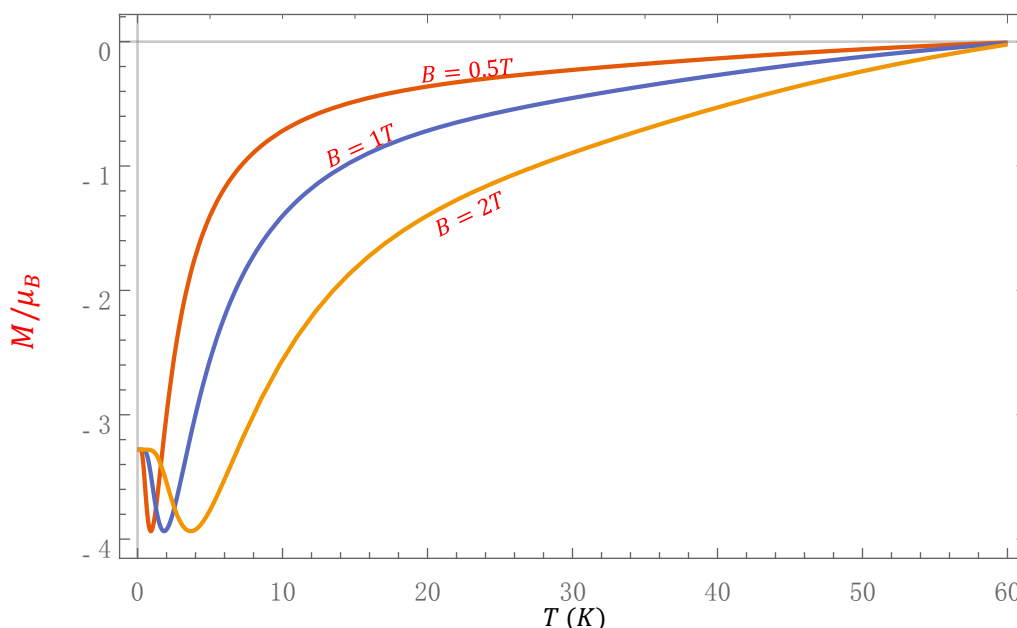


Figure 7. Magnetization ( $M/\mu_B$ ) vs. temperature ( $T$ ) of 3D parabolic GaAs QD for  $B=0.5, 1$  and  $2$  Tesla

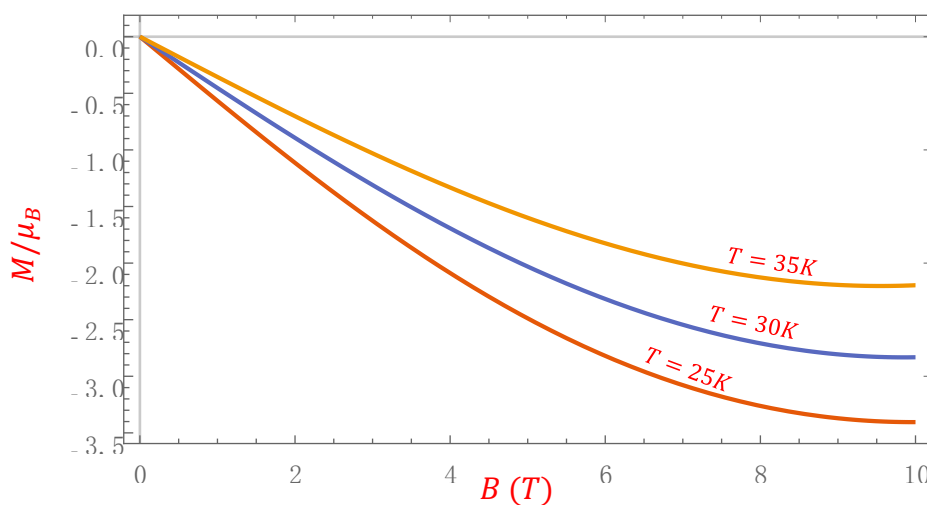


Figure 8. Magnetization ( $M/\mu_B$ ) vs. magnetic field ( $B$ ) of 3D parabolic GaAs QD for  $T=25, 30$  and  $35K$



The characteristic of magnetization of the system produces well through magnetic susceptibility. In Figure 10, the variation of susceptibility with magnetic field is given for different values of temperature. We note from the figure that, susceptibility does not change significantly at low values of the magnetic field for  $B=0.7T$ . But by increasing the temperature, the susceptibility increases significantly even at lower values than the magnetic field. It is noted that above a critical value of magnetic field which depends on the temperature, susceptibility slows down and a crossing behavior is obtained. This is in a full agreement of magnetization behavior presented in Figure 9.

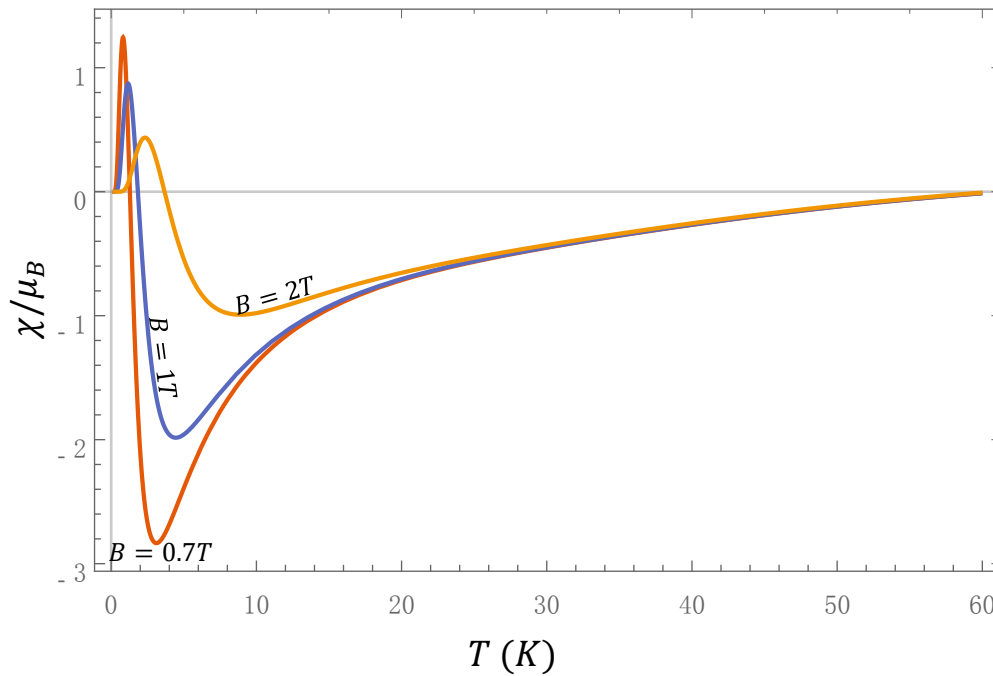


Figure 9. Susceptibility ( $\chi/\mu_B$ ) vs. temperature (T) of 3D parabolic GaAs QD for B=0.7, 1 and 2 Tesla

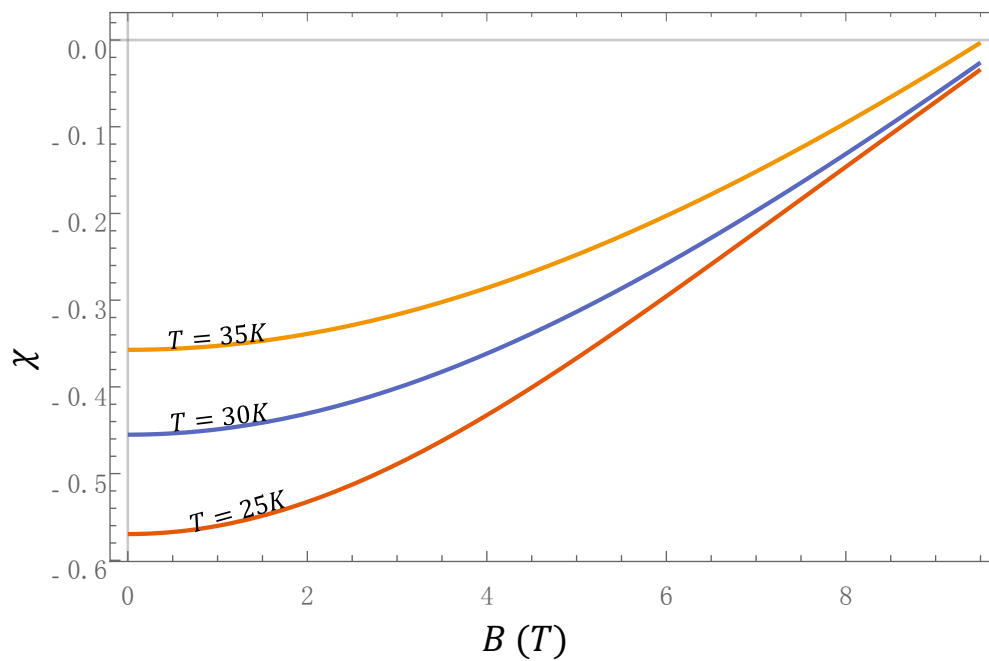


Figure 10. Susceptibility ( $\chi/\mu_B$ ) vs. B of 3D parabolic GaAs QD for T=25, 30 and 35K

### 3. Conclusions

We have studied analytically the problem of single three-dimensional GaAs quantum dot in the presence of magnetic field using the canonical ensemble approach. We have studied the behavior of thermal and magnetic properties of this system as a function of temperature and magnetic field. As a function of temperature, it is noted that heat capacity increases with the temperature and reaches the saturation value of  $1.5K_B$  and the effect of magnetic field is negligible. While at low temperature, heat capacity shows a peak and this peak is shifted to the right and becomes wider as the magnetic field increases, the same behavior was observed for entropy in the low temperature regime. As expected, it was found that entropy increases linearly as the temperature increases. It was also found that the magnitude of magnetization decreases rapidly with increasing temperature and reduces to zero regardless the magnetic field strength, while at low temperatures it increases rapidly, the effect of the magnetic field is tangible. It was also noted that the susceptibility is found to be diamagnetic, its magnitude decreases as the temperature increases and reduces to zero value irrespective of magnetic field strength. But at low temperatures, susceptibility is paramagnetic, and there were peaks that appear at certain values of the magnetic field. As a function of magnetic field. Peaks in heat capacity were observed at certain values of the magnetic field and then decreased rapidly to zero at low temperatures like 1K. The values of the magnetic field that make heat capacity peaks, increase by increasing the temperature, also the width of these peaks is greater in time. It was also observed that, entropy is inversely proportional to the magnetic field, because electron motion is constrained when the magnetic field increases to Landau-type levels, so this leads a decrease in disorder and thus entropy. It is also found that the system is in perfect order at low temperatures like 1K and 5K where entropy decreases to zero value, but at high temperatures like 10K, it decreases and never vanishes due to the competition between thermal energy and the magnetic field. Magnetization is found to decrease with magnetic field while susceptibility is found to be diamagnetic and increases significantly with magnetic field and with further increase in magnetic field, this increase is slow, it exhibits a crossing behavior.

These properties give exciting theoretical observations and can be utilized to decide the real nature of the quantum dot. From fundamental and technological perspectives, the ability to control the magnetic properties of materials will be very desirable, especially in perspective of the current improvements in magneto– hardware and spintronics. The magnetic and thermal properties in materials can be tuned by the size of QD, the mathematical model taken lacks the QD size function, so in the next work the model will be improved by considering the QD size.

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