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Interdependence of External Magnetic and Temperature Effect on Thermodynamic Properties of GaAs Two Electron Quantum Dot

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Abstract: The particular interest of this paper is to investigate the impact of various values of temperature exposed to weak and strong magnetic field strength. A thermodynamic property's oscillatory change as a function of magnetic field effect (B) intensifies the quantization of electron orbits in a constant magnetic field intensity and is the primary contributor to the de Haas-van Alphen effects due to cyclotron frequency and its impact on localizing electron at circular region imposed with the magnetic field that is in contrary to the result of the temperature effect. Thus the interdependent effects of external magnetic field and temperature on thermodynamic properties are studied with harmonic oscillator potentials considering material parameters of GaAs quantum dot. The finite energy state is analytically solved using Nikiforov-Uvarov mathematical formalism. Moreover, the direct impact of the external magnetic fields and temperature on thermodynamic properties of the system is analyzed, and numerically simulated using matlab R2017a version. The dominance of temperature over the external magnetic field and vice versa effect is investigated, thus the value specific heat capacity fluctuated, while the equiponderate impact of temperature and magnetic field shows similar steady values of the specific heat capacity. The study clearly shows the interdependence of magnetic field and temperature affect thermodynamic quantities: partition function, mean energy, entropy, and specific heat capacity.

Keywords: Energy Spectrum, NU Method, Quantum Dot, Partition Function, Means Energy, Entropy and Specific Heat Capacity

1. Introduction

Quantum dots are often referred to as artificial atoms because of their atom-like electron energy spectrum. They are alluring to a wide range of optoelectronic applications [1] due to their optical properties, similar to those of atoms. The Schrödinger equation is one of the fundamental equations in quantum physics which still attracts strong interest of both physics and mathematics. Many advanced mathematical methods have been used to solve it. Among the most popular methods, the variational method [2], the path integral method [3, 4], the functional analysis method [3], super symmetric method [5], the factorization method [6], the Nikiforov-Uvarov method (NU) [7, 8] and the quantization rule approach [9] are well employed to solve the Schrödinger equation of two electron problems. Efficient technique to solve second-order homogeneous differential equations has been the subject of extensive investigation in recent years, particularly when dealing with non-central potential. The Schrödinger equation has been investigated for several potentials such as the Woods-Saxon potential [10, 11]; harmonic oscillator potential [12-14] Coulomb potential [15] and Yukawa potential [16] Calculation of the physical quantities in many physical sciences is the essential work we need to perform. As a consequence, the exact solutions of the Schrödinger and

Dirac wave equations have become the essential part from the beginning of quantum mechanics [17] and such solutions have also become useful in the fields of atomic and nuclear physics. Currently, recent researches on the nanometer scale have opened new fields in fundamental sciences of physics, chemistry, and engineering such as optoelectronic devices, which are termed nanoscience. In fact, the spherical QPDs confinement is one of the most appealing explored applications of semiconductor nanostructures when it is doped with shallow donor impurities [18]. Namely, the impurities are used in both transport and optical properties of physics. However, some researchers have extensively studied topics like confined donors or acceptors in nanostructures [19, 20]. It is well-known that factors such as impurity, electric and magnetic fields, pressure, and temperature play important roles in the electronic, optical and transport properties of low-dimensional semiconductor nanostructures [21-24], hence, many works in 2D quantum dots and semiconductors are studied under the influence of external magnetic field [25].

The paper is organized as follows. In section 2, pseudoharmonic interaction is studied under the influence of external magnetic and reduced to harmonic interaction. The exact analytical expressions for the finite energy level are calculated. The thermodynamic properties like partition function, mean energy, entropy and specific heat capacity with magnetic field and temperature dependence are also investigated. In section 3, results and discussions are performed. Finally, concluding remarks are given in section. 4.

2. Theoretical formalism

2.1. Quantum Dot and Antidot in External Fields

Consider a 2D single charged electron e, with an effective mass μ, interacting via a radials symmetrical dot (electron) and antidot (hole) potential in a uniform magnetic field, AB flux field, applied simultaneously. The Schrödinger equation with interaction potential field has the form

$$[\frac{1}{2\mu}(\vec{p}+\frac{e}{c}\vec{A})^2+V_{con}(r)]\psi(r,\phi)=E\psi(r,\phi) \quad (1)$$

Where E is the energy eigenvalues, $\vec{p}$ is the momentum, μ is the effective mass of an electron and $V_{conf}(r)$ is the scalar pseudoharmonic interaction defined by (Tezcan, 2007) [26].

$$V_{conf}(r)=V_0(\frac{r}{r_0}-\frac{r_0}{r})^2 \quad (2)$$

Where r_0 and V_0 are the zero point effective radius and the chemical potential. Besides, the vector potential $\vec{A}$ in equation (12) may be represented as a sum of two terms ($\vec{A}=\vec{A}_1+\vec{A}_2$), having the azimuthally components $\vec{A}_1=\frac{Br}{2}\hat{\phi}$ and $\vec{A}_1=\frac{\phi_{AB}}{2\pi}\hat{\phi}$ where $\vec{B}=B\hat{z}$ is the applied magnetic field and A_2 describes the additional magnetic flux ϕ_{AB} created by a solenoid inserted inside the antidot (pseudodot). Let us take the wave function $\psi(r,\phi)$ in cylindrical coordinates as

$$\psi(r,\phi)=\frac{1}{\sqrt{2\pi}}\exp(im\phi)\,g(r), \quad (3)$$

where m is the magnetic quantum number ($m=0,\pm1,\pm2,\ldots$). Inserting the wave functions (14) into the Schrödinger equation (12) we obtain a second-order differential equation,

$$g''(r)=\frac{1}{r}g'(r)\left(\gamma^2r^2+\epsilon^2r-\frac{\beta^2}{r^2}\right), \quad (4)$$

with $\epsilon^2=\frac{2\mu}{\hbar^2}(\epsilon+2V_0)-\frac{\mu_c}{\hbar}(m+\alpha),\alpha=\frac{\phi_{AB}}{\phi_0}$ and $\gamma^2=\frac{2\mu V_0}{\hbar^2r_0^2}+(\frac{2\mu\omega_c}{2\hbar})^2$.

Here α is an integer with the flux quantum $\phi_0=\frac{\hbar c}{e}$, $\omega_c=\frac{eB}{\mu c}$ is the cyclotron frequency. A radial wave function g(r) has to satisfy the asymptotic behaviors, that is, $g(0)\to 0$ and $g(\infty)\to 0$. To determine the solution of equation (15) amendable by NU method, it is necessary to introduce the following change of variables $s=r^2$ mapping $r\epsilon(0,\infty)$ into $r\in(0,\infty)$ which in turn recasts equation (15) into the hyper geometric form of equation (1). Applying the basic ideas of reference [7] and comparing it after changing the variable gives the essential polynomials

$$\tilde{\tau}=2,\sigma(s)=2s,\tilde{\sigma}(s)=\gamma^2r^2+\epsilon s-\beta^2 \quad (5)$$

and substituting the polynomials given by equation (16) into equation (6), we obtain $\pi(s)$ as

$$\pi(s)=\pm\sqrt{\gamma^2r^2+(2k-\epsilon^2)s+\beta^2} \quad (6)$$

The expression under the square root of the above equation must be the square of a polynomial of first degree. This is possible only if its discriminant is zero and the constant parameter (root) k can be found by the condition that the expression under the square root has a double zero. Hence, k is described as $k_\pm=\frac{\epsilon^2}{2}\pm\beta r$. In that case, it can be written in the four possible forms of;

$$\pi(s)=\begin{cases}+(\gamma s\pm\beta), for\ k_+=1/2\,\epsilon^2+\beta r\\-(\gamma s\pm\beta), for\ k_-={}^1/_2\,\epsilon^2-\beta r\end{cases}. \quad (7)$$

One of the possible forms of $\pi(s)$ must be chosen to obtain an energy spectrum formula. Therefore, the most suitable physical choice is

$$\pi(s)=\beta-\gamma s. \quad (8)$$

This choice provides the negative derivative of $\tau(s)$ as required. Hence, $\pi(s)$ and $\tau(s)$ are

$$\tau(s)=2(1+\beta)-2\gamma s,\gamma'(s)-2\gamma \quad (9)$$

In this case, a new eigenvalue equation becomes

$$\lambda_n=2\gamma n,n=0,1,2\ldots \quad (10)$$

As it expressed in equation (4) it has been used for the radial quantum number n. Another eigenvalue equation is obtained from the equality $\lambda=k+\pi'$

$$\lambda = \frac{\epsilon^2}{2} - \gamma(\beta + 1) \quad (11)$$

In order to find an eigenvalue equation, the right-hand sides of equation (10) and equation (11) must be compared with each other, i.e., $\lambda_n = \lambda$. In this case the result obtained will depend on $E_{n,m}$ in the closed form:

$$\epsilon^2 = 2\gamma(2n + 1 + \beta) \quad (12)$$

Upon the substitution of the terms in equation (12) we can immediately arrive at the energy spectrum formula in the presence of pseudo-harmonic potential

$$E_{n,m}(\alpha, B) = \hbar\Omega(2n + 1 + |\beta|) + \frac{1}{2}\hbar\omega_c(m + \alpha) - 2V_0 \quad (13)$$

Where $\beta = \sqrt{(m+\alpha)^2 + a^2}$ where, energetic spectrum formula (13) for the energy levels of the electron (hole) is usually used to study the thermodynamics properties of quantum structures with dot and antidot in the presence and absence of magnetic field. In the absence of $2V_0$ term, the above formula becomes the Bogachek Landman [27] energy levels in the presence of magnetic and AB flux intensity of quantum dot it could be harmonic potential energy spectrum from reference [28].

$$E_{n,m}(\alpha, B) = \hbar\Omega(2n + 1 + |\beta|) + \frac{1}{2}\hbar\omega_c(m + \alpha) \quad (14)$$

In the absence repulsive radius AB flux intensity (a=0, $\alpha = 0$) finite energy level as reference [29] for the non-relativistic harmonic oscillator potential, we can obtain,

$$E_{n,m} = \hbar\Omega(2n + 1 + m) + \frac{1}{2}\hbar\omega_c(m) \quad (15)$$

2.2. Thermodynamic Properties

Thermodynamic properties of quantum systems have become very attractive due to their potential applications in thermoelectric devices [30] tunneling and decoherence [31]. Thermodynamic properties of quantum systems now aid in the investigation of the dynamical entropy [32, 33]. Recently, different definitions of specific heat are discussed [34] and the entropy for a quantum oscillator in an arbitrary heat bath at finite temperature is examined [35, 36]. Experiments [37] show the feasibility of processing quantum information (QI) via the manipulation of optically excited electron spins [38] in a diamond. Considering the system to be at equilibrium with a heat bath at temperature T, for the finite energy level of harmonic oscillator given in equation (14) the canonical partition function is,

$$z = \sum_{n,m} \exp\left(-\beta\hbar\Omega(2n+1)\right) \exp\left(-\beta\hbar\Omega(m+\alpha) - \beta\hbar\omega_c(m+\alpha)\right), \quad (16)$$

where $\beta = \frac{1}{k_B T}$, k_B is the Boltzmann constant. The sum is over the discrete energy levels given equation (25) without pseudo-potential. Introducing dimensionless variables $\upsilon_{1=\beta\hbar\Omega}$ and $\upsilon_2 = \frac{\beta\hbar\omega_c}{2}$ the equation of partition function may be simplified as given in reference [39].

$$z = \frac{sinh\upsilon_1}{4\sinh\left(\frac{\upsilon_1+\upsilon_2}{2}\right)\sinh\left(\frac{\upsilon_1-\upsilon_2}{2}\right)sinh\upsilon_1}. \quad (17)$$

It is well known that partition function of the system is calculated from bound state energy level where as all thermodynamics quantities are derived from the partition function of the system. The internal energy U for the system is given by

$$U = -\frac{\partial lnz}{\partial\beta}. \quad (18)$$

The Helmholtz free energy (F) and the entropy (s) is;

$$F = -\frac{lnz}{\beta}, \quad (19)$$

$$s = \frac{1}{T}\left[-\upsilon_1\coth(\beta\upsilon_1) + \frac{\upsilon_1+\upsilon_2}{2}\coth\left(\beta\frac{\upsilon_1+\upsilon_2}{2}\right) + \frac{\upsilon_1-\upsilon_2}{2}\coth\left(\beta\frac{\upsilon_1+\upsilon_2}{2}\right) + \upsilon_1\coth(\beta\upsilon_1)\right] + k_B\left[\ln(sinh(\beta\upsilon_1) - sinh\left(\beta\frac{\upsilon_1+\upsilon_2}{2}\right)) - \ln(sinh\left(\beta\frac{\upsilon_1-\upsilon_2}{2}\right) - sinh(\beta\upsilon_1)) - ln4\right] \quad (20)$$

The specific heat capacity is given as

$$C_v = k_B\beta^2\frac{\partial^2 lnz}{\partial\beta^2} \quad (21)$$

3. Discussion and Result

The thermodynamic properties of a two interacting electrons harmonically oscillator confined interacting electrons in a GaAs quantum dot with parabolic confinement are investigated as a function of interdependence of temperature and magnetic field. We obtained the energy spectrum of the system in closed form by solving Schrödinger equation analytically and then we solved partition function, mean energy, heat capacity, entropy, specific heat capacity using the canonical ensemble approach. A partition function as temperature increases quickly increased for the lower magnetic fields. As function of temperature, it was demonstrated that the heat capacity exhibits a highest fluctuations with strong magnetic fields influences at a very low temperature and vice versa. We also found that, at low temperature entropy increases steeply as the temperature increases, and at very high temperatures the entropy reaches the saturation limit.

We used material parametric values of GaAs $\hbar\omega = 1.05243\hbar\omega_c$, $\hbar\omega_c = 0.1157705$ B and $\hbar\Omega = 0.269777$*B are taken from Ref [29]. This study lays on noticeably distinctive physical phenomenon of the effects energy spectrum on thermodynamic quantities under influence of magnetic field with respect to temperature is explored.

In Figure 1 we plot Partition function as function of temperature with different values of magnetic field strength. For the lower values of magnetic field strength partition function is rapidly raised to its possible maximum due to dominance of temperature value over magnetic field in contrary the fact at low temperature partition function attains its lower value do to dominance of magnetic fields. Generally for higher magnetic field partition functions take the lower phase because of inter influences of temperature and external magnetic field effect.

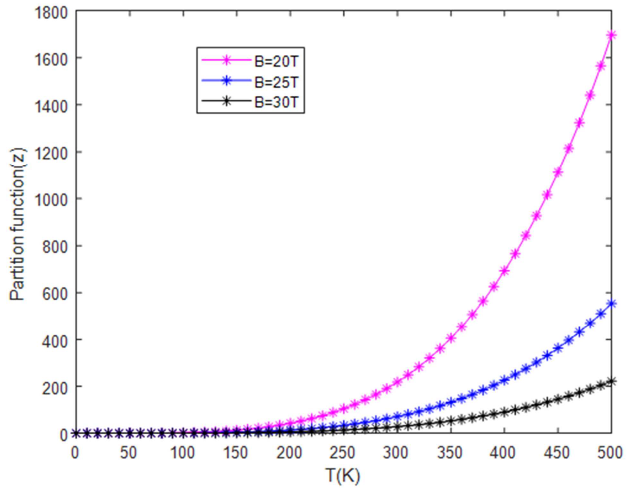

Figure 1. *Partition function versus temperature with various magnetic fields ($B = 20T, B = 25T$ and $B = 30T$).*

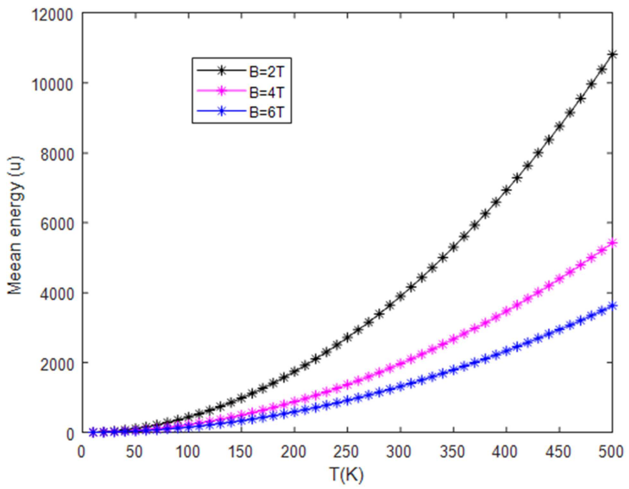

Figure 2. *Mean energy versus temperature with various values of magnetic field strength ($B = 2T, B = 4T$ and $B = 6T$).*

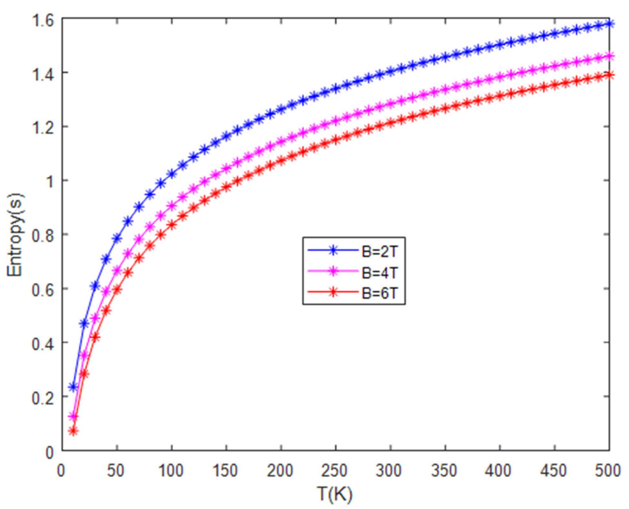

Figure 3. *Entropy (arb.unit) as function Temperature with various values of magnetic field (B=2T, B=4T, B=6T).*

In Figure 2 we plot Mean energy as function of temperature with different values of magnetic field strength. For the lower values of magnetic field strength mean energy is rapidly raised to its possible maximum due to dominance of temperature value over magnetic field. Generally for higher magnetic field mean energy take the lower phase because of inter influences of external magnetic field wins over temperature effect.

In comparison of Figure 1 and Figure 2 partition function is more sensitive to temperature than mean energy. Thus it requires higher external field to be manipulated and maintained under controlled physical properties in higher temperature. That was the defect of previous studies; the researchers confined themselves with very lower temperature effect. Most theoretical investigations are conducted considering very low parameters that are not measurable in real life situation. In our study we considered measurable parameters in real life and clearly shows that the interdependency of temperature and magnetic field yields meaningful physical phenomena.

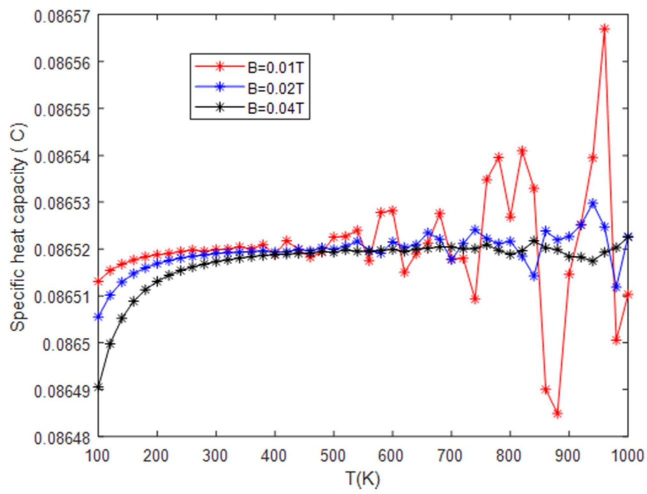

Figure 4. *Specific heat capacity (arb.unit) of GaAs quantum dot as function of strong temperature with the various of low magnetic field strength (B=0.01T, B=0.02T, B=0.04T).*

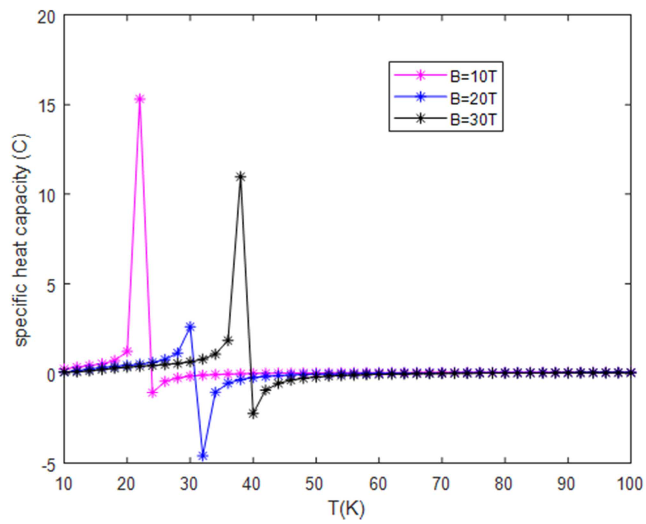

Figure 5. *Specific heat capacity as a function low temperature in T (Kelvin) with various values of strong magnetic field (B=10T, B=20T, B=30T).*

Figure 3 Variation Entropy (arb.unit) with temperature is shown in figure 3 that the entropy increases at sufficiently low temperature and tends to slower as an increment of temperature then it reaches its critical constant value along increment of temperature. For the higher value of external magnetic field entropy is in position to its lower phase value.

As it depicted in Figure 4 specific heat capacity of GaAs quantum dot as function of strong temperature with the various low magnetic field strength ($B = 0.01T$, $B = 0.02T$ and $B = 0.04T$) the dominance of temperature takeover its wining effect over external magnetic field that causes higher fluctuation of specific heat capacity essentially for a strong temperature. That shows unbalanced influence of temperature and magnetic field affect specific heat capacity.

In figure 5 specific heat as function low temperature with strong magnetic field the dominance of against low temperature the most fluctuated specific heat capacity observed at low temperature regime in contrary that have been seen in Figure 5 as such unbalanced interaction of magnetic and temperature entails to occur highly fluctuated specific heat capacity at very low temperature.

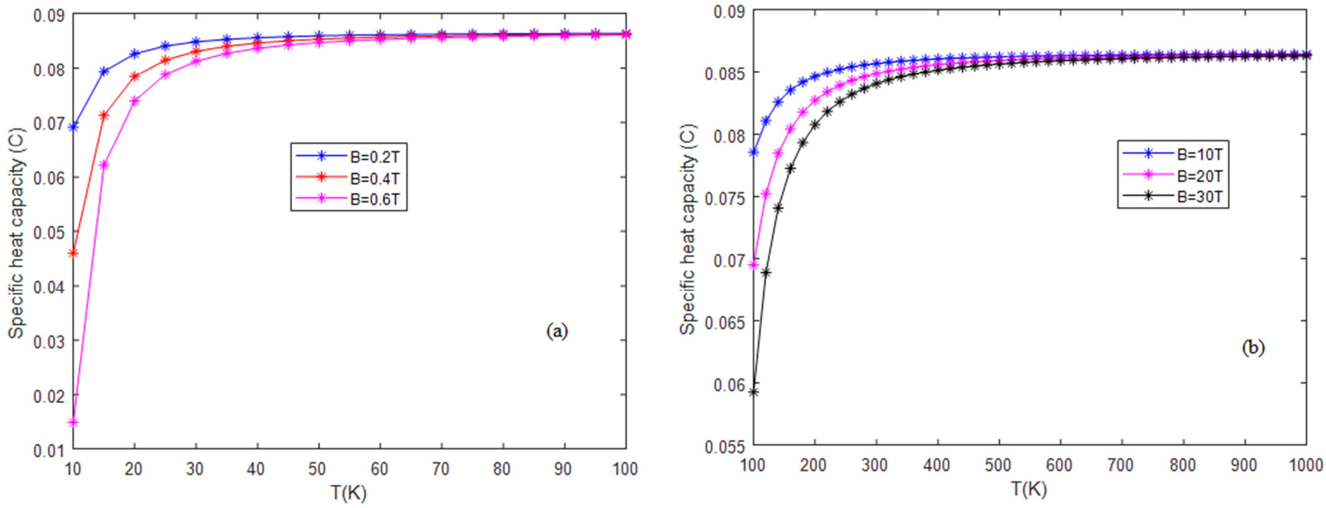

Figure 6. *(a) specific heat capacity (ab.unit) of GaAs quantum dot as function of low temperature with the variation of low magnetic field strength and (b) specific heat capacity as a function of strong temperature in T (Kelvin).*

Figure 6 (a) specific heat capacity of GaAs quantum dot as function of low temperature with the various values of low magnetic field strength and figure 6 (b) specific heat capacity as a function of strong temperature in T (kelvin). Specific heat capacity monotonously increase at low temperature in meanwhile increase slowly reached its saturated to its constant value along temperature to get merged exhibiting its constantan value which is independent of magnetic field and temperature. Here very interesting physical phenomena in both figure 6 (a-b) shows that equally dominating magnetic field and temperature gives almost equal value of specific heat capacity of our system where as one dominating over another parameters results asymmetric physical properties.

4. Conclusion and Remark

We have studied the interdependence of magnetic field and temperature effect on thermodynamic properties of two interacting electron GaAs quantum dot confined in harmonic oscillator potential. The dominance of one over the other generally determines the quantities of thermodynamic behavior on other hand win-win (equiponderance) effect of temperature and magnetic field tunes to fix different values the thermodynamic quantities. In our study we have used a model of two electrons trapped in GaAs quantum dot in nanostructure semiconductor materials. Noticeably deal the thermodynamics properties under magnetic fields and temperature dependence. We have calculated its dependence of thermodynamic quantities partition function, mean energy, entropy and specific heat capacity on interdependence of applied magnetic field and temperature.

Conflict of Interest

The authors report there are no conflicts of interest.

Data Availability Statement

The authors confirm that the data supporting the findings of this study are available within the article.

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