An-Najah National University

Faculty of Graduate Studies

Heat Capacity and Entropy of Donor Impurity in Quantum Dot with Gaussian Confinement

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Dedication

For my father and my mother and for my wonderful family for their love, care and support.

Acknowledgments

All thanks to Allah, who give me health and knowledge to complete my thesis. I would like to express my thanks to my supervisor and instructor Prof. Mohammad Elsaid for his guidance, assistance, supervision and contribution of valuable suggestions.

I can't forget to thank Dr. Khalid Ilaiwi for his help and experience especially in Mathematica. Finally, I would like to thank all friends for providing encouragement and support.

الإقرار

أنا الموقع أدناه مقدم الأطروحة التي تحمل عنوان:

Heat Capacity and Entropy of Donor Impurity in Quantum Dot with Gaussian Confinement

أقر بأن ما اشتملت عليه هذه الرسالة إنما هو نتاج جهدي الخاص، باستثناء ما تمت الإشارة إليه حيثما ورد وأن هذه الرسالة ككل أو جزء منها لم يقدم من قبل لنيل أية درجة أو بحث علمي أو بحثي لدى أية مؤسسة تعليمية أو بحثية أخرى.

Declaration

The work provided in this thesis, unless otherwise referenced, is the researcher's own work, and has not been submitted elsewhere for any other degree or qualification.

Student's name: **اسم الطالب:**

Signature: **التوقيع:**

Date: **التاريخ:**

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List of Symbols and Abbreviations

QD	Quantum dot
3D	Three dimension
2D	Two dimension
1D	One dimension
0D	Zero dimension (quantum dot)
nm	Nanometer
DOS	The density of state
C_v	Heat capacity
S	entropy
$V(r)$	Confinement potential
E_B	Binding energy
GaAs	Gallium Arsenide
AlGaAs	Aluminum Gallium Arsenide
e	Charge of electron
m	Mass of electron
m^*	Effective mass of electron
φ	Wave function
N	Dimension
ϵ	The dielectric constant of material
R^*	Effective Rydberg unit
$\hbar$	Reduced Blank's constant
R	QD radius
r	position coordinate of the electron
l	orbital angular momentum.
ω	an harmonic frequency parameter
K	Kelvin Degree
T	Temperature
n	Principle quantum number
n_r	Radial quantum number

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Abstract

In the present work, The ground state energy of shallow donor impurity in GaAs/AlGaAs heterostructure with Gaussian potential using the shifted $1/N$ expansion method had been calculated. The effects of the impurity on the ground state energy, the dot radius R, confining potential depth V_0 and dimension N had been investigated. The impurity binding energy of the ground state has been calculated as a function of dot radius R, confining potential depth V_0 and dimension N. we had found that the impurity binding energy of the ground state increases as confining potential depth V_0 increases while it decreases as dot radius R and dimension N increases . In addition, we had also computed the heat capacity C_v and entropy S of donor impurity in QD and investigated the dependence of these quantities on dot radius R, confining potential depth V_0, dimension N and temperature T. the comparison shows that our results are in very good agreement with the reported work.

Chapter One
Introduction

1.1 Nanotechnology and Quantum Confinement Effect

Nano science is the study of phenomena and manipulation of materials at atomic, molecular and macromolecular scales (quantum-scale), where properties differ significantly from those at a larger scale.

Nanotechnology is the field of understanding and manipulation of matter with at least one characteristic dimension measured in nanometers (A nanometer is one-billionth of a meter: ten times the diameter of a hydrogen atom) with novel size-dependent physical and chemical properties.

The nanoscopic scale is the size at which fluctuations in the averaged properties begin to have a significant effect on the behavior of a system (due to the motion and behavior of individual particles).

The most popular term in the Nano world is quantum confinement effect which is essentially due to changes in the atomic structure as a result of direct influence of ultra-small length scale on the energy band structure [1]. Quantum confined structure is one in which the motion of the carriers (electron and hole) are confined in one or more directions by potential barriers.

As the size of particle decrease till we reach a nano scale (the decrease in confining dimension) makes the energy levels discrete which means

confine the motion of randomly moving electron to restrict its motion in specific energy levels. The presence of many atoms in a bulk material causes splitting of the electronic energy levels, giving continuous energy bands separated by a forbidden zone. When the particle dimension of a semiconductor near to and below the bulk semiconductor Bohr exciton radius (the distance in an electron-hole pair) the continuous energy bands of a bulk material collapse into discrete, atomic like energy levels.

Based on the confinement direction, a quantum confined structure will be classified into:

1) Three-dimensional (3D) structure or bulk structure: No quantization of the particle motion occurs, i.e., the particle is free.

2) Two-dimensional (2D) structure or quantum well: Quantization of the particle motion occurs in one direction, while the particle is free to move in the other two directions.

3) One-dimensional (1D) structure or quantum wire: Quantization occurs in two directions, leading to free movement along only one direction.

4) Zero-dimensional (0D) structure or quantum dot (sometimes called “quantum box”, “nano Crystal”): Quantization occurs in all three directions.

The confinement phenomena change significantly the density of states of the system and the energy spectra. In solid-state and condensed matter physics, the density of states (DOS) of a system describes the number of

states per interval of energy at each energy level that are available to be occupied by electrons. For QD the density of state shows a discrete behavior unlike to the other confinements which have a continuous density of state as shown in figure (1-1).

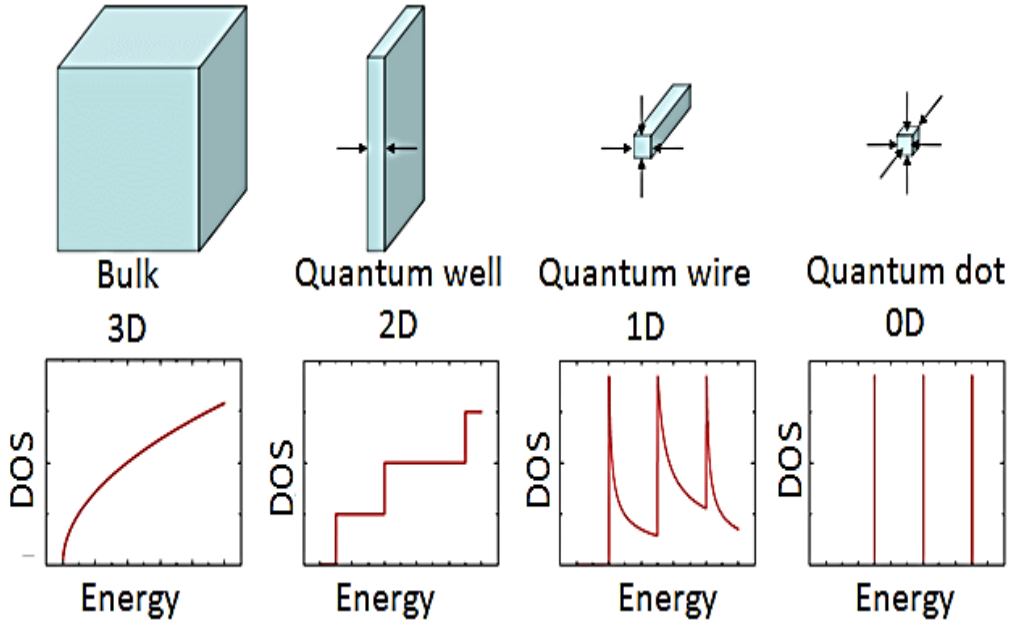

Figure (1-1): Quantum confinement in nanostructure and density of state as function of energy.

The properties of materials will be different at the nano scale for two main reasons. First, nanomaterial's have a relatively larger surface area ,this can make materials more chemically reactive, and affect their strength or electrical properties. Second, quantum effects can begin to dominate the behavior of matter at the nano scale affecting the optical, electrical and magnetic behavior of materials.

The nanofabrication techniques allow us to control precisely both the size and the shape of the low dimensional system. In the last few years there was a rapid progress in the fabrication and processing of nanostructures.

The nanotechnology will have major impacts on all aspects of the world, and its ability to further improve daily life is limitless, nanotechnology seems to hold the key into the future of the world. This technology has allowed for specific properties such as strength, durability, reactivity, conductance, and several other traits to be tailored towards each project of interest [2, 3].

The applications and uses of nanomaterial in electronic and mechanical devices, in optical and magnetic components, quantum computing, tissue engineering, and other biotechnologies, with smallest features, widths well below 100 nm, are the economically most important parts of the nanotechnology nowadays and presumably in the near future.

1.2 Quantum Hetrostructure and Quantum Dots

Nano science is a very interesting and technologically relevant area of condensed matter physics. With the development of modern technology it is now possible to produce zero dimensional (0 D) systems called quantum dots (QDs).

Quantum dots(QDs) are the typical examples of ultra-small systems in the areas of electronics and optoelectronics where the electrons are confined in all three dimensions.

Quantum dot (QD) is a conducting island (semiconductor crystals) of a size comparable to the Fermi wavelength (wavelength that correspond to the highest occupied energy level of a material at absolute zero

temperature). QDs are that usually ranging from (2 to 10) nanometers and (10 to 50) atoms in diameter.

The electrons are confined in all three spatial dimensions using artificial confining potentials. The number of electrons can be manipulated easily by conventional nanofabrication methods.The number of electrons in atoms can be tuned by ionization, while in QDs by changing the confinement potential [4,5].

When we apply energy in the form of electric field or heat the electrons can freely move within an area from a few nanometers to a few hundred of nanometers (defined by the Bohr radius which represents the mean radius of electron around the nucleus of hydrogen atom in its lowest energy level) in a bulk semiconductor so the continuous conduction and valence energy bands exist which are separated by an energy gap . Contrary, in a quantum dot, discrete atomic like states with energies that are determined by the quantum dot radius appear because the excitons (excited electron and an associated hole) cannot move freely.

The effect of the strong electron confinement in a nano structure leads to a small energy separation between the sub bands, increase the dipole transition value, and achieve resonance condition [6]. This is very similar to the famous particle-in-a-box and can be understood by the Heisenberg Uncertainty Principle , the more spatially confined and localized a particle becomes, the wider the range of its momentum/energy.

QDs band gap can be controlled by its size. So we can engineer their optical and electrical properties. Smaller QDs have large band gaps as shown in figure (1-2).

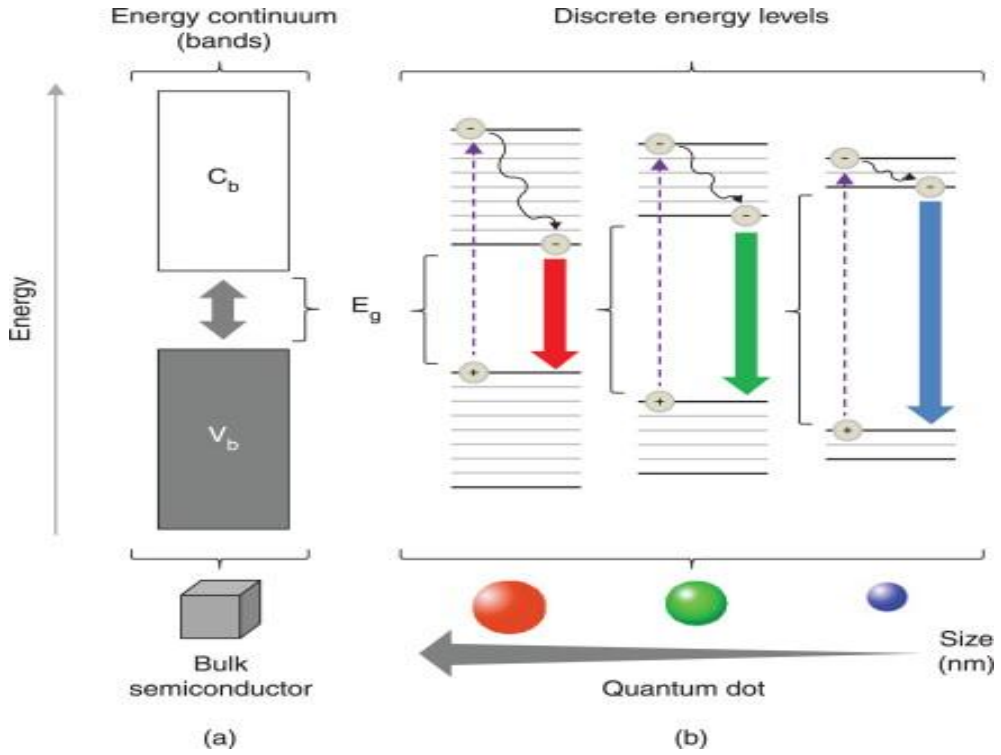

Figure (1-2): Controlling the band gap by quantum dots size.

New potential application in optoelectronics will be discovered by changing in the electronic and optical properties of QDs which may be controlled by an appropriate selection of the sample geometry and material parameters so the size and shape of quantum dots can be experimentally tuned over a wide range [10]. Therefore, quantum dots are sometimes called artificial atoms [11]. Quantum dots have great potential for applications in micro-electronic devices such as quantum dot lasers, solar cells, single electron transistors and quantum computers [12, 13].

The physics of shallow donor impurity states in QDs is an interesting subject so many theoretical and experimental studies of impurity related properties in low dimensional heterostructure have been reported in the last decade . Because their presence can dramatically alter the performance of QDs and their optical and transport (electrical) properties. The donor impurity binding energy increasing continuously as the QD size decreases; also it depends on the donor impurity position [8,9].

In this work we will focus on the heterostructure with impurity, where the electron interacts with the impurity ion by Coulomb potential. The structure of our system is sketched in figure (1.3).

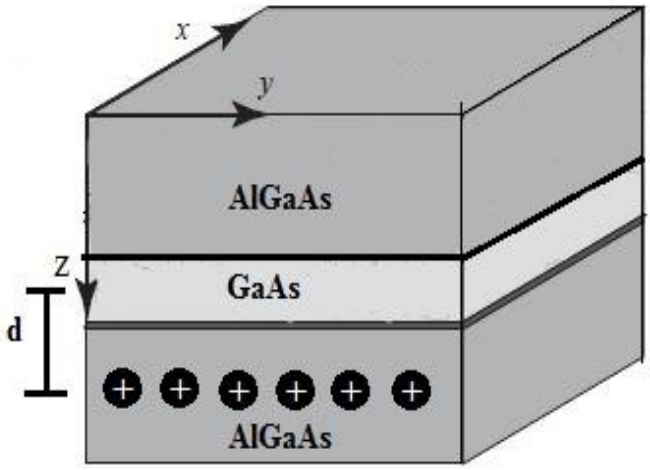

Figure (1-3): The structure of two-dimensional electron confined in GaAs layer bounded to an off donor impurity located in the AlGaAs layer.

The heterostructure in the (x-y) plane with the impurity in the (z) axis at the distance (0, 0, d), which include two AlGaAs layers separated by GaAs layer, one of the AlGaAs layer doped with silicon donor impurity located at

distance (d) along the growth axis in order to have free electrons in the heterostructure (n- type AlGaAs).

The (n-AlGaAs) layer is the source of free electrons in the heterostructure these free electrons move from AlGaAs layer with high band gap to lower band gap GaAs layer. The electrons are trapped in the quantum well of GaAs layer. In this way the 2D structure where the motion of the electrons is quantized along growth axis (z direction) while the electron is free to move in (x-y) plane can be created as shown in figure (1-4).

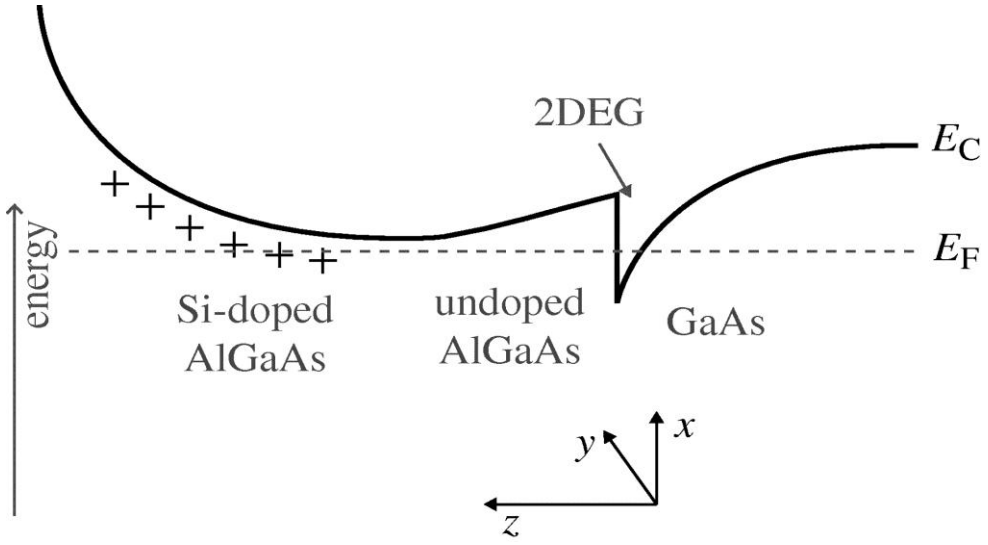

Figure (1-4): A sketch of forming 2DEG.

The QDs can be fabricated by two different ways , the first one is made by using lithography etching techniques of microchip manufacturing and the second is molecular beam epitaxy which can be done by applying chemical processes to get a QD from bulk material [7].

1.3 Literature survey

The binding energy of the hydrogenic impurity in the quantum dot is extensively studied. Most of the theoretical works carried out on shallow donors in spherical quantum dots employ variational approaches [14], or alternatively, perturbation method limited to the strong confinement regime [15], while the exact solution has been obtained for centered impurities [16].

Zhu et al. solved the finite potential well for impurity in the center of spherical quantum dot and obtained the exact solution by using the method of series expansion [17, 18]. Bose et al. obtained the binding energy of a shallow hydrogenic impurity in a spherical quantum dot with a parabolic potential shape by perturbation method [32]. Using variational and fractional-dimensional space approaches, Porras-Montenegro and Perez-Merchancano and Oliveira et al. have calculated the binding energy for shallow- donor impurities in rectangular quantum dots for both finite and infinite potential confinement [19].

A computational scheme yields to exact energies of a spherical nanocrystallite with a shallow donor impurity located anywhere inside is presented by Movilla and Planelles[20]. Gharaati and Khordad used a modified Gaussian potential to calculate energy levels for spherical quantum dot within effective mass approximation [21]. Boda et al. investigated the Gaussian confinement of hydrogenic donor impurity by a very simple variational wave function [22].

The method of $1/N$ expansion has been developed, which was proposed by Sukhatme and Imbo [23, 24] to calculate the spectra of an electron and a donor in QD. Elsaid had studied the quantum dot Hamiltonian by this method in different works [30, 31]. It is a powerful tool to solve Schrodinger equation for spherical symmetric potentials and it is used in different branches of theoretical physics.

The method is simple, and it gives accurate results of energy eigenvalues calculations of the system without dealing with robust numerical calculations or trail wave functions . The shifted $1/N$ expansion surpasses most approximation methods in its domain applicability and the accuracy of its result while the $1/N$ expansion method is applicable to the entire range of the magnetic field strength, while the perturbation theory is limited to a weak range only.

In this work, we shall apply the shifted $1/N$ expansion method to calculate the eigenenergies of donor impurity in QD with Gaussian confinement.

1.4 Research objectives

The main aims of this research can be summarized as follows:

Firstly, The energy and binding energy spectrum of an electron donor impurity in spherical QD related to the Gaussian potential will be calculated by using the shifted $1/N$ expansion method. The obtained results will be compared with previous studies. In addition the computed

state energies will be calculated as a function of dot radius (R) and confining potential depth (V_0) and dimension (N).

Secondly, the effect of dimensionality on the state energy of the quantum dot system will be investigated. The heat capacity (C_v) and entropy (S) as a thermal quantities of the QD system will be calculated.

1.5 Outlines of thesis

In this work, the heat capacity (C_v) and entropy (S) of donor impurity in QD system have been calculated as a thermodynamic quantities of the system as a function of dot radius (R), confining potential depth (V_0), dimension (N) and temperature (T). Since, the eigenvalues of an electron donor impurity in QD related to the Gaussian potential will be the starting point to calculate the physical properties of the system, the shifted $1/N$ expansion method has been used to solve QD Hamiltonian and obtain the eigen energies. Second, the eigen energies spectra have been calculated to display theoretically the behavior of the heat capacity (C_v) and entropy (S) of the QD as function of dot radius (R) , confining potential depth (V_0), dimension (N) and temperature (T).

The rest of thesis is organized as follows: Hamiltonian of donor impurity in QD with Gaussian potential, the principle of the Shifted $1/N$ expansion method and how to calculate the heat capacity (C_v) and entropy (S) of the QD system from the mean energy expression are presented in chapter II. In chapter III, the results of energy and heat capacity (C_v) and entropy (S) of our work have been displayed and discussed, while the final chapter devoted for conclusions and future work.

Chapter Two
Theory of Impurity Confined in Heterostructure

This chapter consists of three main parts: the Hamiltonian of donor impurity in QD with Gaussian potential, Shifted $1/\mathrm{N}$ Expansion Method, The Heat capacity($\mathrm{C_v}$) and Entropy (S).

2.1 Hamiltonian of Donor Impurity in QD with Gaussian Potential

The standard Hamiltonian of an electron in the presence of a hydrogenic donor located at the center of quantum dot can be written as follows:

$$\hat{\mathrm{H}}_0 = -\nabla^2 - \frac{2z}{r} + V(r) \qquad (1)$$

where:

$V(r)$: symmetric attractive Gaussian confinement potential , given by:

$$V(r) = -\mathrm{V}_0\, e^{-r^2/2R^2} \qquad (2)$$

with:

V_0= potential well depth.

R = quantum dot radius (the range of the confinement potential).

r: electron position coordinate, $r = (x, y)$ for the 2D and $r = (x, y, z)$ for the 3D.

Coulomb attractive interaction between the donor electron and the hydrogenic nucleus is represented by second term in Hamiltonian.

$z = 0$ When the donor impurity is absented and $z = 1$ as donor impurity is presented.

Gaussian confining potential can be treated as parabolic potential plus a perturbation because the deviation of Gaussian confining from the parabolic potential is small enough.

2.2 Shifted $1/N$ Expansion Method

The solution of donor impurity Hamiltonian , equation (1) , with Gaussian potential , equation (2) , cannot be obtained in analytic closed form. In this thesis, we intend to solve the Hamiltonian by using the shifted 1/N expansion method. The radial part Schrodinger equation in N dimensional space can be expressed as:

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

where:

m^* : Electron effective mass.

$\hbar$: Planck Constant.

N : Number of spatial dimensions.

The term $l(l+N-2)\,\hbar^2$ is the eigenvalue of the square of the N dimensional orbital angular momentum and $l = |m|$ where m is the magnetic quantum number ($= 0, \mp 1, \pm 2, \ldots\ldots\ldots$) which labels the QD energy states.

The first derivative term in N- dimensional Schrodinger equation, Eq.(3) can be removed by appropriate substitution:

$$\varphi(r) = r^{-\frac{N-1}{2}} u(r) \tag{4}$$

Equation (3) will take the following form :

$$\left(-\frac{\hbar^2}{2m^*} \frac{d^2}{dr^2} + \frac{\left(\bar{k} + a - 1\right)\left(\bar{k} + a - 3\right)\hbar^2}{8m^* r^2} + V(r) \right) u(r) = E u(r) \tag{5}$$

Where $\bar{k}$=$N + 2l - a$, and a is suitable shift parameter that can be determined later.

To calculate the energy eigenvalues, $E(n, l)$, we will expand Schrodinger equation in terms of parameter ($\bar{k}$) and shift parameter (a). The complete mathematical steps that lead to the QD energy eigenvalues expressions in terms of powers of $1/\bar{k}$ are given in Appendix.

The energy eigenvalues, $E(n, l)$, are given by:

$$E(n, l) = E_0 + E_1 + E_2 + E_3 + \cdots$$

Where the radial and principle quantum numbers are related by:

$$n = n_r + l + 1$$

The shift parameter a can be determined by making the term E_1 vanishes namely ($E_1 = 0$) :

$$a = 2 - 2(2n_r + 1)\frac{m^*\omega}{\hbar} \tag{6}$$

Where ω is the an harmonic frequency parameter, which is given by equation A4 in Appendix as:

$$\omega = \frac{\hbar}{2m^*}\left[3 + \frac{r_0 \frac{d^2V}{dr^2}_0}{\frac{dV}{dr_0}}\right]^{1/2} \tag{7}$$

The root r_0 for the corresponding value of ω and corresponding QD state is determined from the following relation:

$$N + 2l - 2 + (2n_r + 1)\left[3 + \frac{r_0 \frac{d^2V}{dr^2}_0}{\frac{dV}{dr_0}}\right]^{\frac{1}{2}} = \left[\frac{4m^* {r_0}^3 \frac{dV}{dr_0}}{\hbar^2}\right]^{\frac{1}{2}} \tag{8}$$

Having determined r_0 , all the energy eigen values can be computed.

The difference of the energy for that state in the absence of donor atom $(z = 0)$ and in its presence $(z = 1)$ gives the binding energy of the impurity in the QD. The computed energy spectra for different states and various QD physical parameters are listed in Table (3-1).

A Mathematica computer code is written to produce the listed numerical energy levels. The computed energies are used to study the thermodynamics properties of donor impurity in QD such as the heat capacity (C_v) and entropy (S) .

2.3 The Heat Capacity (C_v) and Entropy (S)

The heat capacity (C_v) is considered the most important thermal property which describes the heat stored in the quantum dot system [25,26] .

To calculate the heat capacity of the system we have evaluate the mean energy from the statistical energy expression:

$$< E(T, V_0, R, N) > = \frac{\sum_{j=1}^{i} E_j \ e^{-E_j/K_\beta T}}{\sum_{j=1}^{i} e^{-E_j/K_\beta T}} \quad (9)$$

The summation is taken over the sufficient converging energy levels of the QD . In the present work ,we have ensured the convergence of numerical calculations which was found to be satisfied at $i = 15$. The QD average thermal energies or partition function are computed for different ranges of temperature and confining potential strength.

Now the heat capacity can be calculated from equation (9) by taking the temperature derivative of the mean energy:

$$C_v(T, \mathrm{V}_0, R, N) = \frac{\partial <E(T,\mathrm{V}_0,R,N)>}{\partial T} \quad (10)$$

The entropy (S) indicates to the degree of disorder or randomness in the system which can be calculated by equation:

$$S(T, V_0, R, N) = \frac{\partial (K_\beta T \ln <Z(T,V_0,R,N)>)}{\partial T} \quad (11)$$

where:

$$< Z(T, V_0, R, N) > = \sum_{j=1}^{i} e^{-E_j/K_\beta T} \quad (12)$$

The dependence of the QD heat capacity (C_v) and entropy (S) on the QD physical parameters: temperature (T), confinement length (R), depth of the confining potential (V_0), dimension (N), will be shown in various plots.

Chapter Three
Results and discussion

In this chapter we will show and discuss our computed results for energy of hetero structure system made from (GAAs)material (dielectric constant $\epsilon = 12.74$, effective Rydberg $R_D = 5.825\, meV$ and the effective mass of an electron $m^* = 0.067\, m_e$ at zero temperature and pressure) with the impurity in the (z) axis at the distance (d) from electron in GAAs layer. Which are essential input data to calculate the average energy as a first step. Next, we compute the heat capacity (C_v) and entropy (S) by using the energies which we obtained. Diagram and tables were used to illustrate the results. The results will be compared against reported ones.

3.1 Energy and Binding energy of the donor impurity

Shifted $1/N$ expansion method is used to compute the energy states of spherical quantum dot (3D) with confinement potentials .The eigen energies of the donor impurity obtained by $1/N$ expansion method against different computation methods are listed in table (3-1) for $V_0 = 400\, R_D$ and dot radius $R = 1/\sqrt{2}\, a_D$.

The calculation are carried out to the third order correction of the shifted $1/N$ expansion energy series. The analytic expression for the energies $E(n, l)$ yield accurate results for a wide range values of (n, l) in comparison with all computational methods which solving Schrodinger equation by using suitable trial wave function. However we observed a little deviation

between Diagonalizing method and other reported work at table (3-1) particularly at states (2f, 3d).

We had plotted the computed energy results of this work against the radius of QD (R) for both impurity and without impurity in figure (3- 1). The energy with impurity and without impurity have a similar dependence on (R), the decreasing in QD radius (R) leads to increase the state energy of the impurity monotonically.

The electron wave function is mainly distributed inside the well region of the QD so the existence of impurity leads to increase the energy . The coulomb interaction is highly large which means increasing in energy when the impurity is at the center of the QD [33]. The impurity modifies the energy levels of QDs and it affects their electronic and optical properties.

Table (3-1): Eigen energy states in units R_D for 3D quantum dot (spherical QD) with impurity and $V_0 = 400\, R_D$, dot radius $R = 1/\sqrt{2}\, a_D$.

State	Diagonalizing [27]	Numerov integration algorithm [27,28]	Hypervirial-Pade[29]	Our work
1s	-341.895	-341.892	-341.8952	-341.895
1p	-304.463	-304.463	-304.4628	-304.463
2s	-269.644	-269.640	-269.6445	-269.644
1d	-268.110	-268.111	-268.1107	-268.111
2p	-234.446	-235.450	-235.4500	-235.451
1f	-232.849	-232.895	-232.8753	-232.878
3s	-203.983	-203.979	-203.9835	-203.997
2d	-202.427	-202.431	-202.4313	-202.432
1g	-198.700	-198.798	-198.7983	-198.798
3p	-173.156	-173.244	-173.2443	-173.257
2f	-167.797	-170.639	-170.6393	-170.640
4s	-145.372	-145.373	-145.3779	-145.431
3d	-145.741	-143.809	-143.8091	-143.821

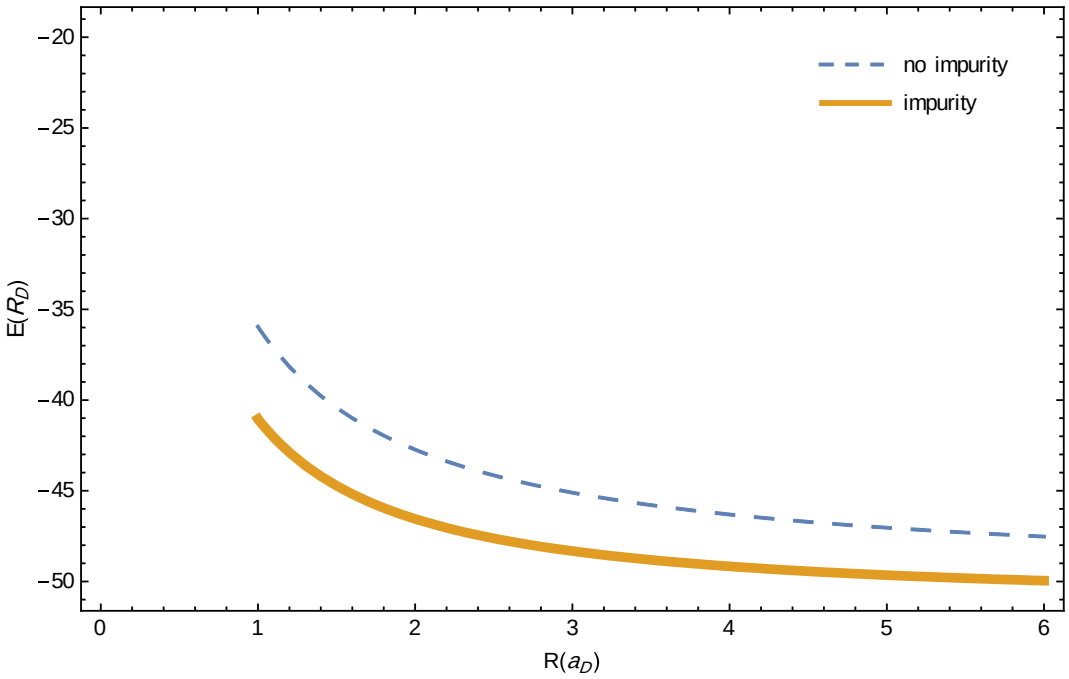

Figure 3- 1: Ground state energy$E(1,0)$ in QD as function of dot radius (R) for $V_0 = 50R_D$, $N = 3D$ $with$ impurity and without impurity**.**

The effect of dot radius (R) and potential well depth (V_0) on the ground state energy E(1,0) (1s state) and the binding energy $E_B(1,0)$ is represented on figures (3-2) and (3-3). The dependence of the confinement of well depth (V_0) is clear in these figures.

The donor binding energy increases as the potential well depth (V_0) increases which means confining the electron close to the donor regime. It is shown that the binding energy $E_B(1,0)$ increases until it reaches a maximum value of the system stability as the dot radius (R) decreases. At larger radius of QD the binding energy will not depend strongly on (V_0) .

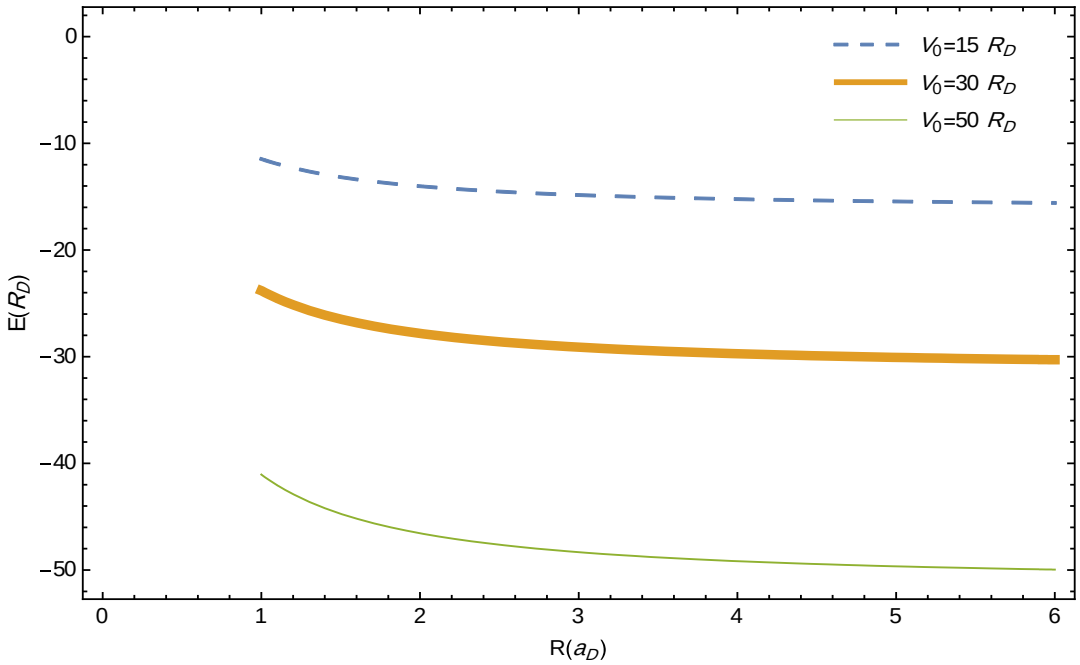

Figure (3-2): Ground state energy levels E(1,0) in QD as function of dot radius (R) for different values of $V_0 = 15R_D, 30R_D, 50R_D$, $N = 3D$.

When the electron is confined in the (Z) direction the coulomb interaction will be more sensitive to the lateral confinement potential (negative voltage due to the heterostructure of the QD which is applied to reduce further confinement region) .Because the decrease in spatial confinement between the electron and the donor impurity (small QD size) the binding energy $E_B(1,0)$ becomes larger. The sharp decrease in binding energy $E_B(1,0)$ to a limiting value will happen for further reduction of dot radius this is due to non-localized charge (In the limit $R \to 0$ the ground state energy goes to zero and as $R \to \infty$ the ground state energy approaches $\to$ V_0).

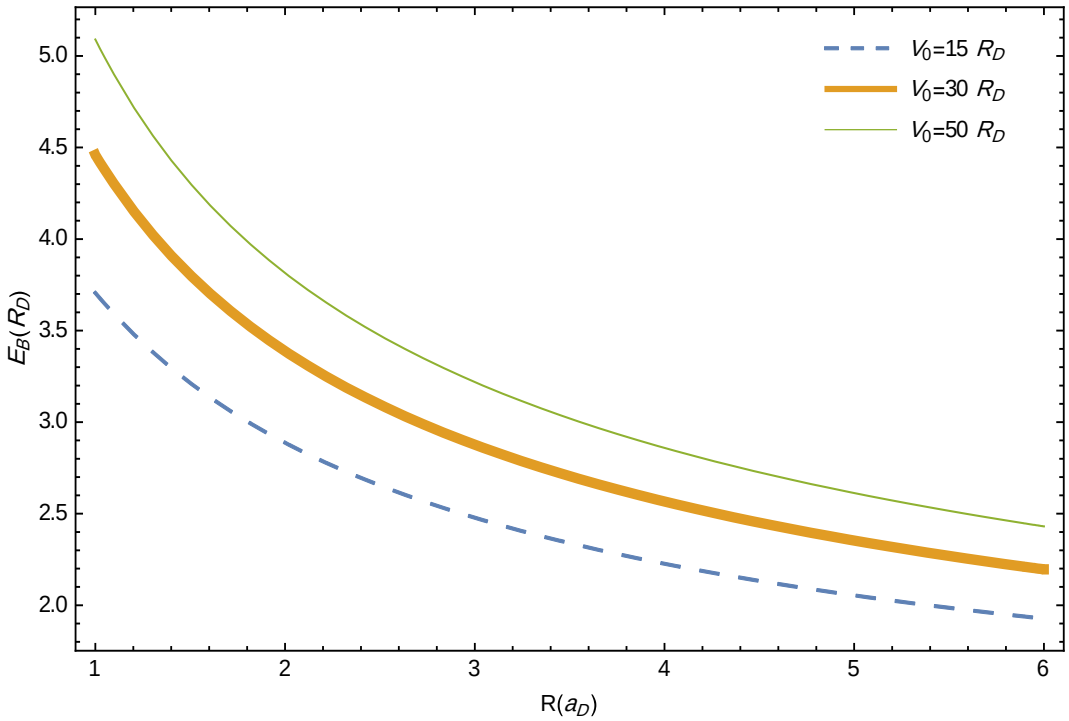

Figure (3-3): Ground state binding energy levels $E_B(1,0)$ in QD as function of dot radius (R) for different values of $V_0 = 15R_D, 30R_D, 50R_D$, $N = 3D$.

The state energy of the impurity may become larger than the confining potential when the dot radius (R) is further decreased. The kinetic energy of the confined electron becomes larger by uncertainty principle and thus increases the probability of the electron leaking outside the well.

The effect of reduction in dimensionality on ground state energy $E(1,0)$ and binding energy $E_B(1,0)$ are shown in figures (3-4) and (3-5) which show that the energy increases as dimension of the system decreases (E(2D) > E(3D)) . The geometric dimension of the system affected on the coulomb interaction intensity between the electron and impurity atom, as the size of the system is reduced the coulomb interaction is promoted.

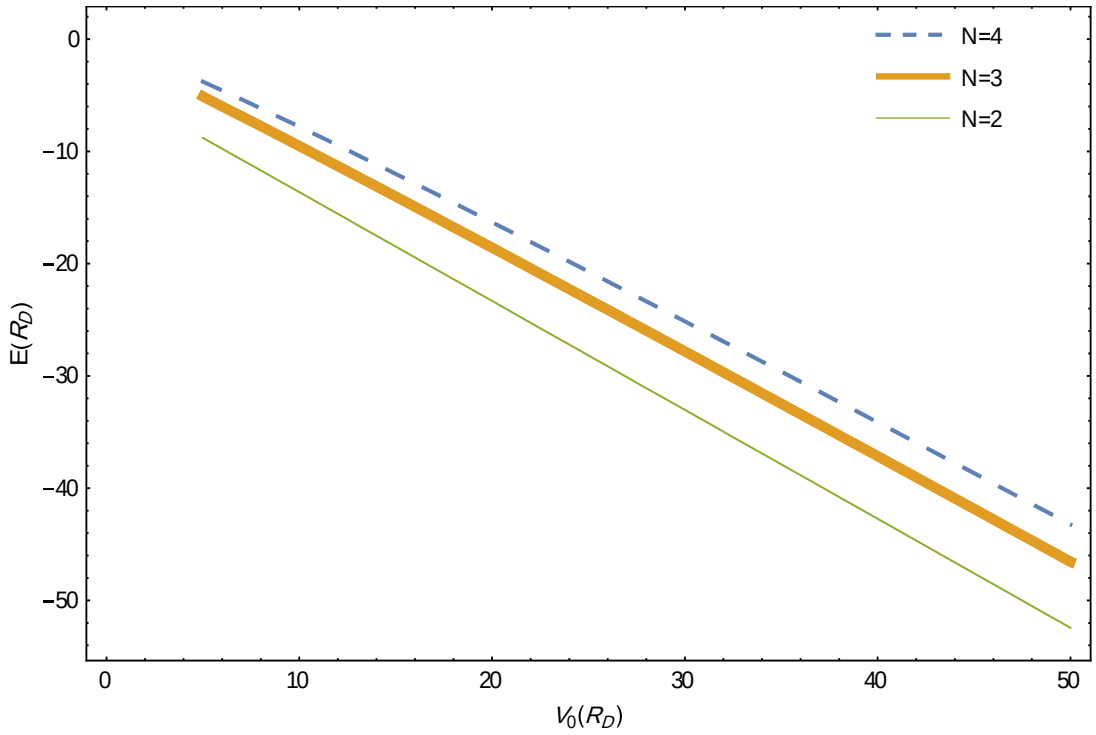

Figure (3- 4): Ground state donor energy$E(1,0)$ as function of potential well depth (V_0) and $R = 2a_D$ for different values of dimension $= 2D, 3D, 4D$.

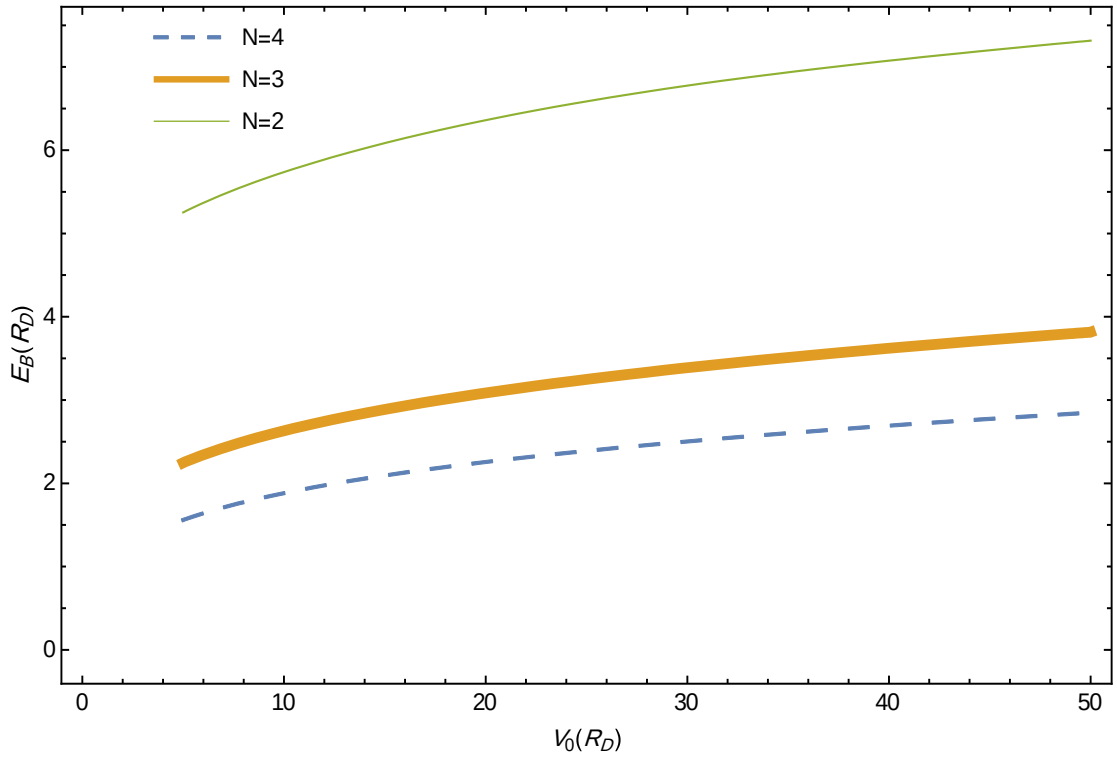

Figure (3- 5): Ground state binding donor energy$E_B(1,0)$ as function of potential well depth(V_0) and $R = 2a_D$ for different values of dimension $N = 2D, 3D, 4D$.

3.2 Heat capacity(C_v) and Entropy (S) of the donor impurity

In this section we will present our computed results for the heat capacity (C_v) and entropy (S) of donor impurity in QD confined by a Gaussian potential. (C_v) and (S) were calculated by using the computed average energy of a confined electron in a QD as essential input data.

3.2 .1 Average Energy of the donor impurity

In figure (3-6) we had shown the behavior of average energy of QD with and without donor impurity as function of temperature (T). We observe that the average thermodynamic energy increases with increasing temperature (T). The reason for this behavior is due to the significant increment in the thermal and the confinement energy contributions.

The behavior of the average energy in QD depends on the density of states because the energy levels are discrete. Consequently, the thermodynamic properties will depend on the energy level distribution and temperature (T) of the occupation probability of the states.

The donor impurity increases the average energy due to its negative coulomb contribution.

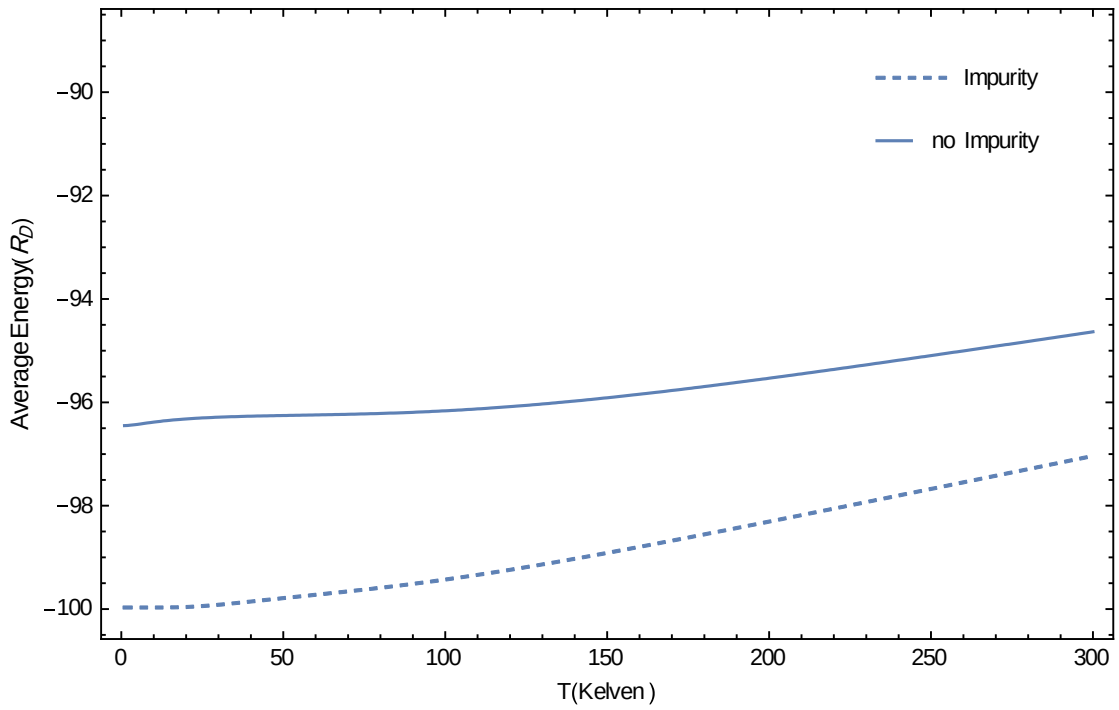

Figure (3-6): Average energy of QD as function of temperature (T) with donor impurity and without impurity at constant $R = 2a_D$, $V_0 = 100R_D$, $N = 3D$.

Figure (3-7) shows the effect of the temperature (T) on the average binding energy of QD. Due to the enhancement of the electron spatial probability density at low temperature (T) it is found that at low temperature (T) of 4K the average binding energy is increased over that associated with temperature (T) near room 300K.

At low temperatures the thermal energy of the system is less than the coulomb interaction which means the increasing in the binding energy, but as the temperature increasing than 20K the kinetic energy (more thermal energy) will be more than the coulomb interaction and that leads to reduce the binding energy. The maximum value of the binding energy approaches to 3.625 R_D at temperature equals 20K.

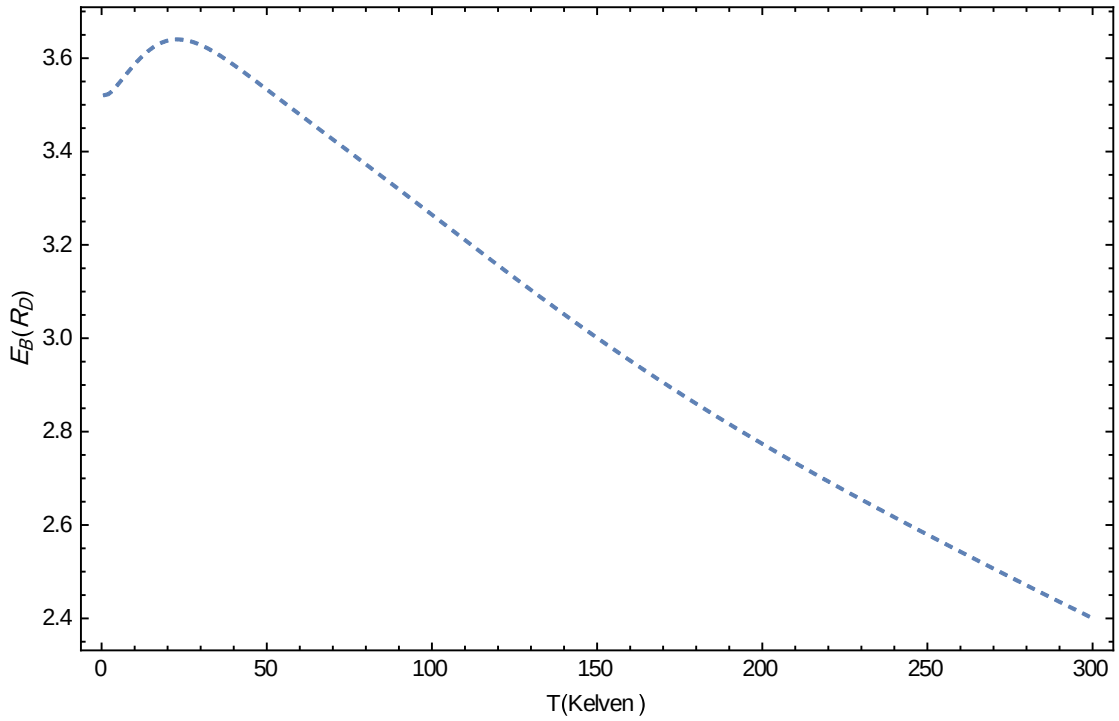

Figure (3-7): 3D Average binding energy of donor impurity in QD as function of temperature (T) at constant $R = 2a_D$, $V_0 = 100R_D$.

3.2 .2 Heat capacity C_v of the donor impurity

Heat capacity (C_v) is a measurable physical quantity which means the ratio of the heat energy absorbed by a substance (or removed from) to the substance's increase in temperature (T), in other words, it is the amount of heat energy required to rise the temperature (T) of a body a specified amount. Figure (3-8) shows the behavior of the heat capacity (C_v) for donor impurity QD versus the temperature (T). The monotonic increase in the heat capacity (C_v) with temperature (T) is expected but as the temperature (T) is increased from absolute zero the heat capacity (C_v) suddenly increases and then decreases giving a peak-like structure. The peak structure is the well-known Schottky anomaly of the heat capacity (C_v), typical for a system where only two states are importance at low

temperature (T) because the thermal energy gained by electrons is enough for only the lowest two levels.

The increase in heat capacity (C_v) with temperature (T) can be attributed to the increase in the thermal energy (E_{th}= K_BT) for electrons which makes more and more states available for thermal excitation.

However as the temperature (T) keeps increasing the heat capacity finally saturates where all the energy levels are populated evenly (there no substantial change). The saturation value of the heat capacity (C_v) approaches at room temperature (300K) is found to be about $0.825K_\beta$.

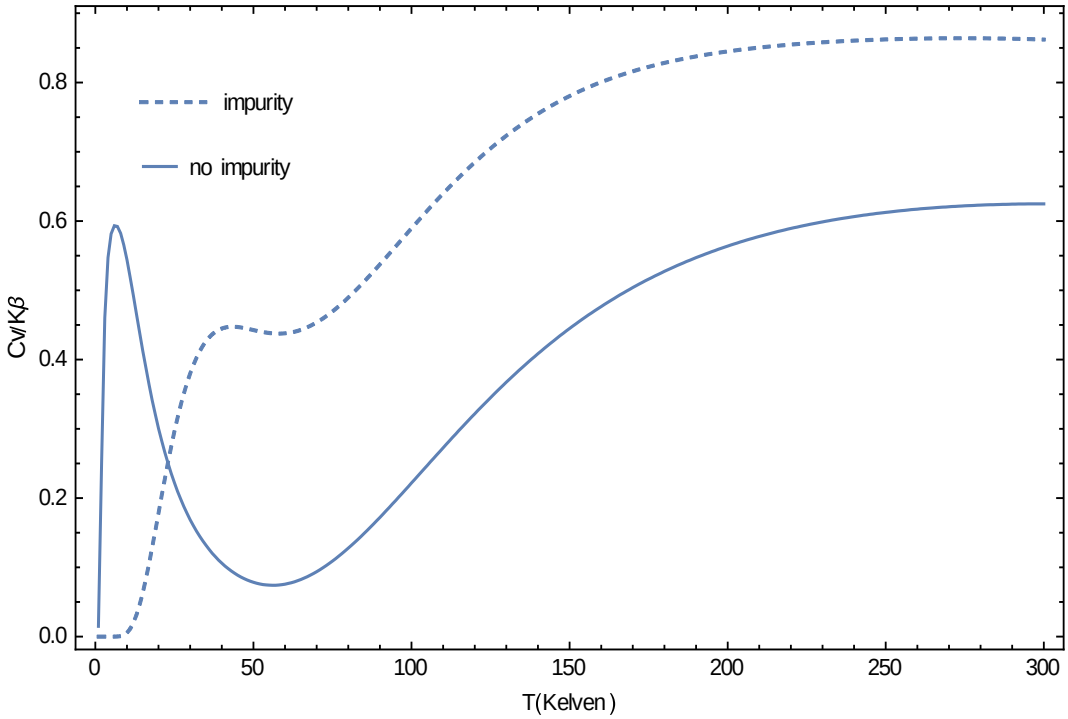

Figure (3-8): Heat Capacity of QD (C_v/K_β) as function of temperature (T) with donor impurity and without impurity at constant $R = 2a_D$, $V_0 = 100R_D$, $N = 3D$

In figure (3-9) we had plotted the behavior of thermal heat capacity (C_v) of donor impurity QD as function of temperature (T) for different values of confinement potential depth (V_0) while keeping R unchanged . It is important to note that increasing in (V_0) leads to an actual drop in the magnitude of the heat capacity (C_v) . As increasing in (V_0) (more confinement energy) the excitation energies for the low-lying excited states become large ,so the environments thermal energy will not excite the system and that leads to a very low heat capacity (C_v).

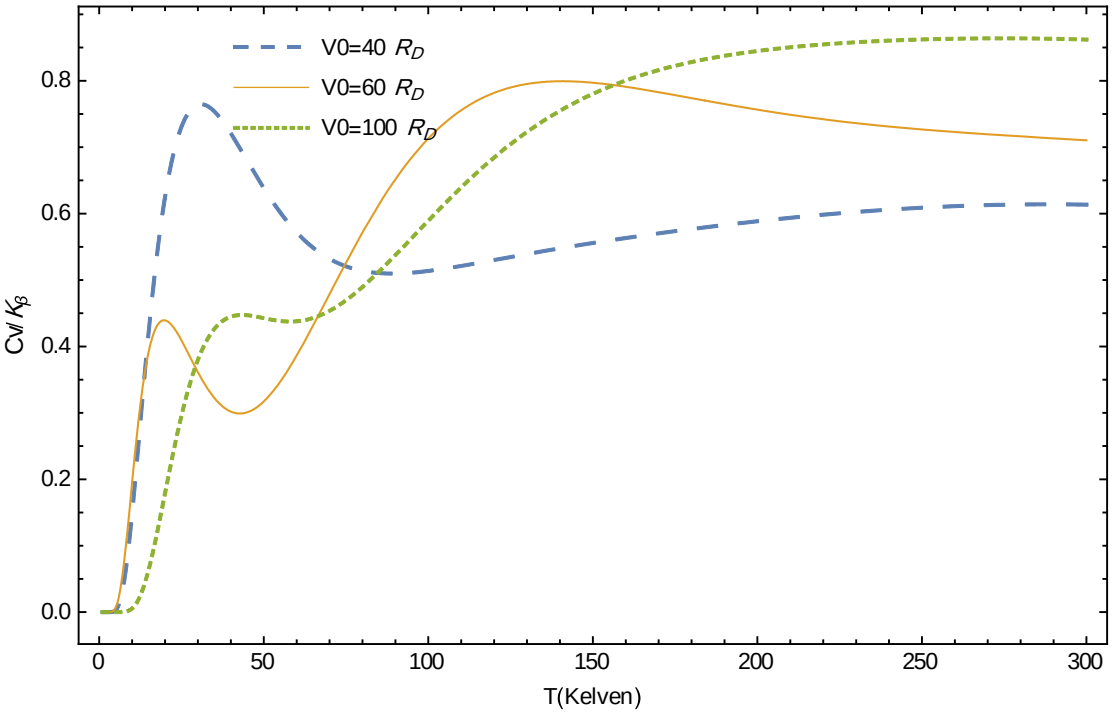

Figure (3-9): Heat Capacity of donor impurity QD (C_v/K_β) as function of temperature(T) for different values $V_0 = 40R_D$, $60R_D$, $100R_D$ at constant $R = 2a_D$, $N = 3D$.

The heat capacity (C_v) of donor impurity QD as function of temperature(T) for different values of QD radius (R) is presented in figure (3-10). We can observe the heat capacity increases monotonically as

R increases . The zero value of heat capacity below a certain critical dot size may be because of the occurrence of the large sub bands energy spacing at low R. Figure(3-11) shows the dependence of the heat capacity(C_v) of donor impurity QD on the dimension(N) for fixed values of (V_0) and (R). We can see that heat capacity curves cross at the same temperature point (known as crossing temperature) which almost equals 170K (energy level crossing).

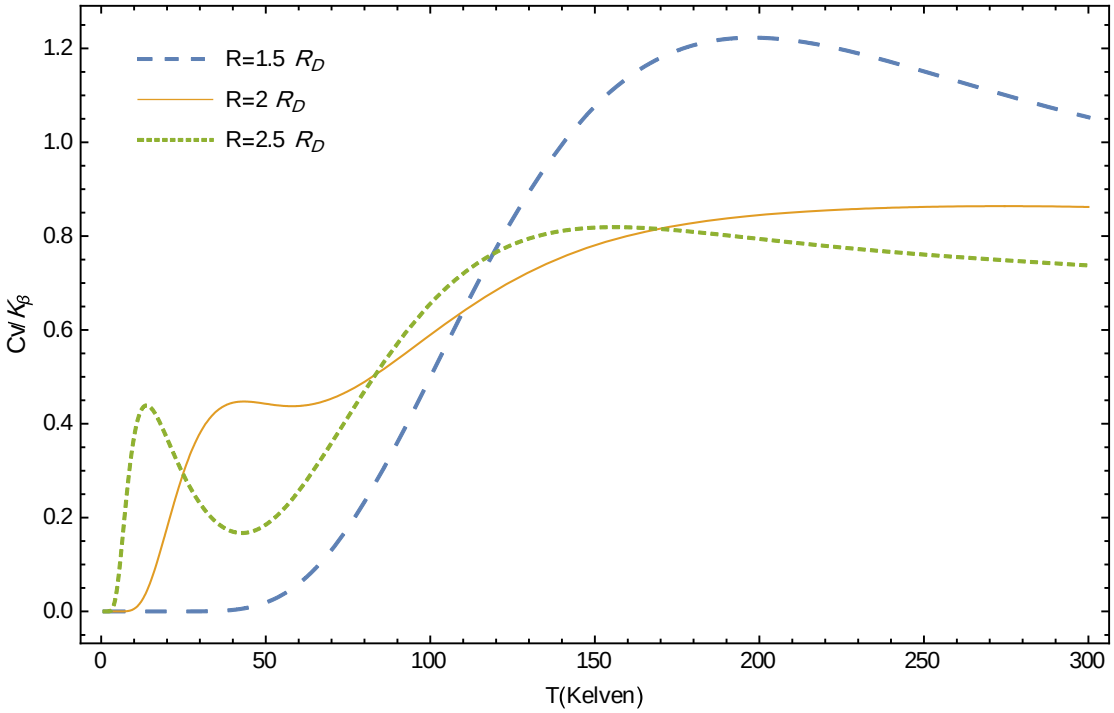

Figure (3-10): Heat Capacity of donor impurity QD (C_v/K_β) as function of temperature (T) for different values of $R = 1.5a_D$, $2a_D$, $2.5a_D$ at constant $V_0 = 100R_D, N = 3D$.

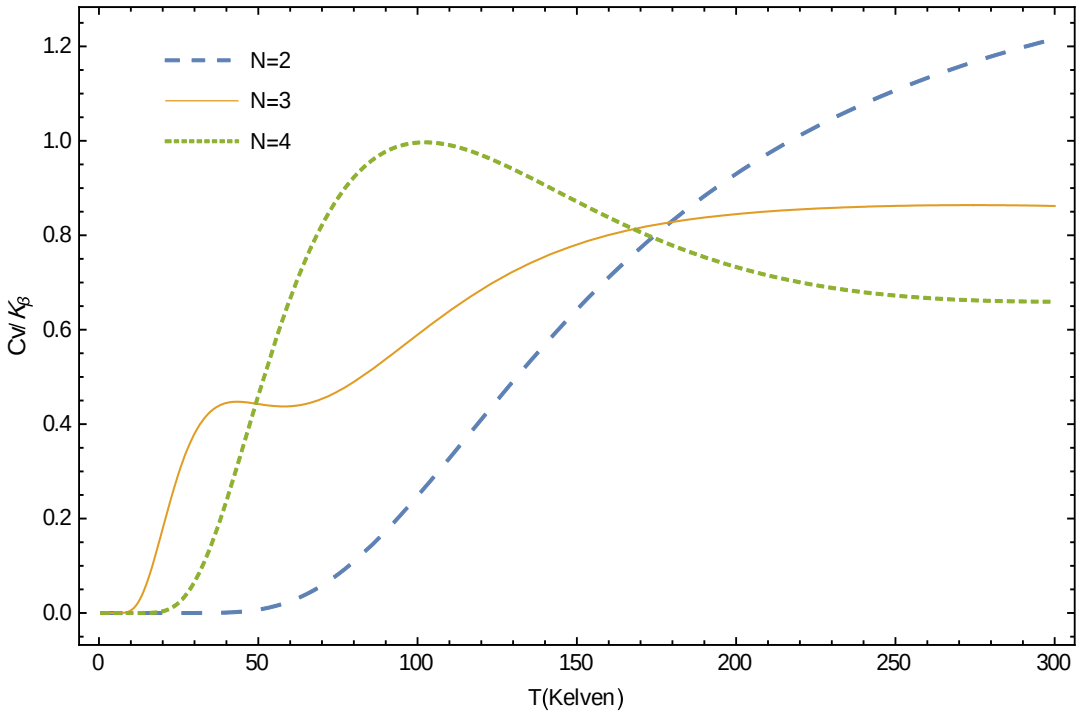

Figure (3-11): Heat Capacity of donor impurity QD (C_v/K_β) as function of temperature(T) for different $values\ of\ N = 2D, 3D, 4D$ at constant $V_0 = 100R_D$, $R = 2a_D$.

3.2.3 Entropy S of the donor impurity

Another important thermodynamics quantity we have studied is the entropy (S) which is real physical quantity and is a definite function of the state of the body. We have calculated the entropy(S) as function of temperature (T) as shown in figure (3-12) with impurity and without impurity. The increasing in entropy (S) of QD with increases the temperature (T) is expected , at lower temperatures the behavior is qualitatively different as compared to that at relatively higher temperatures, the entropy increases monotonically at high value of temperatures but at low temperatures the entropy increases quite rapidly. The thermal energy of electrons will bring more and more disorder in the form of random motion so the entropy (S) increases with temperature (T) increasing. At zero temperature (T) only the

lowest energy level is occupied so the entropy (S) is zero and there is a very little probability of a transition to a higher energy level. As the temperature (T) increases there is an increase in entropy (S) and thus the probability of a transition goes up.

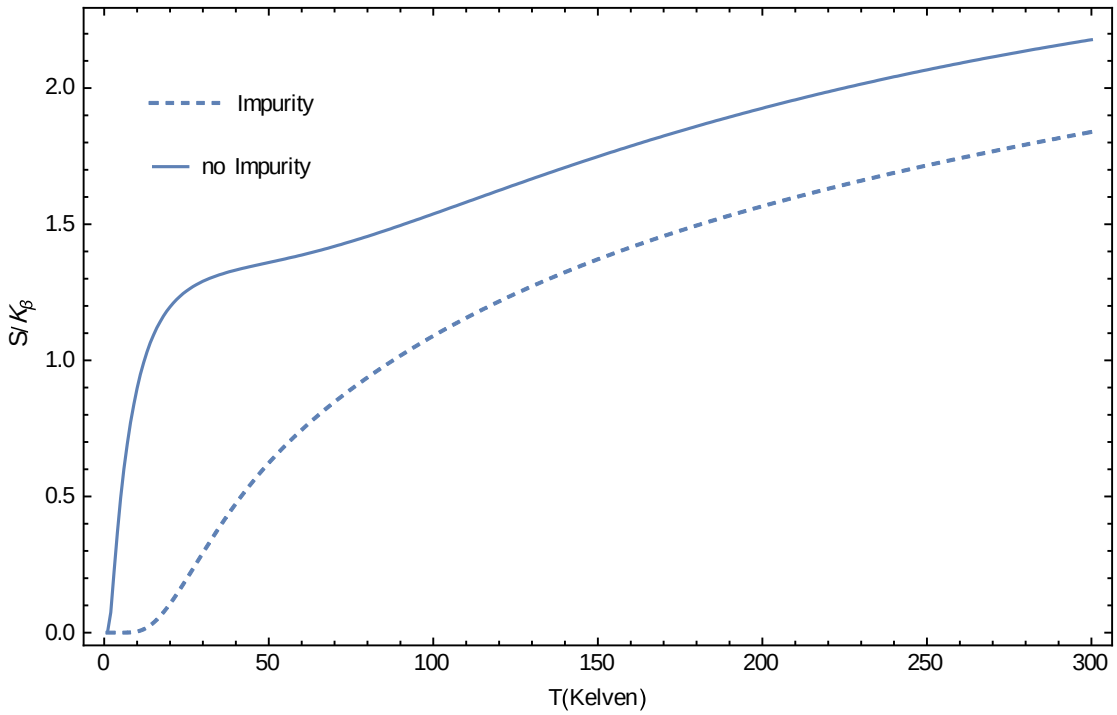

Figure (3-12): Entropy of QD (S/K_β) as function of temperature (T) with donor impurity and without impurity at constant $R = 2a_D$, $V_0 = 50R_D$, $N = 3D$.

The variation of entropy (S) with respect to the QD radius (R) at different temperature (T) is shown in figure (3-13). The figure shows that the entropy (S) increases as the QD radius (R) increases because the increasing in radius will lead to the more ways there are to distribute the atom in that size which means higher entropy (S). Figure (3-14) shows the effect of the potential depth (V_0) on the behavior of the curve of the entropy (S) at different temperatures (T). The figure shows clearly the change in the entropy (S) curves as we increase the confining Gaussian

potential V_0 . The Gaussian potential term ($-V_0 e^{-r^2/2R^2}$) increases greatly the total energy state due to its large Gaussian energy confinement.

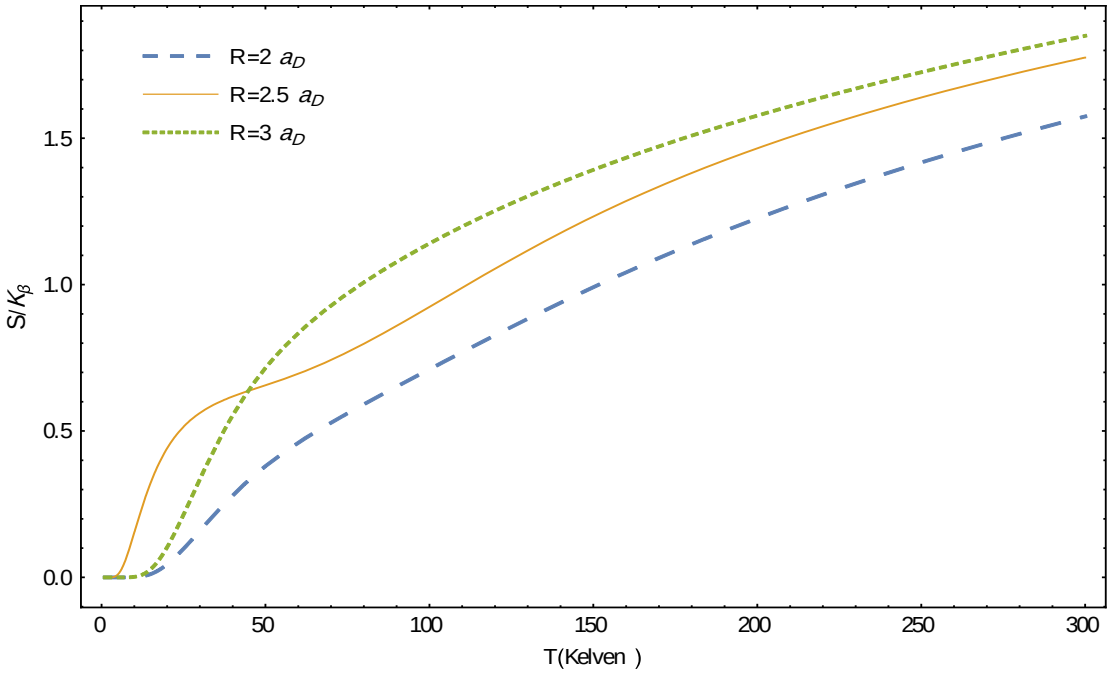

Figure (3-13): Entropy of donor impurity in QD (S/K_β) as function of temperature (T) for different values of $R = 1.5a_D$, $2a_D$, $2.5a_D$ at constant $V_0 = 100R_D$, $N = 3D$.

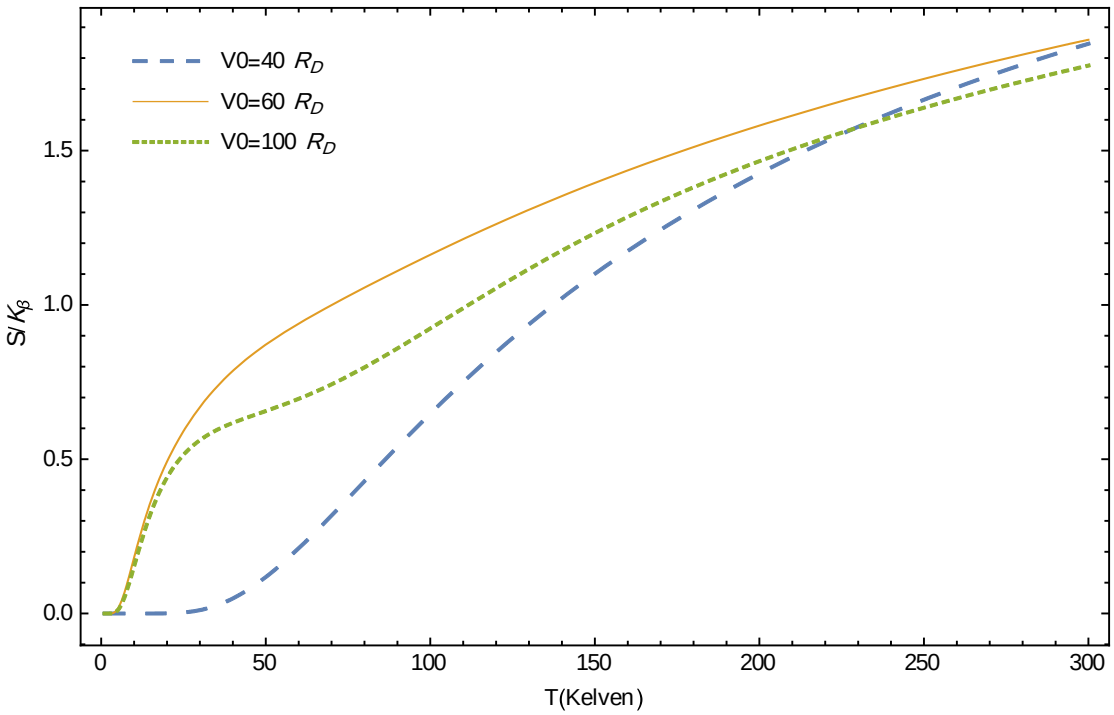

Figure (3-14) : Entropy of donor impurity in QD (S/K_β) as function of temperature (T) for different values of $V_0 = 40R_D$, $60R_D$, $100R_D$ at constant $R = 2.5a_D$, $N = 3D$.

To emphasize The effect of dimension (N) on entropy (S) we had plotted in figure(3-15) the entropy S/K_β as function of temperature (T) but at different values of dimension (N) .The entropy change is due to the difference in spectral density of QD states.

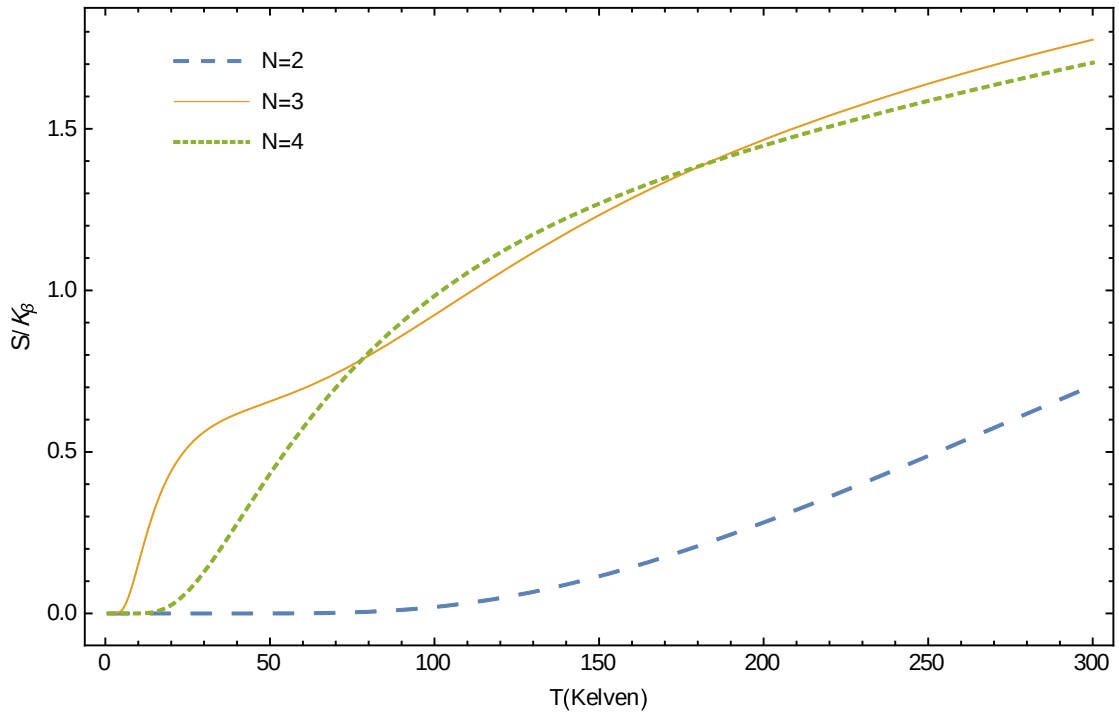

Figure (3-15): Entropy of donor impurity in QD (S/K_β) as function of temperature (T)for different values of $N = 2D\ ,3D\ ,4D$ at constant $R = 2.5a_D\ , V_0 = 100R_D$.

Chapter four
Conclusion

We had solved the donor impurity in GaAs/AlGaAs QD with Gaussian potential Hamiltonian using the shifted $1/N$ expansion method. We have presented a calculation for the donor binding energies associated with the ground state in two, three and four dimension. We have considered the effects of impurity, dot radius (R), confining potential depth (V_0) and dimension (N) on the ground state energy, the interplay of these effects leads to a dependence of the binding energy on these factors .The computed result shows that the impurity binding energies increase with the decrease in dot size (R). Furthermore the binding energies increase with the increase in potential depth (V_0). The results of this work show that the effects of the V_0, N, R on the binding energy of donor impurity should be considered.

According to the numerical results obtained in this work, we have shown the shifted $1/N$ expansion method is very efficient and accurate in calculating the energy spectrum of the donor impurity in QD.

The heat capacity (C_v) and entropy (S) dependence on dot radius (R)**,** confining potential depth (V_0), dimension (N) and temperature (T) of GaAs/AlGaAs QD had been investigated. The investigations had shown clearly that increasing temperature (T), dot radius (R) and dimension (N) enhance the heat capacity (C_v) and entropy (S),while enhancing the confining potential depth (V_0) decrease the heat capacity (C_v) and entropy (S).

In this work, the impurity presence, dot radius (R), confining potential depth (V_0), dimension (N) and temperature (T) effects on the energy, binding energy, heat capacity (C_v), entropy (S) had been studied. However, the electronic and thermodynamic properties of donor impurities in quantum dot are very interesting issues in the future due to its potential in the device applications. In addition the properties of the donor impurity in heterostructure for full energy spectra are very important subject to be studied.

References

[1] T. Takagahara, K.Takeda. **Theory of the quantum confinement effect on excitons in quantum dots of indirect-gap materials**. Physical Review B, **46**, 15578 (**1992**).

[2] K.D. Sattler. **Handbook of Nanophysics**, Principles and Methods, CRC, New York(**2010**).

[3] B. Bhushan, **Handbook of Nanotechnology**, Springer, Berlin (2004).

[4] R.C.Ashoori , H.L.Stormer , J. S. Weiner, L. N. Pfeiffer, S. J. Pearton, K. W. Baldwin, and K. W.West. **Single-electron capacitance spectroscopy of discrete quantum levels**. Phys. Rev. Lett. **68**, 3088 (**1992**).

[5] O. Ciftja . **Understanding electronic systems in semiconductor quantum dots** . Physica Scripta . **88**,058302 (**2013**).

[6] B.Zh. Poghosyan. **Binding Energy of Hydrogen-Like Impurities in Quantum Well Wires of InSb/GaAs in a Magnetic Field** . Nanoscale Res. Lett. **2**, 515 (**2007**) .

[7] H.Ganjipour , Gh. Safarpour. **The effects of pressure and hydrogenic donor impurity on the linear and nonlinear optical properties of a GaAs/GaAlAs nanowire superlattice**. Physica E .**74**, 496504 (**2015**).

[8] J. Zhu, Y. Cheng and J. Xiong . **Exact solutions for two-dimensional hydrogenic donor states in a magnetic field**. Phys. Let. A. 145, 358 (1990).

[9] A.Mmadi, K. R ahmani, I. Zorkani, and A. Jorio. **Diamagnetic susceptibility of a magneto-donor in Inhomogeneous Quantum Dots**. Superlattices and Microstruct. **57**, 27-36 (**2013**).

[10] C. B .Murray, C. R. Kagan, M. G. Bawendi. **Synthesis and Characterization of Monodisperse Nanocrystals and Close Packed Nanocrystal Assemblies**. Annual Review of Materials Science **30**, 545610 (**2000**).

[11] M. A. Kastner. **Artificial Atoms**. Physics Today **46**, 24 (**1993**).

[12] D. loss and D.P. Divincenzo. **Quantum computation with quantum dots.** phys. Rev. A **57**,120 (**1998**).

[13] G. Burkard, D. Loss and D.P. Divincenzo. **Coupled quantum dots as quantum gates**. phys. Rev. B **59**, 2070 (**1999**).

[14] C. Bose. ***Binding energy of impurity states in spherical quantum dots with parabolic confinement***. **J. Appl. Phys**. **83**, 3089 (**1998**).

[15] C. Bose, C.K. Sarkar, **Solid State Electron**. **42**,1661 (**1998**).

[16] W. Xie. **Negative donor centers in a GaAs parabolic quantum dot**. Phys. Lett. A **263** ,127 (**1999**).

[17] Jia-Lin Zhu, Jia-Jiong Xiong, **Bing-Lin Gu. Confined electron and hydrogenic donor states in a spherical quantum dot of $GaAs-Ga_{1-x}Al_xAs$**. phys. Rev. B 41, 6001 **(**1990).

[18] Jia-Lin Zhu, Jian Wu, R.T.Fu, Hao Chen, Yoshiyuki kawazoe. **Effects of quantum size and potential shape on the spectra of an electron and a donor in quantum dots** . Phys. Rev. B **55**, 1673 (**1997**).

[19] N.Porras-Monteegro, S.T. **Perez- Merchancano. Hydrogenic impurities in GaAs-(Ga,Al)As quantum dots**. phys. Rev. B **46**,9780 (**1992**).

[20] J.L. Movilla, J.Planelles. **Image charges in spherical quantum dots with an off-centered impurity: algorithm and numerical results**. Comp. Phys. Comm., **170**, 144 (**2005**).

[21] A. Gharaati, R.Khordad. **A new confinement potential in spherical quantum dots: Modified Gaussian potential**. Superlattices and Microstruct. **48**, 276 (**2010**).

[22] Aalu Boda, Ashok Chaterjee. **Ground state and binding energies of (D^0), (D^-) centres and resultant dipole moment of a (D^-) centre in a GaAs quantum dot with Gaussian confinement** .Physica E **45**, 36 (**2012**).

[23] U. Sukhatme , T. Imbo. **Shifted expansions $1/N$ for energy eigenvalues of the Schrödinger equation**. Phys. Rev. D **28**,418 (**1983**).

[24] T. Imbo, A . pagnamenta ,U . Sukhatme. **Energy eigenstates of spherically symmetric potentials using the shifted $1/N$ expansion**. Phys .Rev. D **29**,1669 (**1984**).

[25] Nag T. T. Nguyen and F.M peters. **Magnetic field dependence of the many-electron states in a magnetic quantum dot: The ferromagnetic-antiferromagnetic transition.** Phys. Rev. B **78**, 045321 (**2008**).

[26] S. A. Mikhailov. **Quantum-dot lithium in zero magnetic field: Electronic properties, thermodynamics, and Fermi liquid–Wigner solid crossover in the ground state**. Phys. Rev. B **65**, 115312 (**2002**).

[27] Sergio S. Gomez, Rodolfo H. Romero. ***Few-electron semiconductor quantum dots with Gaussian confinement.*** Cent Eur. **J . Phys**. **7** (**2009**).

[28] J.M. Thijssen . **Computational Physics**. Cambridge University Press, Cambridge, (**1999**).

[29] C. S. Lai. ***On the Schrodinger equation for the gaussian potential - A exp(-λ r^2)*** . **J. Phys**. A: Math.Gen, 16 L181 (**1983**).

[30] M.EL-Said . ***Energy States of Two Electrons in a Parabolic Quantum Dot in a Magnetic Field*** . **Journal de Physique** I ,**5**,1027-1036 (**1995**).

[31] M.EL- Said. **The ground-state electronic properties of a quantum dot with a magnetic field** .Pysics Scripta,**75**, 436 (**2007**).

[32] C. Bose , C.K.Sarkar . **Effect of a parabolic potential on the impurity binding energy in spherical quantum dots** . Physica B, **253** (**1998**).

[33] Sheng Wang ,Yun Kang, Xian- LiLi . **Binding energy of the ground and first few excited states of hydrogenic donor impurity in a rectangular GaAs quantum dot in the presence of electric field**. Superlattices and Microstructures,**76**, (**2014**)

Appendix

The shifted $1/N$ expansion method consists in solving equation (5) systematically in terms of the expansion parameter $1/\bar{k}$. The leading contribution to the energy comes from the effective potential:

$$V_{eff}(r) = \frac{\hbar^2}{8m^* r^2} + \frac{V(r)}{Q} \tag{A1}$$

Where Q is a constant which rescales the potential (in large $\bar{k}$ limit), $Q = \bar{k}^2$. To obtain such an expansion it is necessary to remove linear parts with respect to the coordinates in the potential. Therefore we develop the potential around its minimum.

$V(r)$ is assumed to be well behaved so that $V_{eff}(r)$ has minimum at $r = r_0$ and there are well-defined bound states. Q is then determined from the following equation:

$$4m^* r_0{}^3 \frac{dV}{dr_0} = \hbar^2 \, Q \tag{A2}$$

In order to shift the origin of the coordinate to the position of the minimum of the effective potential it is convenient to define a new variable x

$$x = \frac{\bar{k}^{\frac{1}{2}}}{r_0}(r - r_0) \tag{A3}$$

By using the Taylor expansion around the effective potential minimum r_0, respectively $x = 0$ we will define an oscillator potential :

$$\omega = \frac{\hbar}{2m^*}\left[3 + \frac{r_0 \frac{d^2V}{dr_0}}{\frac{dV}{dr_0}}\right]^{1/2} \tag{A4}$$

The energy eigenvalues are given by an expansion in powers of $1/\bar{k}$ where $\bar{k} = N + 2l - a$, N being the number of spatial dimensions and (a) so-called shifted parameter.

The shift parameter is defined by equation:

$$a = 2 - 2(2n_r + 1)\frac{m^*\omega}{\hbar} \quad \text{(A5)}$$

For any value of the radial quantum number $n_r(n_r = n - l - 1)$ and for any value of l the energy $E(n_r, l)$ is given by:

$$E(n, l) = E_0 + E_1 + E_2 + E_3 + \cdots \quad \text{(A6)}$$

The binding energy $E_B(n, l)$ in a given state is defined by

$$E_B(n, l) = E_B(n, l, w = 0) - E_B(n, l, w = 1)$$

where:

$$E_0 = V(r) + (Q/(8 * m^* * r^2)$$

$$E_1 = (c_1 * c_3)/(8 * m^*)$$

$$E_2 = (E_1 + \alpha_1)/r^2$$

$$E_3 = \alpha_2/(\bar{k} * r^2)$$

where:

$$Q = (N + 2 * \ell - a)^2$$

$$c_1 = (1 - a)$$

$$c_2 = (2 - a)$$

$$c_3 = (3 - a)$$

$$\alpha_1 = \mathrm{n}_1 * \mathrm{e}_2 + 3 * \mathrm{n}_2 * \mathrm{e}_4 - \mathrm{c}_5 * (\mathrm{e}_1{}^2 + 6 * \mathrm{n}_1 * \mathrm{e}_1 * \mathrm{e}_3 + \mathrm{n}_4 * \mathrm{e}_3{}^2)$$

$$\alpha_2 = \mathrm{t}_7 + \mathrm{t}_{12} + \mathrm{t}_{16}$$

$$c_5 = \omega^{-1}$$

The explicit forms of the previous parameters are given in the following

$$t_7 = t_1 - c_5 * (t_2 + t_3 + t_4 + t_5 + t_6)$$

$$t_{12} = c_5{}^2 * (t_8 + t_9 + t_{10} + t_{11})$$

$$t_{16} = -c_5{}^3 * (t_{13} + t_{14} + t_{15})$$

With:

$$t_1 = n_1 * d_2 + 3 * n_2 * d_4 + 5 * n_3 * d_6$$

$$t_2 = n_1 * e_2{}^2 + 12 * n_2 * e_2 * e_4$$

$$t_3 = 2 * e_1 * d_1 + 2 * n_5 * e_4{}^2$$

$$t_4 = 6 * n_1 * e_1 * d_3 + 30 * n_2 * e_1 * d_5$$

$$t_5 = 6 * n_1 * e_3 * d_1 + 2 * n_4 * e_3 * d_3$$

$$t_6 = 10 * n_6 * e_3 * d_5$$

$$t_8 = 4 * e_1{}^2 * e_2 + 36 * n_1 * e_1 * e_2 * e_3$$

$$t_9 = 8 * n_4 * e_2 * {e_3}^2$$

$$t_{10} = 24 * n_1 * {e_1}^2 * e_4 + 8 * n_7 * e_1 * e_3 * e_4$$

$$t_{11} = 12 * n_8 * {e_3}^2 * e_4$$

$$t_{13} = 8 * {e_1}^3 * e_3 + 108 * n_1 * {e_1}^2 * {e_3}^2$$

$$t_{14} = 48 * n_4 * e_1 * {e_3}^3$$

$$t_{15} = 30 * n_9 * {e_3}^4$$

Where $(n's)(d's)$ *and* $(e's)$ *are parameters given as :*

$$n_1 = 1 + 2 * n_r$$

$$n_2 = 1 + 2 * n_r + 2 * {n_r}^2$$

$$n_3 = 3 + 8 * n_r + 6 * {n_r}^2 + 4 * {n_r}^3$$

$$n_4 = 11 + 30 * n_r + 30 * {n_r}^2$$

$$n_5 = 21 + 59 * n_r + 51 * {n_r}^2 + 34 * {n_r}^3$$

$$n_6 = 13 + 40 * n_r + 42 * {n_r}^2 + 28 * {n_r}^3$$

$$n_7 = 31 + 78 * n_r + 78 * {n_r}^2$$

$$n_8 = 57 + 189 * n_r + 225 * {n_r}^2 + 150 * {n_r}^3$$

$$n_9 = 31 + 109 * n_r + 141 * {n_r}^2 + 94 * {n_r}^3$$

$$c_4 = 2 * m^* * \omega$$

$$e_1 = \epsilon_1/\sqrt{c_4}$$

$$e_2 = \epsilon_2 / c_4$$

$$e_3 = \epsilon_3 / {c_4}^{3/2}$$

$$e_4 = \epsilon_4 / {c_4}^{2}$$

$$d_1 = \delta_1/\sqrt{c_4}$$

$$d_2 = \delta_2/c_4$$

$$d_3 = \delta_3/{c_4}^{3/2}$$

$$d_4 = \delta_4/{c_4}^{2}$$

$$d_5 = \delta_5/{c_4}^{5/2}$$

$$d_6 = \delta_6/{c_4}^{3}$$

Furthermore:

$$\epsilon_1 = c_2/(2 * m^*)$$

$$\epsilon_2 = -3 * c_2/(4 * m^*)$$

$$\epsilon_3 = -1/(2 * m^*) + (r_5 * der_3(r))/(6 * Q)$$

$$\epsilon_4 = 5/(8 * m^*) + (r_6 * der_4(r))/(24 * Q)$$

$$\delta_1 = -c_1 * c_3/(4 * m^*)$$

$$\delta_2 = 3 * c_1 * c_3/(8 * m^*)$$

$$\delta_3 = c_2/m^*$$

$$\delta_4 = -5 * c_2/(4 * m^*)$$

$$\delta_5 = -3/(4 * m^*) + (r_7 * der_5(r))/(120 * Q)$$

$$\delta_6 = 7/(8 * m^*) + (r_8 * der_6(r))/(720 * Q)$$

Where:

$$der_1(r) = \frac{dV}{dr}$$

$$der_2(r) = \frac{d^2V}{dr}$$

$$der_3(r) = \frac{d^3V}{dr^3}$$

$$der_4(r) = \frac{d^4V}{dr^4}$$

$$der_5(r) = \frac{d^5V}{dr^5}$$

$$der_6(r) = \frac{d^6V}{dr^6}$$

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قدمت هذه الأطروحة استكمالاً لمتطلبات الحصول على درجة الماجستير في الفيزياء، بكلية الدراسات العليا، في جامعة النجاح الوطنية، نابلس- فلسطين.

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الملخص

في العمل الحالي، تم حساب طاقة المستوى الأرضي للشوائب المانحة الضحلة في نقاط كمية والمحصورة بجهد جاوس باستخدام طريقة المفكوك وقد قمنا بدراسة اعتماد طاقة المستوى الأرضي على كل من الشوائب، ونصف قطر النقطة وعمق الجهد المحصور والبعد وقد تم حساب طاقة الربط للشوائب في المستوى الارضي بدلالة نصف قطر النقطة وعمق الجهد المحصور والبعد وجدنا ان طاقة الربط للشوائب في المستوى الارضي تزداد بزيادة عمق الجهد المحصور بينما تقل بزيادة نصف قطر النقطة والبعد. بالإضافة الى ذلك قمنا بحساب السعة الحرارية والعشوائية للشوائب المانحة في نقاط كمية مع دراسة اعتماد هذه الكميات على نصف قطر النقطة وعمق الجهد المحصور والبعد والحرارة. وأظهرت المقارنات توافق كبير بين نتائجنا مع نتائج أعمال أخرى منشورة.