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The heat capacity of a semiconductor quantum dot in magnetic fields

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The heat capacity of two interacting electrons confined in a quantum dot presented in a magnetic field has been calculated by solving the Hamiltonian using the exact diagonalization method. The statistical average energies for confined and interacting electrons have been computed for various values of magnetic fields, confining frequency and temperature. We had investigated the dependence of the heat capacity on quantum dot Hamiltonian's parameters and temperature. The singlettriplet transitions in the ground state of the quantum dot spectra and the corresponding jumps in the heat capacity curves had been shown. The comparisons show that our results are in very good agreement with theoretical reported works.

Keywords: quantum dot, magnetic field, exact diagonalization, heat capacity.

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1. Introduction

Semiconductor quantum dots (QDs) have been the subject of interest and hot research area due to their physical properties and significant electronic device applications such as quantum dot lasers, quantum memories, solar cells, single electron transistors, light emitting diodes, biological markers and quantum computers [1–5] The application of a magnetic field perpendicular to the dot plane will introduce an additional structure on the energy levels and correlation effects, of the interacting electrons confined in a quantum dot.

Many authors have used different numerical methods and computational techniques to solve the two electrons QD Hamiltonian, including the effect of an applied magnetic field, and obtain the eigenenergies [6–12]. The energy levels of the interacting electrons show transitions in the angular momentum of the ground states. Computed energies have been used to calculate the statistical average energies of the QD and then, to investigate theoretically the magneto-thermodynamic properties of the two-interacting electron in a quantum dot [13–25].

In this work, we had calculated the heat capacity as a thermodynamic quantity for a quantum dot helium atom in which both the magnetic field and the electron-electron interaction are fully taken into account. Since, the eigenvalues of the electrons in the QD are the starting point to calculate the physical properties of the QD system, we had, first, applied the exact diagonalization method to solve the QD Hamiltonian and obtain the eigenenergies. Second, we had used the computed eigenenergies spectra to display theoretically the heat capacity behavior of the QD as a function of magnetic field strength, confining frequency and temperature.

The rest of this paper is organized as follows: the Hamiltonian formalism, computation exact diagonalization technique and how to calculate the heat capacity from the mean energy expression are presented in Section 2. The final section will be devoted for numerical results and conclusions.

2. Theory

In this section we will describe in detail the main three parts which consist the theory, namely: quantum dot Hamiltonian, exact diagonalization method and the heat capacity.

2.1. Quantum dot Hamiltonian

The effective mass Hamiltonian for two interacting electrons confined in a QD by a parabolic potential in a uniform magnetic field of strength B, applied along z direction is given by:

$$\widehat{H} = \sum_{j=1}^{2} \left(\frac{1}{2m^*}(\vec{p}(\vec{r}_j) + \frac{e}{c}\vec{A}(\vec{r}_j))^2 + \frac{1}{2}m^*\omega_0^2 r_j^2\right) + \frac{e^2}{\epsilon\,|\overrightarrow{r_1} - \overrightarrow{r_2}|} \tag{1}$$

where m^* is the effective mass of electron, e is the electron charge, c is the speed of light, ω_0 and ϵ are defined as the confining frequency and the dielectric constant for the GaAs medium, respectively. Here, r_1 and r_2 describe the positions of the first and second electron in the xy plane; ω_c is the cyclotron frequency and the symmetric gauge

$A = \frac{1}{2}B \times r$ has been used for the vector potential. The complete two electron QD Hamiltonian can be separated into center of mass Hamiltonian H_{CM} and relative Hamiltonian part H, as shown below:

$$H = H_{CM} + H_r \tag{2}$$

$$H_{CM} = \frac{1}{2M}(\overrightarrow{P}_R + \frac{Q}{c}\vec{A}(R))^2 + \frac{1}{2}M\omega_0^2 R^2 \tag{3}$$

$$H_r = \frac{1}{2\mu}(\overrightarrow{p}_r + \frac{q}{c}\vec{A}(r))^2 + \frac{1}{2}\mu\omega_0^2 r^2 + \frac{e^2}{\epsilon\,|r|} \tag{4}$$

where M is the total mass $2m^*$, Q is the total charge$= 2e$, μ is reduce mass$= \frac{m^*}{2}$, and q is the reduce charge $= \frac{e}{2}$.

The corresponding energy of this Hamiltonian equation (1) is

$$E_{total} = E_{CM} + E_r \tag{5}$$

The center of mass Hamiltonian given by equation (3) is a harmonic oscillator type with well-known eigenenergies:

$$E_{CM} = (2n_{CM} + |m_{CM}| + 1)\hbar\sqrt{\frac{\omega_c^2}{4} + \omega_0^2} + m_{CM}\frac{\hbar\omega_c}{2} \tag{6}$$

where n_{CM}, m_{CM} are the radial and angular quantum numbers, respectively.

However, the relative motion Hamiltonian part (H_r), given by equation (4) does not have an analytical solution for all ranges of ω_0 and ω_c. In this work, an exact diagonalization method will be applied to solve the relative part of the Hamiltonian and obtain the corresponding eigenenergies, E_r.

2.2. Exact diagonalization method

For non-interacting case the relative Hamiltonian in equation (4) can be reduced to a single particle problem with eigenstates $|n_r, m_r\rangle$ known as Fock-Darwin states [9] given by the following form:

$$|n_r, m_r\rangle = N_{n_r,m_r}\frac{e^{im_r\varphi}}{\sqrt{2\pi}}(\alpha r)^{|m_r|}e^{-\alpha^2 r^2/2}L_{n_r}^{|m_r|}(\alpha^2 r^2) \tag{7}$$

where the functions $L_{n_r}^{|m_r|}(\alpha^2 r^2)$ are the standard associated Laguerre polynomials. The normalization constant N_{n_r,m_r} can be calculated from the normalization condition of the basis, $\langle n_r, m_r\,|n_r, m_r\rangle = 1$, to give:

$$N_{n_r,m_r} = \sqrt{\frac{2n_r!\alpha^2}{(n_r + |m_r|)!}} \tag{8}$$

$\alpha = \sqrt{\frac{m\omega}{h}}$, is a constant which has the dimensionality of an inverse length.

The eigenenergies of the QD Hamiltonian which are given by equation (5), consist of the sum of the energies for the center of mass Hamiltonian, and the eigenenergies obtained by direct diagonalization to the relative Hamiltonian part. For the interacting case, we shall apply exact diagonalization method to solve equation (4) and find the corresponding exact eigenenergies for arbitrary values of ω_0 and ω_c.

The matrix element of the relative Hamiltonian part using the basis can be expressed as:

$$h_{nn'} = \langle n_r, m_r\,|H_r|n_r, m_r\rangle = \langle n_r, m_r|\,-\frac{\hbar^2}{2\mu}\nabla^2 + \frac{1}{2}\mu\omega^2 r^2\,|n_r, m_r\rangle + \langle n_r, m_r|\,\frac{e^2}{\epsilon r}\,|n_r, m_r\rangle \tag{9}$$

The corresponding relative dimensionless energies are:

$$\frac{E_r}{\hbar\omega_0} = \frac{h_{nn'}}{\hbar\omega_0} = ((2n + |m_z| + 1)\sqrt{1 + \frac{\gamma^2}{4}} - \frac{\gamma}{2}\,|m_z|)\delta_{nn'} + \frac{\lambda}{\sqrt{2}}\sqrt{\frac{n'!n!}{(n' + |m_z|)!(n + |m_z|)!}} \times I_{nn'}\,|m_z| \tag{10}$$

where $\gamma = \frac{\omega_c}{\omega_0}$, $\lambda = \frac{e^2\alpha}{\hbar\omega_0}$ are dimensionless parameters and $\omega^2 = \frac{\omega_c^2}{4} + \omega_0^2$ is the effective confining frequency. $I_{nn'}$ is the coulomb energy matrix element that can be evaluated in a closed form by using the following Laguerre relation [17]:

$$\int_0^\infty t^{\alpha-1}e^{-pt}L_m^\lambda(at)L_n^\beta(bt)dt = \frac{\Gamma(\alpha)(\lambda+1)_m(\beta+1)_n p^{-\alpha}}{m!n!}\sum_{j=0}^{m}\frac{(-m)_j(\alpha)_j}{(\lambda+1)_j j!}\left(\frac{a}{p}\right)^j\sum_{k=0}^{n}\frac{(-n)_k(\alpha+j)_k}{(\beta+1)_k k!}\left(\frac{b}{p}\right)^k. \tag{11}$$

This closed form result of the coulomb energy reduces greatly the computation time needed in the diagonalization process.

In our calculation, we had used the basis, $|n_r, m_r\rangle$ defined by equation (16) to diagonalize the relative QD Hamiltonian and obtained its corresponding eigenenergies E_r.

2.3. Heat Capacity

The heat capacity C_v of the QD system is evaluated as the temperature derivative of the mean energy of the QD:

$$C_v(T, \omega_c, \omega_0) = \frac{\partial \langle E(T, \omega_c, \omega_0) \rangle}{\partial T} \tag{12}$$

where the statistical average energy is calculated as:

$$\langle E(T, \omega_c, \omega_0) \rangle = \frac{\sum_{\alpha=1}^{N} E_\alpha e^{-E_\alpha / K_B T}}{\sum_{\alpha=1}^{N} e^{-E_\alpha / K_B T}} \tag{13}$$

and the sum is taken over energy levels of the QD.

The dependence of the computed heat capacity C_v on the magnetic field ω_c, confining frequency ω_0 and temperature are displayed in the next section.

3. Results and conclusions

Our computed results for two interacting electrons in a quantum dot made from GaAs material ($R^* = 5.825$ meV) are presented in Fig. 1 to 4 and Table 1. We tested the calculated energy against different works. In Table 1, we listed the calculated energy results by the exact diagonalization method for different number of single particle basis s_p against Ciftja's work [9]. The comparison clearly shows excellent agreement between both works. In Fig. 1 we plotted the computed energy results of this work against the strength of the magnetic field for $\omega_0 = \frac{2}{3}R^*$. The present results also show very good agreement compared with Dyblaski [18], where the authors had used the variational method.

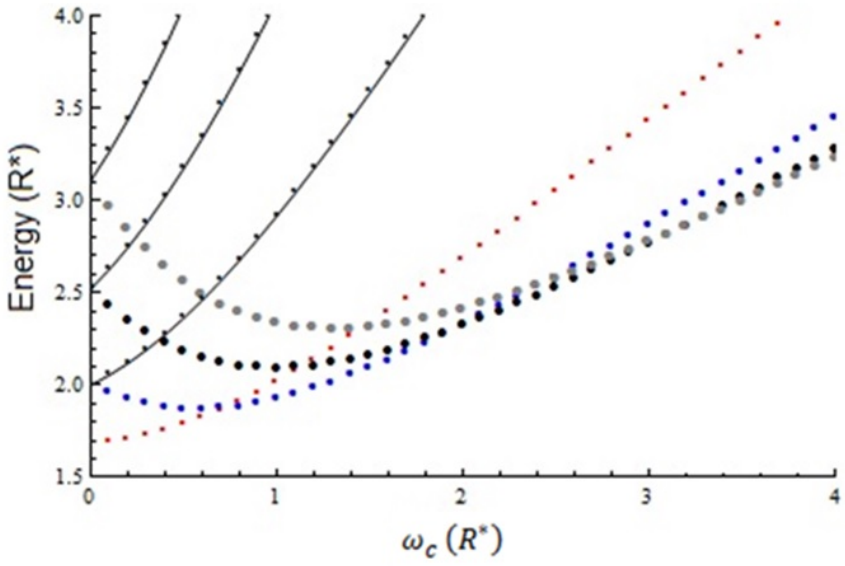

FIG. 1. The computed eigenenergy spectra of two electron quantum dot against the strength of the magnetic field for $\omega_0 = \frac{2}{3}R^*$, and angular momentum $m_r = 0, \pm 1, \pm 2, \pm 3$

Fig. 1 shows clearly the transition in the angular momentum of the ground state of the QD system as the magnetic field increases. The origin of these transitions is due to the effect of coulomb interaction energy in the QD Hamiltonian. These transitions in the angular momentum of the QD system correspond to the (S-T) transitions are expected to manifest themselves as cusps in the heat capacity curve of the QD.

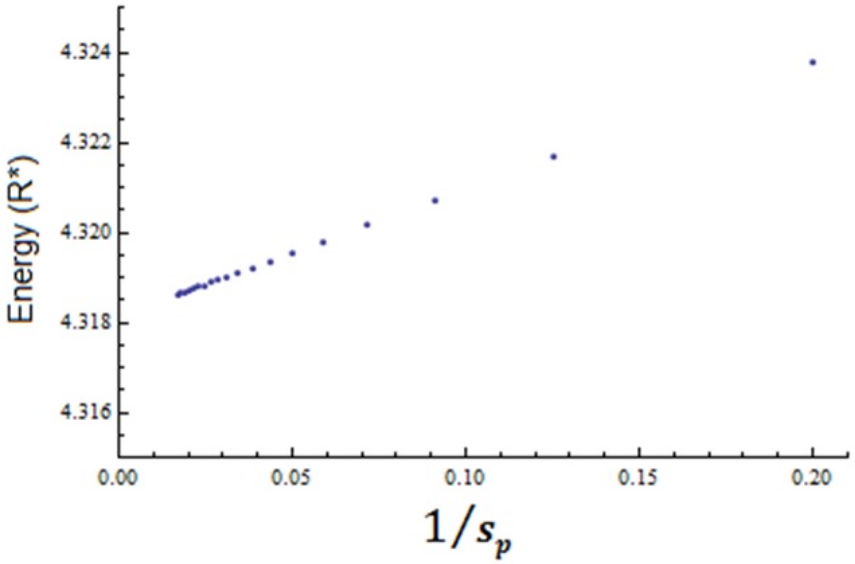

FIG. 2. The computed ground state energy of a two-electron quantum dot in zero magnetic field and $\lambda = 3$, against the inverse of the number of basis taken in diagonalization process

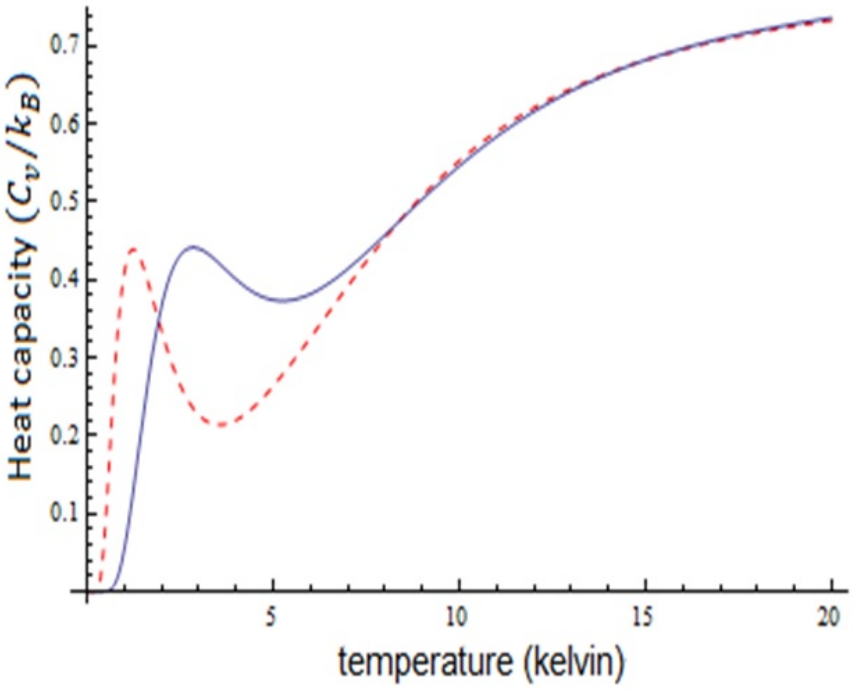

FIG. 3. The dependence of the heat capacity on the temperature for fixed value of magnetic field and various confinement frequencies: $\omega_0 = 0.5R^*$ and $\omega_0 = 0.67R^*$

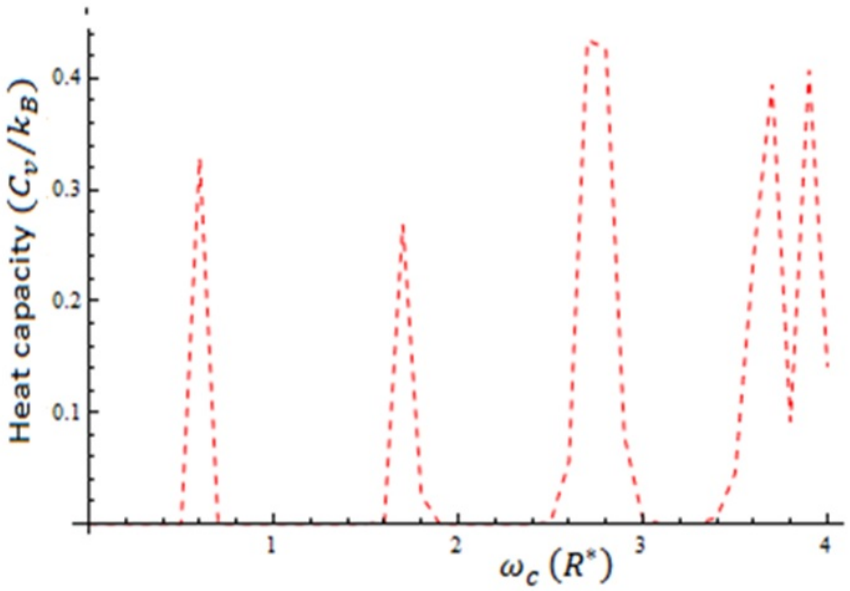

FIG. 4. The heat capacity as function of magnetic field strength for fixed value of temperature (0.01 K) and confinement frequency ($\omega_0 = \frac{2}{3}R^*$)

TABLE 1. Ground state energies in units of $\hbar\omega_0$ of exact diagonalization method at zero magnetic field for different values of dimensionless parameter $\lambda = \frac{e^2\alpha}{\hbar\omega_0}$. The computed results are shown for various number of basis (s_p) against the result which are taken from [9]

λ	Energy $\hbar\omega_0$			
	Ref. [9]	Present work		
		$s_p = 5$	$s_p = 50$	$s_p = 60$
0	2.00000	2.00000	2.00000	2.00000
1	3.00097	3.00122	3.00097	3.00080
2	3.72143	3.72166	3.72143	3.72128
3	4.31872	4.31885	4.31872	4.31863
4	4.84780	4.84787	4.84780	4.84775
5	5.33224	5.33227	5.33224	5.33222
6	5.78429	5.78431	5.78429	5.78428
7	6.21129	6.21129	6.21129	6.21128
8	6.61804	6.61805	6.61804	6.61804
9	7.00795	7.00795	7.00795	7.00795
10	7.38351	7.38351	7.38351	7.38351

In all steps of calculations, we had ensured the issue of convergence. For example, the ground state energy is plotted in Fig. 2 against the inverse of number of basis $\left(\frac{1}{s_p}\right)$, which clearly shows the numerical stability of the ground state energy as the number of basis increased. The diagonalization scheme was found to be very efficient in reproducing the exact energies of the QD system. For example, at $\lambda = 10$, we had found that only five bases are sufficient to reproduce the exact energy value, $\frac{E}{\hbar\omega_0} = 7.38351$ as shown in the table.

In Fig. 3 we showed the behavior of the heat capacity C_v against the temperature for different values of the confining frequency ω_0, while keeping ω_c unchanged. For particular confining frequency, the heat capacity curve shows a peak value at low temperature, while keeping ω_c unchanged. For particular confining frequency, the heat

capacity curve shows a peak value at low temperature, while at high temperature, the heat capacity saturate. These peaks are attributed to the Schottky anomaly. This behavior for the heat capacity is in agreement with the findings of [19, 20]. As the confining frequency increases, the peak of the heat capacity shifts to a higher temperature.

In Fig. 4 we had shown the dependence of the heat capacity on the magnetic field strength for fixed values of the confining frequency and temperature. The heat capacity shows a peak structure which is a result of the transition in the angular momentum of the ground state energy as shown and discussed previously in Fig. 1. For example, the first peak corresponds to the transition in the angular momentum of the ground state from $m_r = 0$ to $m_r = 1$.

In conclusion, we have applied the exact diagonalization method as a theoretical approach to solve the Hamiltonian for interacting electrons confined parabolically in a quantum dot subjected to a magnetic field. We had used the Fock Darwin states as bases to evaluate the coulomb matrix element and to give the result in a closed form. In addition, we had shown the angular momentum transitions in the ground state of GaAs quantum dot spectra. These level crossings cause oscillations in the heat capacity curve of the quantum dot. The results of both, the eigenenergies and the heat capacity, calculated by exact diagonalization method show very good agreement comparable with other recent works.

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