Chinese Journal of Physics 54 (2016) 391–397

Contents lists available at ScienceDirect

Chinese Journal of Physics

journal homepage: http://www.journals.elsevier.com/chinese-journal-of-physics/

Variational calculations of the heat capacity of a semiconductor quantum dot in magnetic fields

Ayham Shaer, Mohammad K. Elsaid*, Musa Elhasan

Physics Department, Faculty of Science, An- Najah National University, Nablus, West Bank, Palestine

ARTICLE INFO

Article history:
Received 27 February 2016
Received in revised form 21 April 2016
Accepted 28 April 2016
Available online 29 April 2016

Keywords:
Heat capacity
Variational method
Quantum dot
Magnetic field

ABSTRACT

The heat capacity of two interacting electrons confined in a quantum dot presented in a magnetic field had been calculated by solving the relative Hamiltonian using variational method. We had investigated the dependence of the heat capacity on temperature, magnetic field and confining frequency. The singlet triplet 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 reported works.

1. Introduction

Quantum dots (QDs), or artificial atoms, had been the subject of interest research due to their physical properties and great potential device applications such as quantum dot lasers, solar cells, single electron transistors 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.

Different approaches had been used to solve the two electrons QD Hamiltonian, including the effect of an applied magnetic field, to obtain the eigenenergies and eigenstates of the QD-system. Maksym and Chakraborty [6] had used the diagonalization method to obtain the eigenenergies of interacting electrons in a magnetic field and show the transitions in the angular momentum of the ground states. They had also calculated the heat capacity curve for both interacting and non-interacting confined electrons in the QD presented in a magnetic field. The interacting model shows very different behavior from non-interacting electrons, and the oscillations in these thermodynamic quantities like magnetization ($\mathcal{M}$) and heat capacity (C_v) are attributed to the spin singlet-triplet transitions in the ground state spectra of the quantum dot. Wagner et al. [7]. had also studied this interesting QD system and predicted the oscillations between spin-singlet (S) and spin-triplet (T) ground states.

Taut [8] had managed to obtain the exact analytical results for the energy spectrum of two interacting electrons through a coulomb potential, confined in a QD, just for particular values of the magnetic field strength. Ciftja and Golam Faruk [9,10] had solved the QD-Hamiltonian by variational method and obtained the ground state energies for various values of magnetic field (ω_c), and confined frequency (ω_0). In addition, they had performed exact numerical diagonalization for the Helium QD-Hamiltonian and obtained the energy spectra for zero and finite magnetic field strength. Kandemir [11] had found the closed

* Corresponding author.
E-mail address: mkelsaid@najah.edu (M.K. Elsaid).

http://dx.doi.org/10.1016/j.cjph.2016.04.024

form solution for this QD Hamiltonian and the corresponding eigenstates for particular values of the magnetic field strength and confinement frequencies. Elsaid et al. [12] had used the dimensional expansion technique, in different works, to study and solve the QD-Hamiltonian and obtain the energies of the two interacting electrons for any arbitrary ratio of coulomb to confinement energies. In addition, he had given an explanation to the level crossing. De Groote et al. [13] had also calculated the magnetization, susceptibility and heat capacity of helium like confined QDs and obtained the additional structure in the heat capacity. In a detailed study, Nguyen and Peeters [14] had considered the QD helium in the presence of a single magnetic ion and applied magnetic field taking into account the electron-electron correlation in many quantum dot. They had shown the dependence of these thermal and magnetic quantities: C_V, $\mathcal{M}$ and χ on the strength of the magnetic field, confinement frequency, magnetic ion position and temperature. They had observed that the cusps in the energy levels show up as peaks in the heat capacity and magnetization.

Very recently, Boyacioglu and Chatterjee [15] had studied the behavior of heat capacity of a single quantum dot confined with a Gaussian potential model. They observed that the heat capacity curve shows peaks structure at low temperature. Helle et al. [16] had computed the magnetization of a rectangular QD in a high magnetic field and the results show the oscillation and smooth behavior in the magnetization curve for both, interacting and non-interacting confined electrons, respectively.

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 [17–19]. Since, the eigenvalues of the electrons in the QD are the starting point to calculate the physical properties of the QD system, we had used the variational method to obtain the eigenenergies. We have adopted a single variational parameter wave function to describe accurately the motion of two confined electrons in a single quantum dot used previously by the authors of Ref. [20]. Next, we had used the computed eigenenergies spectra to display theoretically the dependence of heat capacity 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 theory and computation variational technique of the interacting quantum helium atom are presented in Section 2. In Section 3, we show how to calculate the heat capacity from the mean energy expression. 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, variational calculation 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

$$H = \sum_{j=1}^{2}\left\{\frac{1}{2m^*}\left[\mathbf{p}(\mathbf{r_j}) + \frac{e}{c}\mathbf{A}(\mathbf{r_j})\right]^2 + \frac{1}{2}m^*\omega_0^2 r_j^2\right\} + \frac{e^2}{\varepsilon|\mathbf{r}_1 - \mathbf{r}_2|} \tag{1}$$

where ω_0 is the confining frequency and ε is the dielectric constant for the GaAs medium. $\mathbf{r}_1$ and $\mathbf{r}_2$ describe the positions of the first and second electron in the xy plane. ω_c is the cyclotron frequency and the symmetric gauge $\mathbf{A} = ½\,\mathbf{B} \times \mathbf{r}$ is used.

The quantum dot Hamiltonian can be decoupled into center of mass and relative parts by using the standard coordinate transformation.

The center of mass Hamiltonian is a harmonic oscillator type with well known eigenenergies:

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

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

However, the relative Hamiltonian part (H_r), given by the following equation:

$$H_{rm} = \frac{1}{2\mu}\left[p_r + \frac{e}{c}\mathbf{A}(\mathbf{r})\right]^2 + \frac{1}{2}\mu\omega_0^2 r^2 + \frac{e^2}{\varepsilon|\mathbf{r}|} \tag{3}$$

where $\mu = m^*/2$ does not have an analytical solution for all ranges of ω_0 and ω_c.

2.2. Variational calculation method

Dyblaski and Hawrylak, in a recent work [20], had used successfully the variational method to solve the Hamiltonian and study the electronic structure of the quantum dot. Encouraged by the accuracy of the variational method used by the authors of Ref. [20], we shall apply the variational technique to calculate the complete eigenenergy spectra of the QD Hamiltonian and