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The effects of pressure and temperature on the energy levels of a parabolic two-electron quantum dot in a magnetic field

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Abstract In the present work, we have calculated the energy levels of GaAs parabolic quantum dot under the combined effects of external pressure, temperature and magnetic field. The eigenenergies have been obtained by solving the two electron quantum dot Hamiltonian using the exact diagonalization method. The obtained results show that the energy levels of the quantum dot depend strongly on the pressure and temperature. We have found that the energy levels enhance as the pressure increases for fixed temperature and magnetic field while the quantum dot energy levels decrease as the temperature increases for fixed pressure and magnetic field. The comparisons show that our results are in very good agreement with the reported works.

1. Introduction

Quantum dots (QDs), or artificial atoms, are 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 (Owji et al., 2016; Boda and Chatterjee, 2016; Ciftja, 2013; Kastner, 1992). 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 that are confined in a quantum dot.

Different approaches were used to study the electronic and thermodynamic properties of the quantum dot .Theoretically, many authors had solved the two electron QD Hamiltonian, including the effect of an applied magnetic field, to obtain the eigenenergies and eigenstates of the QD-system (Wagner et al., 1992; Taut, 1994; Ciftja and Kumar, 2004; Ciftja and Golam Faruk, 2005; Kandemir, 2005; Elsaid, 2000; Elsaid et al., 2008; Nguyen and Peeters, 2008; Nammas et al., 2011; Boyacioglu and Chatterjee, 2012; Helle et al., 2005; Schwarz et al., 2002; Nguyen and Das Sarma, 2011) .The results of these studies predicted the oscillations between spin-singlet (S) and spin-triplet (T) ground states. The thermodynamic quantities like: heat capacity (C_v), magnetization (M) and magnetic susceptibility (χ) of the quantum dot had also been calculated (Sanjeev Kumar et al., 2016; Avetisyan et al., 2016; Boyacioglu and Chatterjee, 2012; Nguyen and Peeters,

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2008). The computed results show that the interacting model behaves very differently from non-interacting electrons, and the oscillations in these magnetic and thermodynamic curves of the magnetization and heat capacity were attributed to the spin singlet–triplet transitions in the ground state spectra of the quantum dot. Experimentally, the magnetization of electrons in GaAs/AlGaAs semiconductor QD as function of applied magnetic field at low temperature 0.3 K had been measured (Schwarz et al., 2002). They had observed oscillations in the magnetization. To reproduce the experimental results of the magnetization, they found that the electron–electron interaction should be taken into account in the theoretical model of the QD magnetization. Very recently, the effects of pressure and temperature on the electronic and optical properties of a quantum dot presented in external magnetic and electric fields had been also considered (Owji et al., 2016; Dybalski and Hawrylak, 2005).

In this work, we consider a two electron parabolic quantum dot placed in a magnetic field and study the pressure and temperature effects. We applied the exact diagonalization method to solve the QD Hamiltonian and obtain the energy states for various values of physical parameters: pressure, temperature, parabolic confinement and magnetic field strength.

The rest of this paper is organized as follows: Section 2 presents the Hamiltonian of two interacting electron in a quantum dot, and the diagonalization technique of the interacting quantum artificial atom. We devoted the final section for numerical results and conclusions.

2. Theory

In this section we describe in detail the theory of the two electron QD which consists of two parts, namely: quantum dot Hamiltonian and exact diagonalization method of the GaAs quantum dot.

2.1. Quantum dot Hamiltonian

In the effective mass approximation the Hamiltonian for two interacting electrons confined in a QD by a parabolic potential in a uniform magnetic field $\vec{B} = B\hat{k}$ can be written in a separable form as:

$$\hat{H} = \hat{H}_{CM} + \hat{H}_r \tag{1}$$

$$\hat{H}_{CM} = \frac{1}{2M}\left[\vec{P}_R + \frac{Q}{c}\vec{A}(\vec{R})\right]^2 + \frac{1}{2}M\omega_0^2 R^2 \tag{2}$$

$$\hat{H}_r = \frac{1}{2\mu}\left[\vec{p}_r + \frac{q}{c}\vec{A}(\vec{r})\right]^2 + \frac{1}{2}\mu\omega_0^2 r^2 + \frac{e^2}{\epsilon|\vec{r}|} \tag{3}$$

where ω_0, $M = 2m^*, \mu = \frac{m^*}{2}$ and ϵ are defined as the confining frequency, total mass, reduced mass and the dielectric constant for the GaAs medium, respectively. $\vec{R} = \frac{\vec{r_1}+\vec{r_2}}{2}$ and $\vec{r} = \vec{r_2} - \vec{r_1}$ are the center of mass and relative coordinates, respectively. $\omega_c = \frac{eB}{m^*}$ is the cyclotron frequency and $A = \frac{1}{2}B \times r$ is the vector potential, (Dybalski and Hawrylak, 2005).

The corresponding energy of the QD Hamiltonian in Eq. (1) is:

$$E_{total} = E_{CM} + E_r \tag{4}$$

The center of mass Hamiltonian given by Eq. (2) is a harmonic oscillator type with well-known eigenenergies:

$$E_{n_{cm},m_{cm}} = (2n_{cm} + |m_{cm}| + 1)\hbar\omega + m_{cm}\frac{\hbar\omega_c}{2} \tag{5}$$

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

$\omega^2 = \omega_0^2 + \frac{\omega_c^2}{4}$ is the effective confining frequency.

However, the relative motion Hamiltonian part (H_r), given by Eq. (3) does not have an analytical solution for all ranges of ω_0 and ω_c. In this work, we applied the exact diagonalization method to solve the relative part of the Hamiltonian and obtained the corresponding eigenenergies E_r.

The two electron wave function $\Psi(\vec{r_1},\vec{r_2}) = \psi(\vec{r_1},\vec{r_2})\chi(\sigma_1,\sigma_2)$ is a product of the spatial part $\psi(\vec{r_1},\vec{r_2})$ and the spin part $\chi(\sigma_1,\sigma_2)$. The spatial part can be separated into a CM (2) and relative (3) parts wave functions: $\psi(\vec{r_1},\vec{r_2}) = \psi_{CM}(\vec{R})\psi_r(\vec{r})$.

The relative part $\psi_r(\vec{r})$ has a parity : $(-1)^m$, under the particle permutation ($\varphi \rightarrow \varphi + 2\pi$ **.** Therefore, the spatial part has an even parity for even m- quantum number, and in this case the spin part must be a singlet state with total spin $S = 0$.The total two-electron wave function becomes antisymmetric as the Pauli exclusion principle requires. On the other hand, if the spatial relative part has an odd parity for odd m-values, in this case the spin part must be triplet with total spin $S = 1$. The angular quantum number (m) and the total spin (S) are related by the expression $S = \frac{[1-(-1)^m]}{2}$, (Wagner et al., 1992).

2.2. Exact diagonalization method

For non-interacting case the relative Hamiltonian in Eq. (3) is a single particle problem with eigenstates $|n_r m_r\rangle$ known as Fock-Darwin states, (Fock, 1928; Ciftja and Kumar, 2004; Ciftja and Golam Faruk, 2005).

$$|n_r m_r\rangle = N_{n_r m_r}\frac{e^{im_r\phi}}{\sqrt{2\pi}}(\alpha r)^{|m_r|}e^{-\alpha^2 r^2/2}L_{n_r}^{|m_r|}(\alpha^2 r^2) \tag{6}$$

where the functions $L_{n_r}^{|m_r|}(\alpha^2 r^2)$ are the standard associated Laguerre polynomials. We calculated the normalization constant $N_{n_r m_r}$ from the normalization condition of the basis, $\langle n_r m_r | n_r m_r\rangle = 1$, which resulted in,

$$N_{n_{rm_r}} = \sqrt{\frac{2n_r!\alpha^2}{(n_r + |m_r|)!}} \tag{7}$$

We used α as a constant which has the dimensionality of an inverse length

$$\alpha = \sqrt{\frac{m\omega}{h}} \tag{8}$$

The eigenenergies of the QD Hamiltonian which are given by Eq. (4) consist of the sum of the energies for the center of mass Hamiltonian (E_{cm}) and the eigenenergies (E_r) which are obtained by direct diagonalization to the relative Hamiltonian part. For interacting case, we applied the exact diagonalization method to solve Eq. (3) and find the corresponding exact eigenenergies for arbitrary values of ω_c and ω_0.

The matrix element of the relative Hamiltonian part using the basis $|n_r m_r\rangle$ can be written as,

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