



Magnetization of Coupled Double Quantum Dot in Magnetic Fields

Eshtiaq Hjaz, Mohammad K. Elsaid*, and Musa Elhasan

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

The magnetization of two interacting electrons confined in a coupled double quantum dot presented in a magnetic field has been calculated by solving the relative Hamiltonian using variational and exact diagonalization methods. We have investigated the dependence of the magnetization on temperature, magnetic field strength, confining frequency and barrier height. The singlet-triplet transitions in the ground state of the quantum dot spectra and the corresponding jumps in the magnetization curves have been shown. The comparisons show that our results are in very good agreement with reported works.

Keywords: Magnetization, Variational Method, Exact Diagonalization, Double Quantum Dot.

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. Wagner, et al.⁶ had studied this interesting QD system and predicted the oscillations between spin-singlet (S) and spin-triplet (T) ground states. Taut⁷ 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. In Refs. [8, 9] the authors 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 values of magnetic field strength. Kandemir^{10,11} had found the closed form solution for this QD Hamiltonian and the corresponding eigenstates for particular values of the magnetic field strength and

confinement frequencies. Elsaid^{12–16} 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 and gave an explanation to the level crossings.

Maksym and Chakraborty¹⁷ 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 also had 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 magnetic and thermodynamic quantities like magnetization (M) and heat capacity (C_v) are attributed to the spin singlet-triplet transitions in the ground state spectra of the quantum dot. De Groote et al.¹⁸ also had calculated the magnetization, susceptibility and heat capacity of helium like confined QDs and obtained the additional structure in magnetization. In a detailed study, Nguyen and Peeters¹⁹ 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 dots. They had shown the dependence of these thermal and magnetic quantities: C_v , 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. In Ref. [20], the authors had used the static fluctuation approximation (SFA) to study the thermodynamic properties of two

*Author to whom correspondence should be addressed.

dimensional GaAs/AlGaAs parabolic QD in a magnetic field. Boyacioglu and Chatterjee²¹ had studied the magnetic properties of a single quantum dot confined with a Gaussian potential model. They observed that the magnetization curve shows peaks structure at low temperature. Helle et al.²² had computed the magnetization of a two-electron lateral quantum dot molecule (QDM) in a high magnetic field at zero temperature and the results show the oscillation and smooth behavior in the magnetization curve for both, interacting and non-interacting confined electrons, respectively.

In an experimental work,²³ the magnetization of electrons in GaAs/AlGaAs semiconductor QD as function of applied magnetic field at low temperature 0.3 K had been measured. 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. Furthermore, the density functional method (DFT) had been used to investigate the magnetization of a rectangular QD in the applied external magnetic field.²⁴ Climente, Planelles and Movilla had studied the effect of coulomb interaction on the magnetization of quantum dot with one and two interacting electrons.²⁵

Very recently, Avetisyan et al.²⁶ had studied the magnetization of anisotropic QD in the presence of the Rashba spin-orbit interaction for three interacting electrons in the dot. In Ref. [27], the authors have studied the electron-electron correlations in many electron single quantum dot confined by parabolic potential in the presence of single magnetic ion and perpendicular magnetic field. They have obtained the energies and have studied the thermodynamic quantities such as the heat capacity, the magnetization and the susceptibility. They have found that the cusps in the curves of these heat quantities are due to the transitions in the angular momentum of the energy levels of the QD. Dybalski and Hawrylak²⁸ had also studied the electronic properties of two electrons in a strongly coupled double quantum dot. They have analyzed the singlet-triplet gap with the barrier height potential and with an external magnetic field. The authors had solved the full Hamiltonian of DQD, by using the variational method to calculate separately the energy matrix elements of SQD term and barrier potential term. Next, the exact diagonalization method is implemented to compute the corresponding energies of the full DQD Hamiltonian. The author of Ref. [29] had used the Huns-Mulliken molecular orbit approach to calculate the energy levels of two electrons confined in two laterally coupled quantum dots, under the influence of applied magnetic field. They had showed that the jumps of the magnetization are due to the singlet-triplet transitions in the energy levels.

The purpose of this work is to calculate the magnetization as a thermodynamic quantity for a coupled double quantum dots presented in a magnetic field taking into account the electron-electron coulomb interaction term.

Since, the eigenvalues of the electrons in the DQD are necessary input quantities to calculate the statistical average energies of the DQD system, to achieve this target we have implemented the variation and exact diagonalization methods to obtain the desired eigenenergies. The computed eigenenergies spectra have been used to study theoretically the dependence of the magnetization curve of the coupled DQD as a function of magnetic field strength, confining frequency barrier height and temperature.

The rest of this paper is organized as follows: the Hamiltonian theory and computation techniques of two interacting and confined electrons in DQD are presented in Section 2. In Section 3, we show how to calculate the magnetization from the mean energy expression. Final section will be devoted for numerical results and conclusion.

2. THEORY OF COUPLED DOUBLE QUANTUM DOT HAMILTONIAN

Consider two interacting electrons inside a double quantum dots confined by a parabolic potential of strength ω_o under the effect of an applied uniform magnetic field of strength ω_c , taken to be along z -direction, in addition to a coupled Gaussian barrier of width Δ and height V_o . This model can be characterized by the Hamiltonian (H_{DQD}),

$$H_{DQD} = \sum_{j=1}^2 \left\{ \frac{1}{2m^*} \left[\mathbf{p}(\mathbf{r}_j) + \frac{e}{c} \mathbf{A}(\mathbf{r}_j) \right]^2 \right\} + \frac{1}{2} m^* \omega_o^2 r_j^2 + \frac{e^2}{\epsilon_o |r_1 - r_2|} + V_o (e^{-x_1^2/\Delta^2} + e^{-x_2^2/\Delta^2}) \quad (1)$$

where \mathbf{r}_j and $\mathbf{p}(\mathbf{r}_j)$ are the position and momentum of the electron inside the QD. In addition, x_1 and x_2 represent the position of each quantum dot along the x -direction.

H_{DQD} can be considered as the sum of the single quantum dot Hamiltonian (H_{SQD}) and the potential barrier term $V_b = V_o (e^{-x_1^2/\Delta^2} + e^{-x_2^2/\Delta^2})$ as follows,

$$H_{DQD} = H_{SQD} + V_b \quad (2)$$

It is obvious that the single quantum dot Hamiltonian, H_{SQD} can be obtained from Eq. (2) by making the barrier potential term vanishes, $V_b = 0$. Using the standard coordinate transformation and adopting the symmetric gauge, the single quantum dot Hamiltonian, can be separated into a center of mass Hamiltonian, H_{CM} , and a relative Hamiltonian part, H_r as shown below,

$$H_{CM} = \frac{1}{2M} \left[P_R + \frac{Q}{c} A(R) \right]^2 + \frac{1}{2} M \omega_o^2 R^2 \quad (3)$$

$$H_r = \frac{1}{2\mu} \left[p_r + \frac{q}{c} A(r) \right]^2 + \frac{1}{2} \mu \omega_o^2 r^2 + \frac{e^2}{\epsilon|r|} \quad (4)$$

where M is the total mass = $2m$, Q is the total charge = $2e$, μ is reduced mass = $m/2$, and q is the reduced charge = $e/2$.

The corresponding energy of the H_{SQD} Eq. (4) is:

$$E_{\text{SQD}} = E_{\text{CM}} + E_r \quad (5)$$

The center of mass Hamiltonian has the harmonic oscillator form with well known fully analytical solution for wave function and energy given, respectively, as,

$$\psi_{n_2, m_2}(R) = (-1)^{n_2} \frac{\beta^{|m_2+1|}}{\sqrt{\pi}} \left[\frac{n_2!}{(n_2+|m_2|)!} \right]^{1/2} \times e^{-\beta^2 R^2/2} R^{|m_2|} L_{n_2}^{|m_2|}(\beta^2 R^2) e^{im_2\phi} \quad (6)$$

$$E_{n_{\text{cm}}, m_{\text{cm}}} = (2n_{\text{cm}} + |m_{\text{cm}}| + 1) \hbar \sqrt{\frac{\omega_c^2}{4} + \omega_o^2} + m_{\text{cm}} \frac{\hbar \omega_c}{2} \quad (7)$$

Where n_{cm} , m_{cm} are the radial and azimuthal quantum numbers, respectively and L_n^m is the associate Laguerre polynomials.⁸

The relative Hamiltonian part Eq. (4) does not have an analytical solution for all ranges of ω_0 and ω_c , due to the existence of both coulomb and parabolic terms, so the variational method has been used as an accurate method to get the energy spectra (E_r) for the relative Hamiltonian in terms of a variational parameter. The adopted variational wave function and the corresponding energy equation are given in the Appendix A.

The calculation the energy matrix elements of the V_b -barrier term using the variational method had been given in Ref. [28] and will not be repeated here. The combined terms of the single quantum dot Hamiltonian energy and barrier energy matrix elements will be diagonalized to give the full matrix elements of the DQD Hamiltonian.²⁸ We would like to emphasize again that our aim in this work is to investigate the effect of barrier height and confining frequency on the magnetization properties of the DQD, so only the essential steps which lead to the main eigenenergy equation of the full DQD Hamiltonian will be shown in the Appendix B.

3. MAGNETIZATION OF DQD

We have computed energies of the DQD system as essential input data to calculate the magnetization (M) of the DQD.

The magnetization of the DQD system is evaluated as the magnetic field derivative of the mean energy of the DQD.

$$M(T, B, \omega_o, V_o, \Delta) = \frac{-\partial \langle E(T, B, \omega_o) \rangle}{\partial B} \quad (8)$$

where the statistical average energy is calculated as:

$$\langle E(T, B, \omega_o, V_o, \Delta) \rangle = \frac{\sum_{\alpha=1}^N E_{\alpha} e^{-E_{\alpha}/k_B T}}{\sum_{\alpha=1}^N e^{-E_{\alpha}/k_B T}} \quad (9)$$

We use Eqs. ((8) and (9)) to investigate the dependence of the magnetization of the double quantum dots on very

rich and tunable physical parameters, namely: the temperature (T), magnetic field strength (ω_c), confining potential ω_0 , barrier height (V_o) and barrier width (Δ).

4. RESULTS AND DISCUSSION

The computed results for two interacting electrons in double quantum dots made from GaAs material ($m^* = 0.067m_e$, $R^* = 5.825$ meV) are presented in Figures 1–7. Figure 1(a) shows the calculated eigenenergy spectra of DQD for angular momentum $m = 0, 1$ and 2 as a function of magnetic field strength $\omega_c = 0.0$ to 4.0, confining frequencies $\omega_0 = 2/3R^*$ and barrier heights $V_o = 1R^*$.

In Figure 1(b) we had plotted also the computed energy results of this work against the strength of the magnetic field for $\omega_0 = 2/3R^*$, $\Delta = 0.5R^*$, $V_o = 1R^*$ for small range of $\omega_c = \{0, 1R^*\}$ to show the level crossing more clearly. The energy level plot shows obviously the transition in the angular momentum of the ground state of the DQD system as the magnetic field strength increases. The origin of these transitions is due to the effect of coulomb interaction energy in the QD systems.²² The singlet-triplet transitions in the angular momentum of the DQD system manifest themselves as cusps in the magnetization curve of the DQD. Our energy spectra results show very good agreement compared with the corresponding one displayed

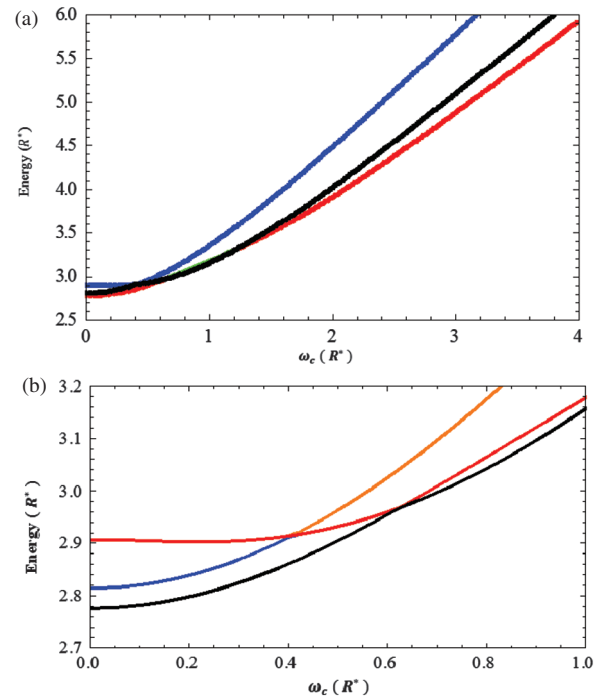


Fig. 1. (a) The computed energy spectra of two interacting electrons in double quantum dots against the strength of the magnetic field for $\omega_0 = 2/3R^*$, $\Delta = 0.5R^*$, $V_o = 1R^*$ for the range of $\omega_c = \{0, 4R^*\}$, and angular momentum $m = 0, 1, 2$. (b) The computed energy spectra of two interacting electrons in double quantum dots against the strength of the magnetic field for $\omega_0 = 2/3R^*$, $\Delta = 0.5R^*$, $V_o = 1R^*$, for the range of $\omega_c = \{0, 1R^*\}$, and angular momentum $m_r = 0, 1, 2$.

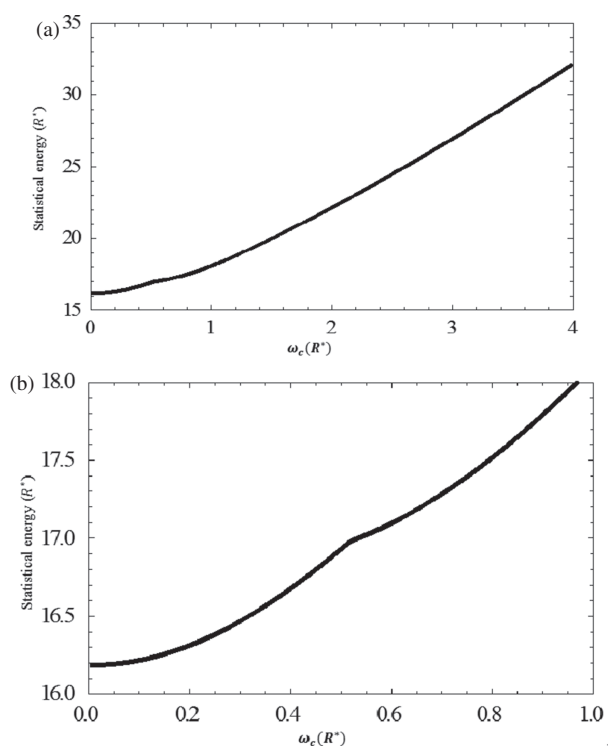


Fig. 2. (a) The statistical energy of two interacting electrons in double quantum dots against the strength of the magnetic field for $\omega_o = 2/3R^*$, $\Delta = 0.5R^*$, $V_o = 1R^*$, (b) The statistical energy of two interacting electrons in double quantum dots against the strength of the magnetic field for $\omega_o = 2/3R^*$, $\Delta = 0.5R^*$, $V_o = 1R^*$. The curve shows a cusp at $\omega_c = 0.5R^*$.

in Figure 3 of Ref. [28] where the authors had used the combined variational and exact diagonalization methods to solve the DQD Hamiltonian.²⁸ In addition we have plotted the statistical energy against the strength of magnetic field for wide range and small range of ω_c in Figures 2(a, b), respectively. These figures show clearly the origin of the cusps in the statistical energy curves that cause the corresponding cusps in the magnetization curve of the DQD.

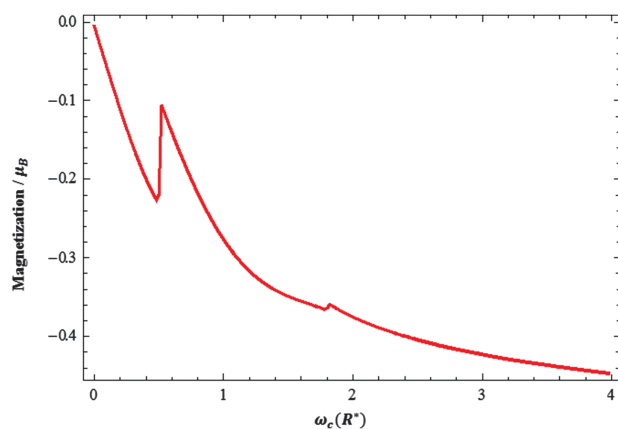


Fig. 3. The magnetization (in unit of $\mu_B = e\hbar/2m^* = 0.87$ meV/T for GaAs) at $T = 0.01$ K, of the two interacting electrons in DQD against the magnetic field strength for $\omega_o = 2/3R^*$, $\Delta = 0.5R^*$, $V_o = 1R^*$.

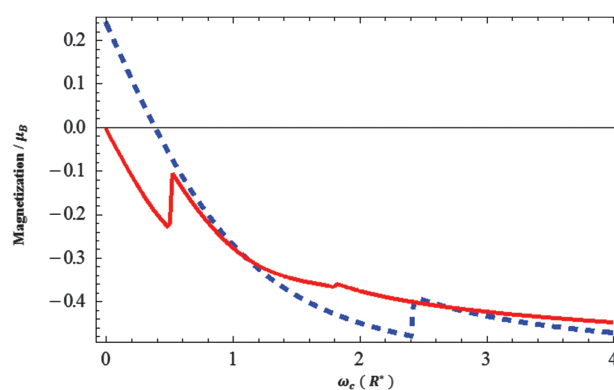


Fig. 4. Comparison between the magnetization (in unit of μ_B) of the two interacting electrons in SQD (dashed) for $\omega_o = 2/3R^*$ and the magnetization of the two interacting electrons in DQD (solid) for $\omega_o = 2/3R^*$, $\Delta = 0.5R^*$, $V_o = 1R^*$ against the magnetic field strength calculated at $T = 0.01$ K.

In Figure 3, we have computed magnetization curve for DQD against the magnetic field strength $\omega_c = 0.0$ to 4.0. The curve clearly shows the cusps at $\omega_c = 0.5$ and 2, which are attributed to the effect of electron–electron interaction in the DQD Hamiltonian. In Figure 4, we have compared the magnetization curves for both DQD and SQD. The magnetization curves for both SQD and DQD show zero magnetization for zero magnetic field and low temperature value, $T = 0.01$ K. Furthermore, the cusp in the magnetization curve of DQD is shifted to lower magnetic value.

Furthermore, we have investigated the effect of the barrier height V_o on the magnetization curve. We have plotted in Figure 5 the magnetization curves independently calculated at three different barrier heights namely, $V_o = 0.5$, 1.0 and 1.5. The comparison clearly shows the gradual shift of the magnetization jumps to lower magnetic field as the barrier height increases.

In addition we have studied the effect of temperature on the magnetization curves of DQD system as function

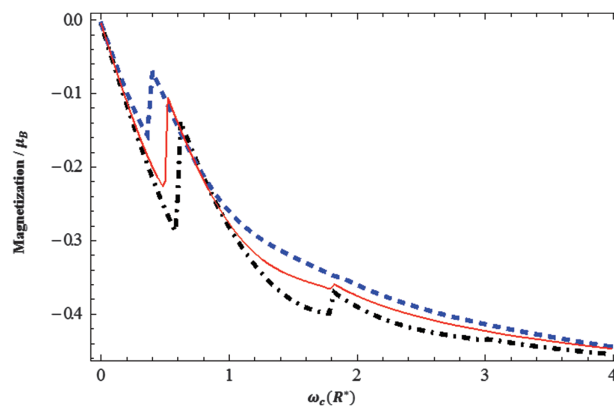


Fig. 5. The magnetization (in unit of $\mu_B = e\hbar/2m^* = 0.87$ meV/T for GaAs) at $T = 0.01$ K, of the two interacting electrons in DQD against the magnetic field strength for $\omega_o = 2/3R^*$, $\Delta = 0.5R^*$. (a) $V_o = 0.5R^*$ (dashed/dotted curve), (b) $V_o = 1R^*$ (solid curve), (c) $V_o = 1.5R^*$ (dashed).

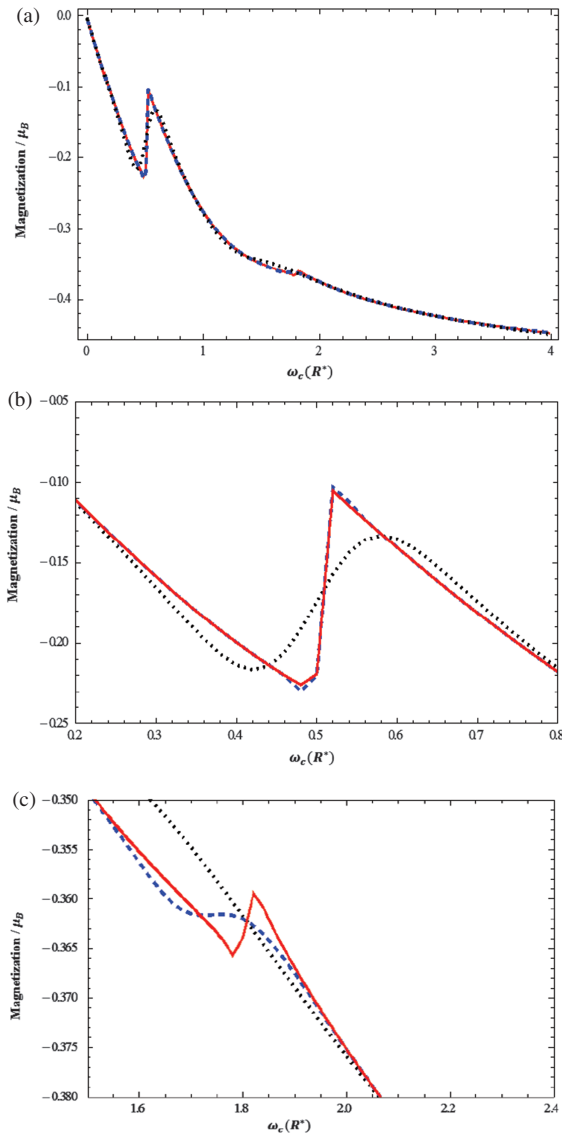


Fig. 6. (a) The magnetization (in unit of $\mu_B = e\hbar/2m^* = 0.87$ meV/T for GaAs) of the two interacting electrons in DQD against the magnetic field of long range strength for $V_0\omega_0 = 2/3R^*$, $\Delta = 0.5R^*$, $V_0 = 1R^*$, (a) at $T = 0.01$ K (solid curve), (b) at $T = 0.1$ K (dashed), (c) at $T = 1$ K (dotted). (b) The magnetization (in unit of $\mu_B = e\hbar/2m^* = 0.87$ meV/T for GaAs) of the two interacting electrons in DQD against the magnetic field of short range strength showing the first cusp, for $\omega_0 = 2/3R^*$, $\Delta = 0.5R^*$, $V_0 = 1R^*$. (a) at $T = 0.01$ K, (b) at $T = 0.1$ K, (c) at $T = 1$ K. (c) The magnetization (in unit of $\mu_B = e\hbar/2m^* = 0.87$ meV/T for GaAs) of the two interacting electrons in DQD against the magnetic field strength showing the second cusp, for $V_0\omega_0 = 2/3R^*$, $\Delta = 0.5R^*$, $V_0 = 1R^*$. (a) at $T = 0.01$ K (solid curve), (b) at $T = 0.1$ K (dashed curve), (c) at $T = 1$ K (dotted curve).

of the magnetic field strength calculated at three different temperatures $T = 0.01$, 0.1 and 1 K as shown in Figures 6(a)–(c). We have seen from the figure that the temperature shows an effect on the cusps of the magnetization curves. To show this effect more clearly we have focused in Figures 6(b, c), on the first and second magnetization cusps, respectively. We have noticed from the

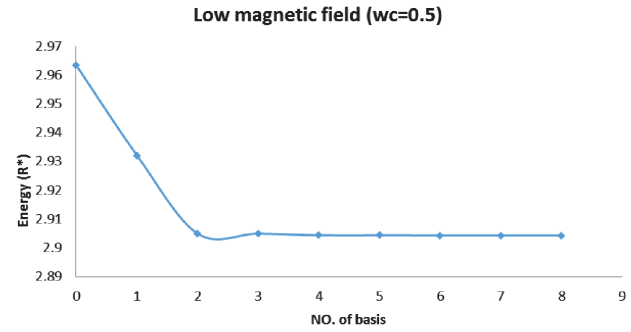


Fig. 7. The energy of DQD for fixed values of $\omega_0 = 2/3R^*$, $\Delta = 0.5R^*$, $V_0 = 1R^*$ against the number of basis and various confining cyclotron frequencies $\omega_c = 0.5R^*$.

figures that the heights of the peaks due to transition jumps are reduced, broadened and shifted to higher magnetic value as the temperature increased.

In all computational steps we have ensured the convergence of the energy spectra have been achieved. For example we have shown, in Figure 7, the computed energy results of DQD for fixed values of $\omega_0 = 2/3R^*$, $\Delta = 0.5R^*$ and $V_0 = 1R^*$ against the number of basis for $\omega_c = 0.5$. The figure clearly shows the stability behavior in the energy of the DQD system as the number of basis increase.

In conclusion, we have applied the exact diagonalization and variational calculation methods to solve the Hamiltonian for two interacting electrons confined in a double-quantum dot presented in a magnetic field. We have investigated the dependence of the magnetization of the DQD on the magnetic field strength, confining frequency, barrier width, barrier height and temperature.

APPENDICES

Appendix A: Energy Variation Calculations of SQD

The purpose of this appendix is to give the main expressions that have been used to compute the eigenenergy expressions of the DQD.

The adopted one parameter variational wave function is taken as:

$$\psi(r) = \sqrt[4]{\alpha} \frac{u_m(\rho) e^{im\phi}}{\sqrt{2\pi}\sqrt{\rho}} \quad (\text{A1})$$

where,

$$u_m(\rho) = \rho^{1/2+|m|} (1 + \beta\rho) e^{-(\rho^2/2)} \quad (\text{A2})$$

$$\rho = \sqrt{\alpha}r, \quad \text{and} \quad \alpha = \frac{1}{4} \sqrt{\frac{\omega_c^2}{4} + \omega_0^2} \quad (\text{A3})$$

Our wave function,

$$u_m(\rho) = C_m \rho^{1/2+|m|} (1 + \beta\rho) e^{-(\rho^2/2)} \quad (\text{A4})$$

with normalization constant can, C_m , be expressed in terms of standard gamma function, $\Gamma(x)$ angular momentum, m , and parameters: α , and β_{\min} .²⁸

We proceed to obtain the energies of the relative part of the single quantum dot Hamiltonian by calculating the

energy matrix elements $E_r = \langle \psi | H_r | \psi \rangle$ as,

$$E_r(\beta) = -\frac{1}{2}m\omega_c + 2\alpha \frac{a+b\beta+c\beta^2}{d+e\beta+f\beta^2} \quad (\text{A5})$$

where a , b and c are constants in terms of quantum numbers m and α .

The energy eigenvalues of H_r can be found by minimizing the energy formula Eq. (A5) with respect to the variational parameter β to give

$$\beta_{\min, m} = \frac{2cd - 2af - \sqrt{(2cd - 2af)^2 - 4(bd - ae)(ce - bf)}}{2(-ce + bf)} \quad (\text{A6})$$

So, the energy expression of the SQD Hamiltonian in terms of the variational parameter, β_{\min} , which satisfies the minimization condition is:

$$E_r(\beta_{\min}) = -\frac{1}{2}m\omega_c + 2\alpha \frac{a+b\beta_{\min}+c\beta_{\min}^2}{d+e\beta_{\min}+f\beta_{\min}^2} \quad (\text{A7})$$

Appendix B: Energy Calculations of DQD by Variational and Exact Diagonalization Methods

To compute the full energy spectra of the DQD system we have set $V_o > 0$ in the Hamiltonian model Eq. (1), so the potential of the barrier is

$$V_b = V_o(e^{-x_1^2/\Delta^2} + e^{-x_2^2/\Delta^2}) \quad (\text{B1})$$

The matrix element of the DQD can be evaluated in terms of elliptic functions, angular quantum number, m , and barrier width, Δ .

The combined terms of the single quantum dot energy ($E_m(\beta_m)$) and barrier energy matrix elements will give the full matrix elements of the DQD Hamiltonian. We had implemented the diagonalization technique to obtain the eigenenergies of the H_{DQD} ,

$$H_{m, n} = [E_m(\beta_m) + E_{\text{CM}}]\delta_{m, n} + \langle u_m | V_b | u_n \rangle \quad (\text{B2})$$

where, E_{CM} , is the center of mass Hamiltonian as define previously in Eq. (8).

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Received: 3 August 2016. Accepted: 30 August 2016.