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ORIGINAL ARTICLE

Energy states and exchange energy of coupled double quantum dot in a magnetic field

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Abstract

The ground state energies of two interacting electrons confined in a coupled double quantum dot (DQD) presented in a magnetic field has been calculated by solving the relative Hamiltonian using variational and exact diagonalization methods. The singlet-triplet transitions in the angular momentum and spin of the quantum dot ground state had been shown.We have studied the magnetic field versus confining frequency and magnetic field versus potential barrier height phase diagram of DQD .Furthermore, we have investigated the dependence of the exchange energy of two electron double quantum dot on the confining frequency, potential height barrier, barrier width and magnetic field strength. The comparisons show that our results are in very good agreement with reported works.

Keywords: *Double quantum dot; Exact diagonalization; Exchange energy; Magnetic field; Variational method.*

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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 [1-4]. Different analytical and numerical methods had been used to solve the two interacting electrons QD- Hamiltonian, including the presence of an applied magnetic field, and had obtained the eigenenergies and eigenstates of the QD-system as a function of magnetic field strength [5-17].The energy spectra shows spin-singlet (S) and spin-triplet (T) ground state oscillations. These spin oscillations show themselves as transition peaks in the spectra of magnetic and thermodynamic quantities like magnetization (M), magnetic susceptibility (X) and heat capacity (C_v) [18-26].

The purpose of this work is to calculate the complete energy spectra of a coupled double quantum dots as a function of parabolic confining frequency, barrier height, barrier width and magnetic field strength, taking into account the electron-electron coulomb interaction term. The obtained eigenenergies have been used to calculate the exchange energy, ($J=E_{singlet} - E_{triplet}$) and to show the effects of barrier height potential and the parabolic confining frequency on the DQD exchange energy .We obtained the magnetic field cyclotron frequency versus parabolic confining frequency and the magnetic field cyclotron frequency versus barrier height phase diagrams for DQD. To achieve our targets, we had implemented the combined variation and exact diagonalization method to obtain the desired eigenenergies.

The rest of this paper is organized as follows: The computation methods of two interacting electrons in DQD are presented in section II. Results and conclusions are given in section III. Final section will be devoted for conclusion.

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EXPERIMENTAL

Computational Methods

Consider two interacting electrons inside double quantum dots confined by a parabolic potential of strength ω_c 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}),

$$H_{DQD} = \sum_{j=1}^{2}\left\{\frac{1}{2m^*}\left[p(r_j) + \frac{e}{c}A(r_j)\right]^2 + \frac{1}{2}\, m^*\omega_0^2\, r_j^2\right\} + \frac{e^2}{\epsilon|r_1 - r_2|} + V_o\left(e^{-x_1^2/\Delta^2} + e^{-x_2^2/\Delta^2}\right). \quad (2.1)$$

where r_j and $p(r_j)$ are the position and momentum of the electron inside the QD. In addition, and represent the position of each electron inside the quantum dot along the *x*-direction.

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,

$$H_{DQD} = H_{SQD} + V_b \quad (2.2)$$

It is obvious that the single quantum dot Hamiltonian, can be obtained from Equation 2.2 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 as shown H_r below,

$$\mathrm{H_{CM}} = \frac{1}{2\mathrm{M}}\left[\mathrm{P_R} + \frac{\mathrm{Q}}{\mathrm{c}}\mathrm{A(R)}\right]^2 + \frac{1}{2}\mathrm{M}\omega_0^2\mathrm{R}^2 \quad (2.3)$$

$$\mathrm{H_r} = \frac{1}{2\mu}\left[\mathrm{p_r} + \frac{\mathrm{q}}{\mathrm{c}}\mathrm{A(r)}\right]^2 + \frac{1}{2}\mu\omega_0^2\mathrm{r}^2 + \frac{\mathrm{e}^2}{\epsilon|\mathrm{r}|} \quad (2.4)$$

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

The corresponding energy of the H_{SQD} equation (2.4) is:

$$E_{SQD} = E_{CM} + E_r \quad (2.5)$$

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

$$\psi_{n_2,m_2}(R) = (-1)^{n_2}\frac{\beta^{|m_2+1|}}{\sqrt{\pi}}\left[\frac{n_2!}{(n_2+|m_2|)!}\right]^{\frac{1}{2}} e^{-\beta^2R^2/2}R^{|m_2|}L_{n_2}^{|m_2|}(\beta^2R^2)e^{im_2\phi} \quad (2.6)$$

$$\mathrm{E_{n_{cm},m_{cm}}} = (2\mathrm{n_{cm}} + |\mathrm{m_{cm}}| + 1)\hbar\sqrt{\frac{\omega_c^2}{4} + \omega_o^2} + \mathrm{m_{cm}}\frac{\hbar\omega_c}{2} \quad (2.7)$$

Where n_2=n_{cm}, m_2=m_{cm} are the radial and azimuthal quantum numbers, respectively, and L_n^m is the associateLaguerre polynomials [7].

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 (2.3) and relative (2.4) 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 ($\varphi \to \varphi + 2\pi$). 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 $= \frac{[1-(-1)^m]}{2}$.

The QD ground state labeled by the quantum numbers: $n_{cm} = 0$, $m_{cm} = 0$, $n = 0$, $m \le 0$, in the presence of an elelctron-electron interaction goes a transition to m=-1 , -2 , -3, ….as the strength of the magnetic field increases .The transitions in the angular momentum of the QD ground state lead also to oscillations in the spin of the ground state between the singlet (S=0) and triplet (S=1) states, [5] .

The relative Hamiltonian part equation (2.4) does not have an analytical solution for all ranges of ω_o 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 Appendix A. 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. We have given, in the Appendices, the essential steps which convert full DQD Hamiltonian into a matrix eigenvalue form. The exact diagonalization method is used in spanning the total Hamiltonian for the selected single electron basis and extracts

the lowest eigenvalues (eigenenergies) of the matrix. The procedure of increasing the number of linearly independent eigenstates is converging to the exact results. In each step the new energy results are compared with previous results from a smaller apace, until satisfactory convergence is achieved. The computed eigenenergies will be used to investigate the effect of barrier height and confining frequency on the dependence of the exchange energy on the magnetic field strength of the DQD.

RESULTS AND DISCUSSIONS

The computed results for two interacting electrons in double quantum dots made from GaAs material (m^*=0.067 m_e, R^*=5.825 meV) are presented in Table 1 and Figs. 1 to 8. The eigenenergies are obtained by diagonalizing the DQD-Hamiltonian in the matrix form (B2) with the single electron basis, $u_m(\rho)$, given by Eq. (A4). Fig. 1a and 1b show the calculated eigenenergy spectra of DQD for angular momentum m=0,1 and 2 as a function of magnetic field strength of long range ω_c=0.0 to 4.0 and short range ω_c=0.0 to 1.0, respectively. The spectra is calculated for fixed values of confining frequencies $\omega_0 = \frac{2}{3}R^*$ and barrier heights V_0=1R^*.

The energy level plot in Fig. 1b 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

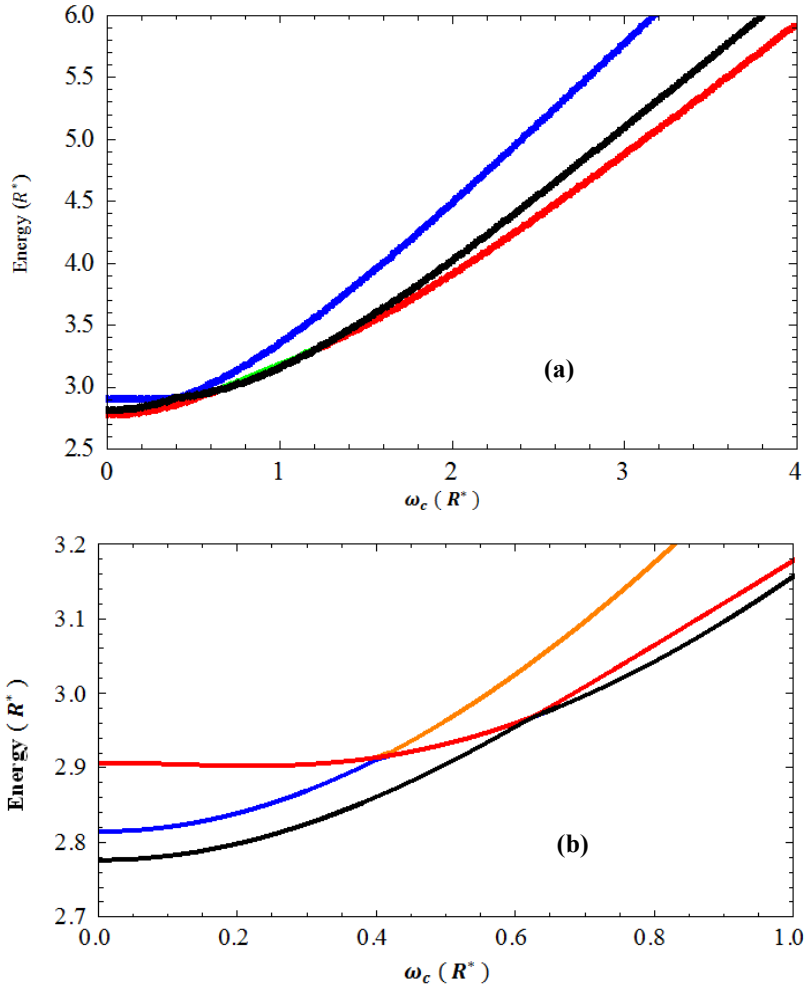

Fig. 1: a) The computed energy spectra of two interacting electrons in double quantum dots against the strength of the magnetic field for $\omega_0 = \frac{2}{3}R^*, \Delta = 0.5\,R^*, V_o = 1R^*$ for the range of $\omega_c = \{0, 4R^*\}$, and angular momentum m = 0,1,2. b) The computed energy spectra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

Table I: The ground state energies of QD (in R^*) as a function of dimensionless coulomb coupling parameter $\lambda = {\alpha e^2}/{\hbar\omega}$ with , $\alpha = \sqrt{{m\omega}/{\hbar}}$, obtained from exact diagonalization method (second column) compared with reported work (third column), Reference [7].

$\boldsymbol{\lambda}$	E (Present work)	E(Ref.[7])
0	2.00000	2.00000
1	3.000969	3.00097
2	3.721433	3.72143
3	4.318718	4.31872
4	4.847800	4.84780
5	5.332238	5.33224
6	5.784291	5.78429
7	6.211285	6.21129
8	6.618042	6.61804
9	7.007949	7.00795
10	7.383507	7.38351

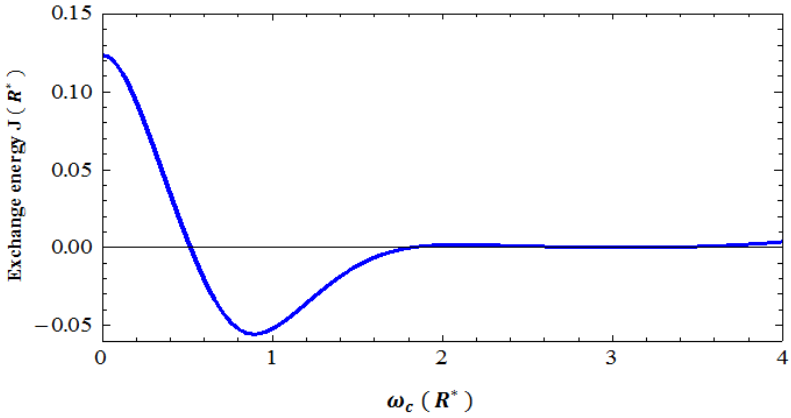

Fig. 2: The computed exchange energy of the two interacting electrons in DQD versus the magnetic field strength for $\omega_o = \frac{z}{3} R^*$, $\Delta = 0.5\ R^*$, $V_o = 1R^*$.

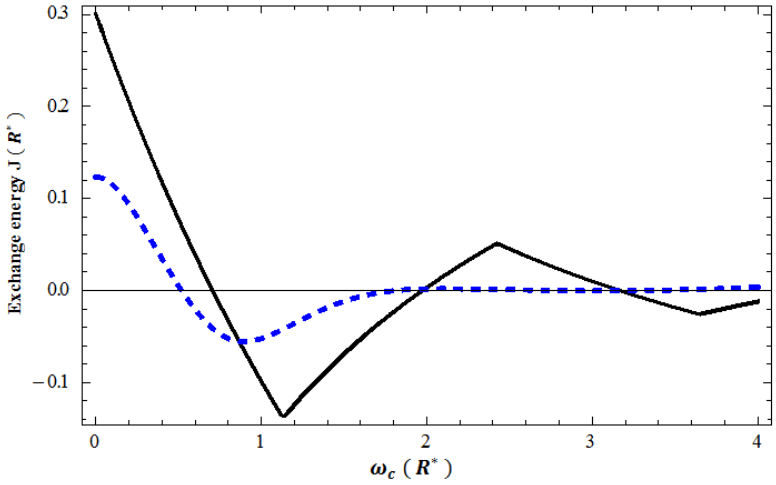

Fig. 3: Comparison between the exchange energy of the two interacting electrons in QD for $\omega_o = \frac{2}{3} R^*$ (V_b =0) in the DQD Hamiltonian (solid curve) , and the exchange energy of the two interacting electrons in DQD for $\omega_o = \frac{2}{3} R^*$, $\Delta = 0.5\ R^*$, $V_o = 1R^*$ against the magnetic field strength (dashed curve).

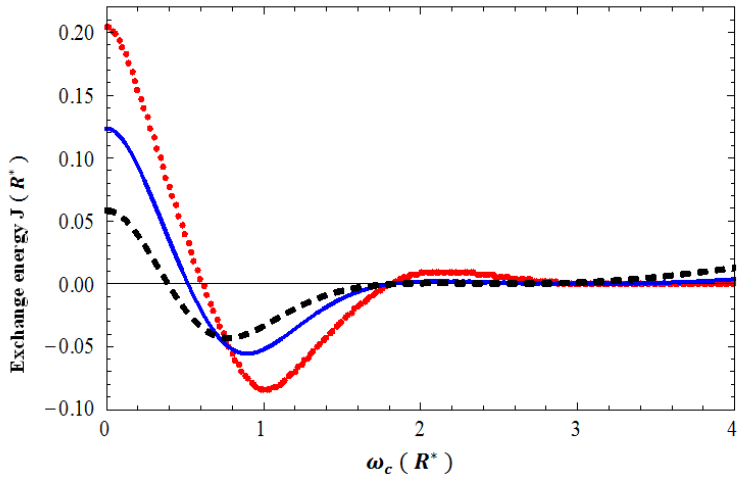

Fig. 4: The exchange energy of two interacting electrons in DQD against the magnetic field strength for $\omega_o = \frac{2}{3} R^*$, $\Delta = 0.5$ R* and different values of V_o : (dotted curve) at V_o = 0.5 R* , (solid curve) at V_o = 1 R* and (dashed curve) at V_o = 1.5 R* .

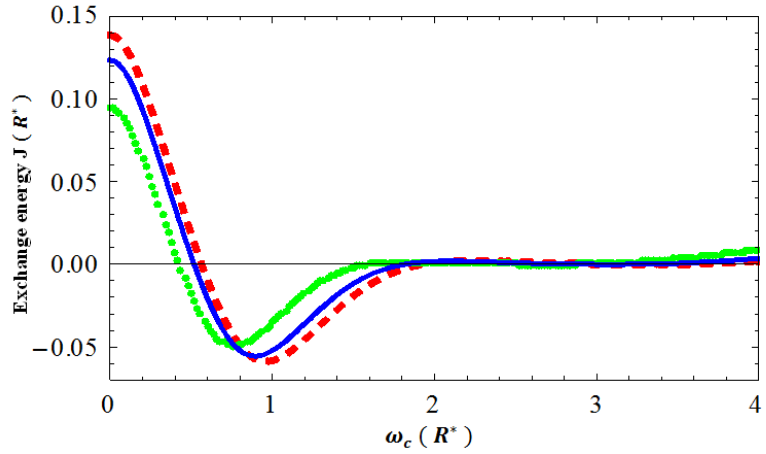

Fig. 5: The exchange energy of two interacting electrons in DQD as a function of the magnetic field strength for $V_o = 1 R^*$, $\Delta = 0.5$ R* and different values of ω_o: (dashed curve) at ω_o= 0.7 R* , (solid curve) at ω_o= $\frac{2}{3}$ R* and (dotted curve) at ω_o= 0.6 R* .

the QD systems [12]. 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 results displayed in Fig. 3 of Ref. [20], where the authors had used the variational method to solve the DQD Hamiltonian.

In Fig. 2, we have computed the results of exchange energy ($J=E_{singlet} - E_{triplet}$) curve for DQD against the magnetic field strength $\omega_c = 0.0\ to\ 4.0$, $\omega_0 = \frac{2}{3}R^*, \Delta = 0.5R^* and\ V_0 = 1R^*$. The curve shows very good agreement with the corresponding one in Ref. [20]. We have compared the exchange energy curves for both single quantum dot (SQD) and DQD in Fig. 3. The exchange energy curve for SQD (---) shows a deep and sharp minimum. Meanwhile the corresponding J-curve in DQD system (---) shows a smooth and shallower minimum. This J-behavior agrees again with the result of Ref. [20].

In Fig. 4, we have studied the effects of barrier height potential, V_0 on the magnetic field dependence of the exchange energy, J(B) , for fixed values of ω_0 and Δ It is observed that as V_b increases the minimum of the J-curve becomes shallower and shifted to higher magnetic field

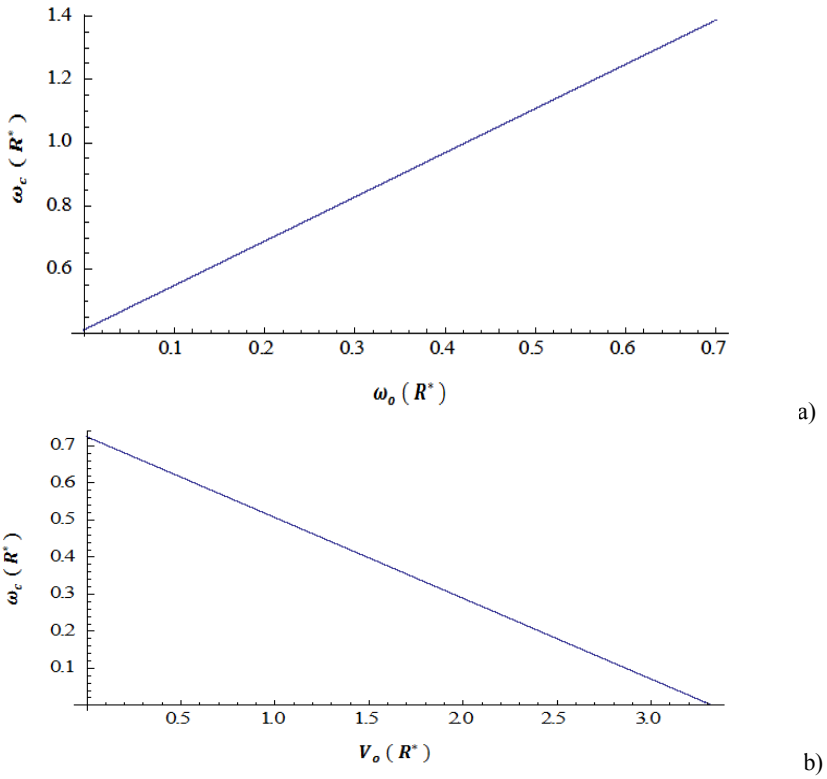

Fig. 6: Phase diagrams for the exchange energy, a) ω_c - ω_0 at $V_o = 1\,R^*$. b) ω_c – V_o at $\omega_0 = \frac{2}{3}R^*$.

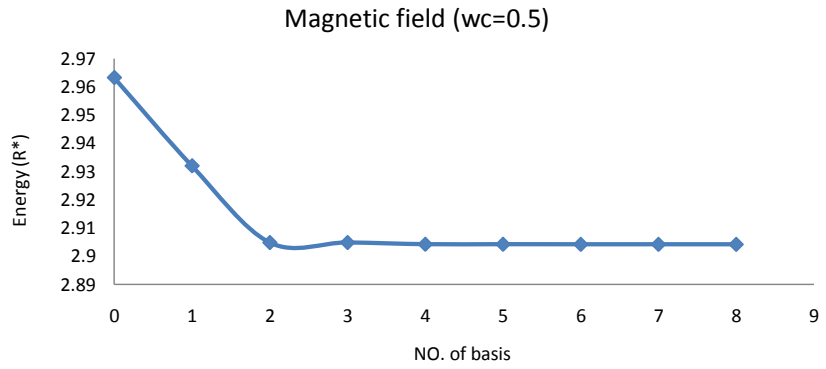

Fig. 7: The energy of DQD for fixed values of $\omega_0 = \frac{2}{3}R^*, \Delta = 0.5\,R^*$, $V_o = 1R^*$against the number of basis and $\omega_c = 0.5R^*$.

strength. A similar qualitative effect for the parabolic confining frequency on the J-curve has shown in Fig. 5.

Furthermore, we have calculated and showed in Fig. 6 (a and b) the magnetic field versus parabolic confining frequency (ω_c-ω_0) and magnetic field versus potential barrier height (ω_c-V_0) phase diagrams of DQD. It is observed from Fig. 6a that the transition magnetic field enhances as the confining frequency increases. This behavior is also reported by Kyriakidis et al. in reference [22]. On the other hand, the transition magnetic field decreases as the potential barrier height increases. In all computational steps, the convergence process of the energy spectra is found to be very fast and is achieved for small number of basis. For example we have shown, in Fig. 7, the computed energy results of DQD for fixed values of $\omega_0 = \frac{2}{3}R^*$, $\Delta = 0.5\,R^* and\ V_0 = 1R^*$ against the number of basis for ω_c=0.5 The figure clearly

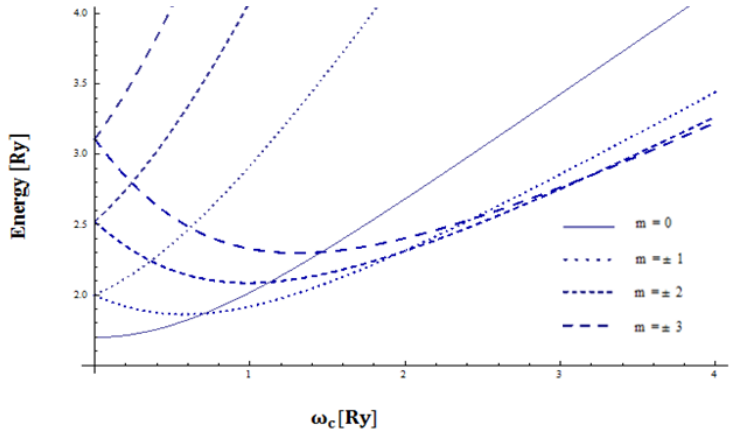

Fig. 8: The computed energy spectra of single quantum dot versus the strength of the magnetic field for $\omega_0 = \frac{2}{3}R^*$, angular momentum $m = 0, -1, -2, -3$.

shows the stability behavior in the energy of the DQD system as the number of basis increases. Fig. 8 displays the present computed results for a single quantum dot for comparison purposes with both: The analytical variational and numerical Numerov results given in Fig. 1 of Dybalski and Hawrylak work [20]. In Table 1, we have listed the computed results for a single QD against the results of Ciftja and Golam Faruk [7]. The comparison shows an excellent agreement between both works.

CONCLUSION

In conclusion, we have applied the combined exact diagonalization and variational calculation methods to solve the Hamiltonian for two interacting electrons confined in double-quantum dots presented in a magnetic field. We have investigated the dependence of the DQD energy levels and exchange energy on the magnetic field strength, confining frequency and barrier width and barrier height. The DQD phase diagrams are also shown.

APPENDICES

Appendix A: Energy expressions of single QD Hamiltonian by variation calculations

The purpose of this Appendix is to give the main expressions that have been used to compute the eigenenergy expressions of the QD. 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,

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

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

Our wave function,

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

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},[20]. The choice of the trial wave function $u_m(\rho)$ is justified as follows. The power term: $\rho^{1/2+|m|}$ and the exponential term: $e^{-\frac{\rho^2}{2}}$, each gives the correct asymptotic behavior of the wave function as $\rho \to 0$ and $\rho \to \infty$, respectively. These terms should be kept unchanged to guarantee the physical behavior of the wave function. The variational parameter, β is a numerical factor and its exact values, for example, are: $\sqrt{2}$ and $\sqrt{2/3}$ for m=0 and m=1 states ,respectively .In this case it seems reasonable to take this numerical factor as a variational parameter, β.

We proceed to reproduce the energies of the relative part of the single quantum dot Hamiltonian by calculating the energy matrix element $E_r = \langle\psi|H_r|\psi\rangle$ 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 equation (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 final 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: The energy calculations of double quantum dot Hamiltonian by combined variational and exact methods.

To compute the full energy spectra of the DQD system we have set V_o>0 in the Hamiltonian model equation (2.1), so the potential of the barrier is

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

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 (β_m)) and barrier energy matrix elements will give the full matrix elements of the DQD Hamiltonian. This converts the problem into a matrix eigenvalue problem. We have implemented the diagonalization technique to obtain the eigenergies of the H_{DQD} ,

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

where, E_{CM}, is the center of mass Hamiltonian as defined previously in Eq. 2.7 .

CONFLICT OF INTEREST

The authors declare that there is no conflict of interests regarding the publication of this manuscript.

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