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Quantum Double Dot as Quantum Computer Unit

A. M. Khalaf , Z. Ali*, Sh. Abdelfattah*, A. M. Selim*
Physics Department, Faculty of Science, Al-Azhar University, Cairo, Egypt
*Physics Department, Faculty of Science (Girls branch), Al-Azhar University, Cairo, Egypt

ABSTRACT

In this work, we have investigated the exchange interaction of two electrons in double lateral quantum dot (which is the base of quantum gate) under effect of external magnetic field, electric field and inter dot distance between double dots. From similarity between double quantum dots and molecule, we have used molecular physics approaches (Hitler – London and Hund – Mullikan approximation method) to investigate our system. We also show the magnetization behavior as function of magnetic field.

Indexing terms/Keywords

Quantum dot - Quantum gate - Exchange interaction

INTRODUCTION

In recent years, quantum computer has a great interest throughout nanotechnology [1]. These computers are a model system based on quantum mechanics, such a device requires two – level system called qubit [1, 2] in order to store information, as well as controllable method to adjust interaction between qubits [2].

Quantum dots [3] seem to be logically can used to form quantum gate. Two types of quantum dot qubits have been obtained the spin and charge of electron as a qubit. Since electron spin has very long coherence time (for GaAs can exceed 100 nm) compared to electron orbital states, thus electron spin may be better choose for qubits. There is another advantage of using spin as a qubit, the intrinsic two – state systems of spin (electron spin up and down) perform one qubit, thus no extra dimensions transition to which could lead to leakage errors in quantum computer [4,5]. A quantum two level system can be in a superposition of its state [6] also qubits may be entangled with each other forming quantum logic gate [4]. Because of supersession and entanglement operation, quantum computers can perform certain problem significantly faster than classical computer [1]. Two quantum dots coupled to form quantum gate, in which electrons may be tunnel between them and produce spin – spin interaction represented by exchange coupling [7]. The coupling between the spins can be switched on and off through externally controlled parameters such as confinement potential and magnetic field [8, 7]. Also detuning (the offset between the energy levels of the two dots) and tunnel coupling which can be changed by applying gate voltage [2].

Our work depends on two spin qubits in double quantum dots (artificial molecule). Due to Pauli Exclusion Principle, the ground state is a singlet state and the first excited state is a triplet state [5, 9]. To evaluate Quantum logic gates as quantum XOR (which use for programming any problem calculated by quantum computation), we first calculate "swap operator" [10] which is unitary time evolution between spins in dots

$$U_{12}(t) = e^{-itH_s(t)/\hbar} \qquad (1)$$

Where Hamiltonian for spin spin interaction is given by $H_s(t) = J_{12}(t)S_1 . S_2$ (where J12 is the exchange interaction given the energy difference between singlet and triplet state), Then we will evaluate a quantum logic gate UXOR as in [11]

$$U_{XOR} = \exp(i(\pi/2)S_1^z)\exp(-i(\pi/2)S_2^z)U_{SW}^{1/2}\exp(i\pi S_1^z)U_{SW}^{1/2}$$

We study the spin dynamics of two electrons inside double quantum dots by evaluating the exchange interaction as a function of magnetic field B , electric field E which control level detuning and distance between two dots 2d. Performing all calculation under Heitler – London and Hund – Mulliken method.

2- Quantum Dots Model

We Consider a system of two double quantum dots of GaAs defined in a two dimensional (x-y plan) separated by a distance 2d from the center of each other, each dot contains electron has spin 1/2 and its effective mass m^* (m^*= 0.067 m_e in GaAs)

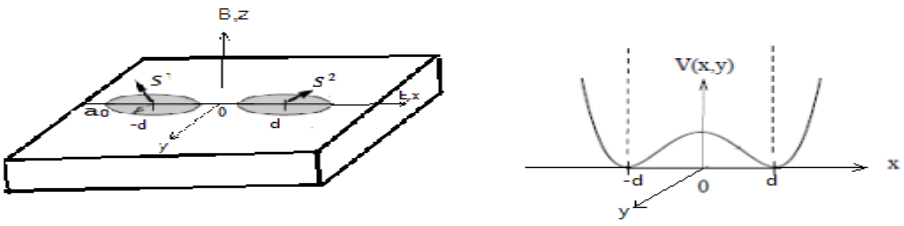

Fig (1): double quantum dot under magnetic field in z- direction where each dot has electron spin 1/2,The two dots separated by 2d distance from each other.

For simplicity, we consider the two quantum dots are identical. If we apply a magnetic field in the z- direction perpendicular to double quantum dot plan and an electric field E in a plane along the x axis, the Hamiltonian describe this system is given by

$$\mathcal{H} = K_1 + K_2 + \mathcal{H}_Z + V_c + \mathcal{H}_{SO} + \mathcal{H}_S = \mathcal{H}_{orb} + \mathcal{H}_Z + \mathcal{H}_S \qquad (2)$$

Where K_i is the single particle energy, $K_i = \frac{1}{2m}(p_i - \vec{A}(r_i))^2 + ex_iE + V(r_i)$

$\vec{A}(r_i)$ is The vector potential which given by $\vec{A}(r_i) = \frac{[\vec{B}\times\vec{r_i}]}{2} \rightarrow A_{\pm}(r_i) = \frac{B}{2}(-y, x, 0)$, $\mathcal{H}_Z$ is Zeeman energy where:

$$\mathcal{H}_Z = g_{eff}\mu_B \sum B S_Z^i$$

Where g_{eff} is the effective g- factor (g = -0.44 for GaAs), and μ_B is the Boher magneton. The ratio between Zeeman energy and orbital energy is small, so we can neglect Zeeman energy. $\mathcal{H}_s$ is a spin spin interaction

Coulomb interaction between two electrons can be represented by:

$$V_c = \frac{e^2}{\varepsilon r_{12}}$$

Where ε is the dielectric constant (in GaAs ε =13.1), r_{12} is the distance between two electrons.

$V(r_i)$ is the confined potential. Since the experimental fact show that the spectrum of single dot (2DEG) has a simple harmonic oscillator [4, 7], thus the best choice of confinement potential for laterally aligned dots is the quartic potential which is given by:

$$V(x,y) = \frac{\omega_o \hbar}{2a_o^2}\left(\left(\frac{x^2}{2a} - \frac{a}{2}\right)^2 + y^2\right) \qquad (3)$$

Which separate double dots as two harmonic well of frequency ω_o and the effective Boher radius of a single isolated harmonic well is $a_0 = \sqrt{\frac{\hbar}{m\omega_o}}$ (is a measure of lateral extension of the electron wave function in the dots).

Since the single dot potentials are harmonic oscillator, so that the ground state single particle orbits wave function $\emptyset(x,y)$ centered at the origin given by

$$\emptyset(x,y) = \sqrt{\frac{m\omega}{\pi\hbar}}\, e^{-m\frac{\omega(x^2+y^2)}{2\hbar}} \qquad (4)$$

Where $\omega = \sqrt{\omega_o^2 + \omega_l^2}$, ω_l is the Larmor frequency given by $\omega_l = \frac{eB}{m^*}$

The single dot ground state centered at $(\pm d, 0)$ given by

$$\emptyset_{\pm d}(x,y) = \exp(\pm iya/2\, l_B^2)\, \emptyset(x \mp d, y) \qquad (5)$$

Where $\exp(\pm iyd/2\, l_B^2)$ is phase factor due to magnetic field, $l_B = \sqrt{\frac{\hbar c}{\omega_l m^*}}$ is magnetic length.

In few electron systems, spin orbit interaction is dominant. The spin–orbit interaction in a quantum dot is given by $H_{so} = \frac{\omega_\delta^2}{2mc^2} S.L$ (**L** is the electron angular momentum which has approximate value ħ). If spin orbit coupling is strong the electron spin is not a good parameter, thus it should be selected material quantum dot with small spin- orbit coupling [1] (for GaAs $H_{so}/\hbar\omega_o \approx 10^{-7}$ it is small value can be ignored [11]).

After all considerations, the two electrons Hamiltonian is a purely orbital take the form

$$\mathcal{H}_{orb} = \frac{1}{2m}\left(p_1 - \frac{e}{c}A(r_1)\right)^2 + \frac{1}{2m}\left(p_2 - \frac{e}{c}A(r_2)\right)^2 + v(x,y) + \frac{e^2}{\varepsilon r_{12}}$$

After some mathematics, the orbital Hamiltonian is given by

$$\mathcal{H}_{orb} = k^0_{-d}(r_1) + k^0_{+d}(r_2) + Q + V_c \qquad (6)$$

Where:

$k^0_{\pm d}(r_i) = \frac{\left(p_i - e\frac{\vec{A}(r_i)}{c}\right)^2}{2m} + \frac{\omega\hbar b}{2a_o^2}((x_i \mp d)^2 + y_i^2)$ is Hamiltonian for particle (electron) in harmonic potential, $Q(x,y) = v(x,y) - \frac{\omega\hbar b}{2a_o^2}((x_1 + d)^2 + (x_2 - d)^2)$ and $V_c = \frac{e^2}{\varepsilon r_{12}}$

For two electron in double quantum dot interacts in a uniform magnetic field corresponding to spin singlet $|s\rangle = \frac{1}{\sqrt{2}}|\uparrow\downarrow - \downarrow\uparrow\rangle$ with total spin S = 0 and triplet $|T_o\rangle = \frac{1}{\sqrt{2}}|\uparrow\downarrow + \downarrow\uparrow\rangle$, $|T_+\rangle = |\uparrow\uparrow\rangle$, $|T_-\rangle = |\downarrow\downarrow\rangle$ with total spin S= 1, (under consideration the temperature is very lower than $\hbar\omega_o$, so we can use ground state (singlet) and first excited state (triplet). The exchange energy between two electrons is the difference between triplet states $|T_o\rangle$, and the ground singlet state $|s\rangle$.

$$J = E_T - E_S$$

We can calculate J by evaluate the expectation value for singlet and triplet state of orbital Hamiltonian operator

$$J = \langle\psi_T|\mathcal{H}_{orb}|\psi_T\rangle - \langle\psi_S|\mathcal{H}_{orb}|\psi_S\rangle \qquad (7)$$

Because of similarity between atoms and quantum dots we use approaches from molecular physics to calculate J so we use Heitler – London and Hund – Mulliken, the validity of this approximations required that at zero magnetic field the ground state must be singlet (at B=0 is J > 0).

2.1 Heitler – London method

Heitler – London method is the simplest approach to calculate exchange splitting in double quantum dots. The basic assumption of this method is that the two electron lowest energy wave function singlet and triplet are written as a combination of single dot single- electron wave function basis. This method is accurate when two dots are at large inter-dot distance from each other, also doubly occupied of dot is neglected

The singlet and triplet state are given by

$$-\psi_{S/T}\rangle = \frac{|\phi_L(1)\phi_R(2)\pm\phi_L(2)\phi_R(1)\rangle}{\sqrt{2(1\pm p^2)}} \times \frac{|\uparrow\downarrow+\downarrow\uparrow\rangle}{\sqrt{2}} \qquad (8)$$

The first term is the orbital contribution with $|\phi_{L/R}(1/2)\rangle$ is the single- dot ground state orbital for electron 1/2 given by equation (5), the second term is the spin dependent part which can neglect here.

The overlap between right and left orbits is denoted by:

$$p = \int \phi^*_{+a}(r)\phi_{-a}(r)\,d^2r = \langle\phi_L|\phi_R\rangle = \exp\left(\frac{-m\omega d^2}{\hbar} - \frac{d^2\hbar}{4l_B m\omega}\right)$$

From equation (6), (7), and (8) the exchange energy due to H-L obtained by

$$J_{HL} = \langle\psi_T|\mathcal{H}_{orb}|\psi_T\rangle - \langle\psi_S|\mathcal{H}_{orb}|\psi_S\rangle$$

This can write as:

$$J_{HL} = \frac{p^2}{1-p^4}(J_Q + J_{V_c})$$

Where J_Q is the single particle confinement potential contribution given by:

$$J_W = \langle\phi_L(1)\phi_R(2)|Q|\phi_L(1)\phi_R(2)\rangle - \frac{1}{p^2}\langle\phi_L(1)\phi_R(2)|Q|\phi_L(2)\phi_R(1)\rangle$$

This contribution provide singlet state, while J_{V_c} is the coulomb interaction contribution between two electron expressed by:

$$J_{V_c} = \langle\phi_L(1)\phi_R(2)|V_c|\phi_L(1)\phi_R(2)\rangle - \frac{1}{p^2}\langle\phi_L(1)\phi_R(2)|V_c|\phi_L(2)\phi_R(1)\rangle$$

$$= J_{V_{c1}} - J_{V_{c2}}$$

It is consist of two parts, the first part is the direct coulomb interaction $J_{V_{c1}}$ and the other is the exchange interaction $J_{V_{c2}}$; both coulomb terms favor triplet state since in triplet state two electrons avoid each other

Solving the matrix element of C and W yield:

$$J_{HL} = \frac{\hbar\omega_o}{\sinh[2\alpha^2(2b-\frac{1}{b})]}\left[\frac{b\alpha^2}{16\pi^2\omega}e^{-10b\alpha^2}(1+e^{b\alpha^2(3-\frac{1}{b^2})})(\omega_0 - \frac{4\omega^2}{\omega_0} + 3\hbar\omega_0) + S\sqrt{b}\,\mathrm{Erf}[2\sqrt{2b}\alpha](e^{-2b\alpha^2} - e^{2\left(b-\frac{1}{b}\right)\alpha^2})\right] \qquad (9)$$

Where **erf** is the error function given by $\mathrm{erf}(z) = \frac{2}{\sqrt{\pi}}\int_0^z e^{-t^2}dt$,

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and $s = \frac{1}{8\sqrt{2}\pi^{3/2}}(\frac{e^2}{\hbar a_0})/\hbar\omega_o$ is the ratio between Coulomb and confining energy, the parameter **b** is the magnetic compressed factor obtained by $b = \frac{\omega}{\omega_o} = \sqrt{1+\frac{\omega_l^2}{\omega_o^2}}$, and $\alpha = \frac{d}{a_0}$ is the dimensionless distance.

The exchange energy **J (B)** as a function of magnetic field is plotted in figure (2). We note that J is positive at zero magnetic fields which are physically true for two particle system. Also we observe that J is changes its sign from positive to negative as magnetic field B increase corresponding to singlet- triplet passing occurring at **B** = 0.9037 T (for $\hbar\omega_o \approx 3\text{mev}$, and α =0.7).

At lower magnetic field **B**, **b** is small and the overlap $\mathbf{p} = e^{-\alpha^2(2b-\frac{1}{b})}$ become large, thus the exchange term reduce result positive J provide that singlet state is the ground state. As a magnetic field increase, the electron orbital compressed by factor **b** leads to the overlap decrease exponentially. Suppression of p is satisfied by growing exchange term $J_{V_{ex}}$ as $e^{2\alpha^2(b-\frac{1}{b})}$ and suppression **J** exponentially with $e^{-2b\alpha^2}$. Lowering overlap make negative term of exchange integral in equation (9) be significant which can larger than direct coulomb term as a result **J** become negative. Once the exchange term increase the long coulomb interaction is dominant leading to triplet state being the ground state (physically, in triplet state two electron avoid each other, leading to repulsion coulomb interaction between them dominant)

We note also that at certain value of **B** (B≈ 2 T for $\hbar\omega_o \approx 3\text{mev}$), the exchange energy returned increase as **B** increase.

This behavior can explain by calculating two terms of equation (9) at different value of b (which depend on B). When **b** increase, the two coulomb terms (the second term) decrease but the exchange terms much decrease and change its sign make **J** return increase again. Since coulomb interaction still dominant, thus remains negative and don't become positive again.

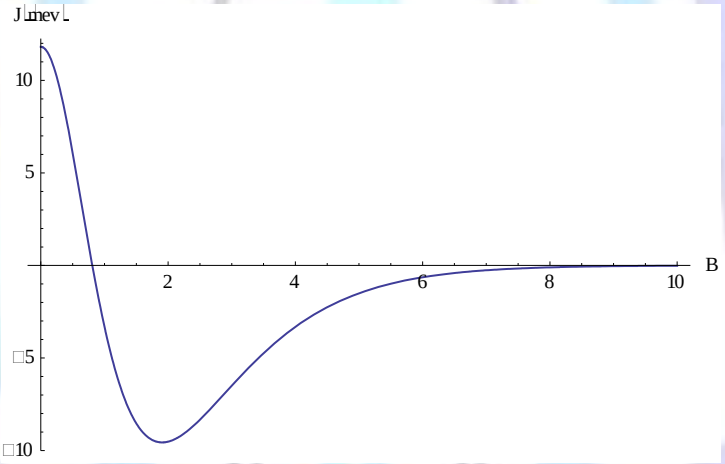

Fig (2): the exchange energy J obtained from H-L as a function of magnetic field B at fixed inter dot distance($\alpha = \frac{d}{a_0} = 0.7$)

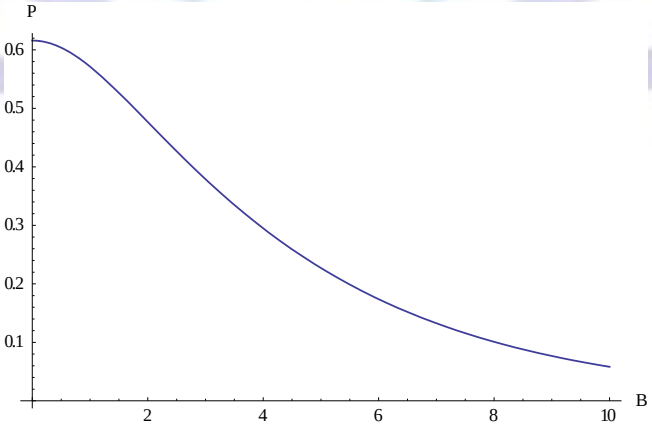

Fig. (3): the overlap P as a function of magnetic field B

Similarly **J** decrease exponentially as **d** increase (as the two dots far apart) because of overlap of wave function reduce for large inter- dot distance d. as two dots come close to each other, the overlap between the electron wave function increase and consequently **J** increase Fig (4)

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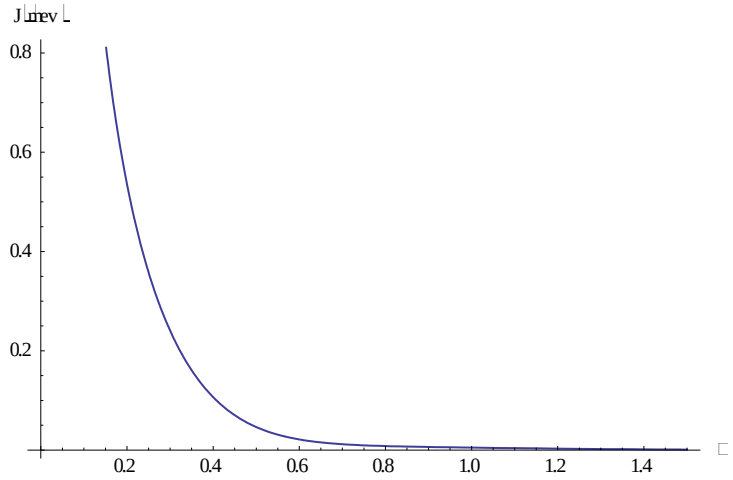

Fig (4): variation of J obtained from H-L with inter dot distance d at zero magnetic field (B=0)

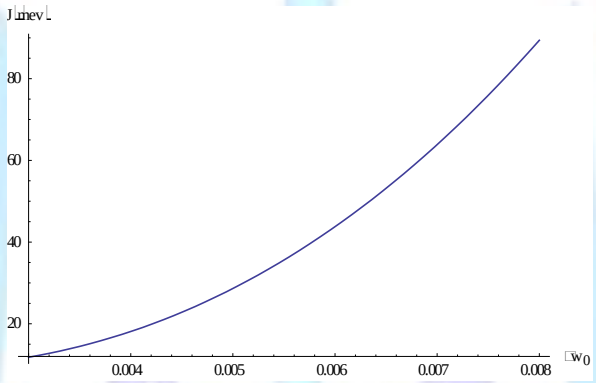

Fig (5): variation of the exchange energy J obtained from H-L as a function of $\hbar\omega_0$

When an electric field mentioned in equation (2) is taken into consideration, the exchange energy as a function of E becomes:

$$J_{HL}(E) = \left(\frac{\hbar w_o}{\sinh[2\alpha^2(2b-\frac{1}{b})]}\right) e^{-10\alpha^2 b}(-1+e^{8\alpha^2 b})(1+e^{(2b\alpha^2+2b\alpha^2(1-\frac{1}{b^2}))})\frac{de^2E^2}{8\pi^2\hbar w_o} \qquad (10)$$

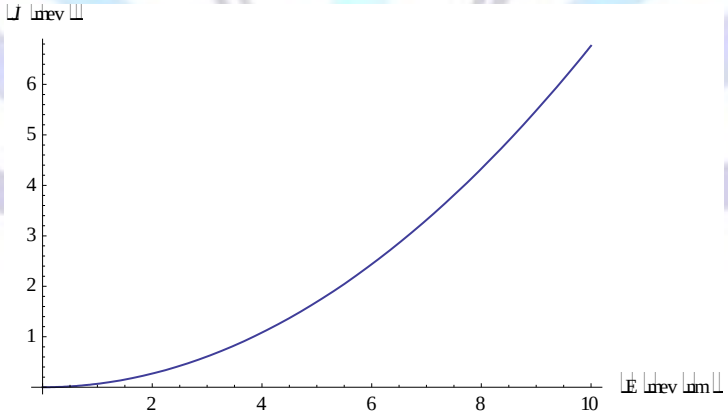

Fig (6): the exchange energy J obtained from H-L as a function of

electric field E at fixed inter dot distance($\alpha = \frac{d}{a_0} = 0.7$) and magnetic field B

The electric field produces shifting of the electron orbital (singlet and triplet state). As a result ground state energy level can tune, this tuning is important for tunneling of electrons between levels. As the electric field increase, levels are detuning and tunneling suppressed as well as overlaps decrease. Thus above equation is valid for small level shifting or as J(B, E) – J(B,0) ≤ J(B, 0)

H-L do not work at short distance [12] (because of the overlap of wave function become large, the ratio of coulomb energy to confinement energy increase at certain value of d (distance between two dots) leads to unphysical negative

value of J even at **B** = 0). So we can use the Hund-Mullikan approximation in this method we add two bases to H-L approximation by including doubly occupied state [13].

2.2 Hund-Mullikan method

Hund- Mullikan is an improvement of H-L approach, where two doubly occupied states (2, 0) and (0, 2) are included with two basis singlet s (1, 1) and triplet T (1, 1) of H-L. We still use only the two single – dot ground state as the basis state, so that according to Pauli- exclusion principle the doubly occupied state must be spin singlet. Therefore two Hilbert space of H-L changes to four Hilbert space consist of three basis of singlet state with anti-symmetric spin part and a symmetric orbital part

$$\psi_L^d = \Phi_L(r_1)\Phi_L(r_2)$$

$$\psi_R^d = \Phi_R(r_1)\Phi_R(r_2)$$

$$\psi_S = \frac{\Phi_L(r_1)\Phi_R(r_2)+\Phi_L(r_2)\Phi_R(r_1)}{\sqrt{2}}$$

while only one basis of triplet state with a symmetric spin part and anti- symmetric orbital part $\psi_T = \frac{\Phi_L(r_1)\Phi_R(r_2)-\Phi_L(r_2)\Phi_R(r_1)}{\sqrt{2}}$. These four wave function forming basis of H-M approximation.

The Hamiltonian corresponding to four basis S (0, 2), S (2, 0), S (1, 1) and T (1, 1) written as:

$$\mathcal{H}_{\text{orb}} = \epsilon_R + \epsilon_L + \begin{pmatrix} L & N & \sqrt{2}t & 0 \\ N & L & \sqrt{2}t & 0 \\ \sqrt{2}t & \sqrt{2}t & W_s & 0 \\ 0 & 0 & 0 & W_T \end{pmatrix} \qquad (11)$$

Yield the eigenvalues singlet and triplet obtained by:

$$E_T = \epsilon_R + \epsilon_L + W_T$$

$$E_{S0} = \epsilon_R + \epsilon_L + L - N$$

$$E_{S-} = \epsilon_R + \epsilon_L + \frac{L}{2} + \frac{W_S}{2} + \frac{N}{2} - \sqrt{\frac{(L-W_S+N)^2}{4} + 4t^2}$$

$$E_{S+} = \epsilon_R + \epsilon_L + \frac{L}{2} + \frac{W_S}{2} + \frac{N}{2} + \sqrt{\frac{(L-W_S+N)^2}{4} + 4t^2}$$

Where

$\epsilon_{R/L} = \langle \Phi_{R/L} - k_{+d}^0 - \Phi_{R/L} \rangle$ are the single–particle energies in the left / right dot, $L = \langle \psi_{L/R}^d - C - \psi_{L/R}^d \rangle$ is the on–site Coulomb repulsion, $N = \langle \psi_{L/R}^d - V_c - \psi_{R/L}^d \rangle$ is inter-dot Coulomb exchange integral, $W_S = \langle \psi_S - V_c - \psi_S \rangle$, $W_T = \langle \psi_T - V_c - \psi_T \rangle$ are the Coulomb energies for the S(1, 1) and T(1, 1) and $t = \langle \Phi_{\Phi_{L/R}} - k_{+d}^0 - \Phi_{R/L} \rangle + \frac{1}{\sqrt{2}} \langle \psi_S - V_c - \psi_{L/R}^d \rangle$ is the inter-dot tunneling matrix element renormalized by long rang Coulomb interaction . Using the basis of orthonormalized single particle states given in Ref. [8] as

$\Phi_{L/R} = (\phi_{L/R} - g\phi_{R/L}) / (\sqrt{1 - 2\,\mathrm{p}\,g + g^2})$ where $g = \frac{(1-\sqrt{1-\mathrm{p}2})}{\mathrm{p}}$

, and p is the overlap between right and left orbits

The exchange interaction J can obtain by diagonalizing the Hamiltonian given in eq. (11), where J is the energy difference between the triplet E_T and lowest singlet state E_{S-}

$$J_{HM} = E_T - E_{S-} = W_T - W_S - \frac{1}{2}(L - W_S + N) + \frac{1}{2}\sqrt{(L - W_S + N)^2 + 16t^2} \qquad (12)$$

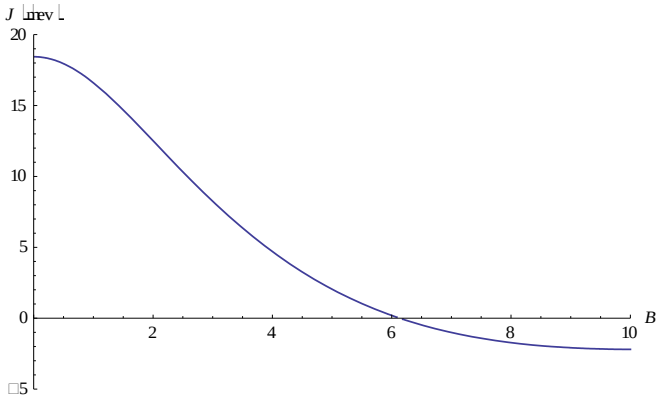

Fig. (7): The Hund-Mullikan exchange energy J as a function of magnetic field at a fixed inter-dot distance

We can see that: as a magnetic field increase, the electron orbits compressed and the confining area that two electron occupied on the same dot become smaller as a result two electron repel each other further leading to a significant energy. We also see for large B, J become negative due to the first term in equation (12). This result Coulomb energ obtained from H-M has a good agreement with that obtained by H-L

3. Magnetization

From thermodynamics relations, we calculate the mean magnetization by $M = KT \frac{\partial \ln Z}{\partial B}$ where Z is partition function which is depend on Hamiltonian, there is a jump in magnetization at B=3.8T which due to singlet triplet crossing

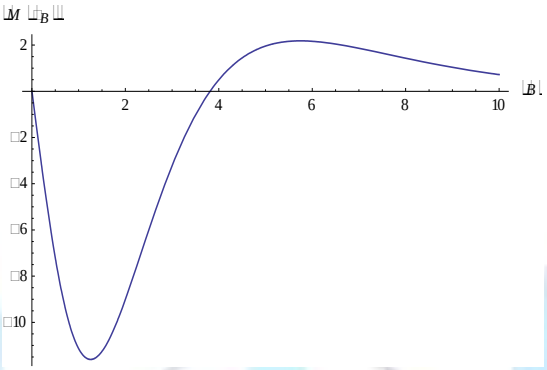

Fig. (8): The magnetization behavior as a function of magnetic field at a fixed inter-dot distance

4. Conclusion

We can form a quantum gate, the basic unit of quantum computer, using double quantum dot where the electron spin represents the qubit, and calculating the exchange energy J between spin of two electron trapped in double dots under effect of external parameter using approximation method from molecular physics Heitler-London and Hund-Mulliken. It is shown that J changes its sign from positive to negative corresponding to singlet-triplet crossing by increasing magnetic field, (which can remark as a jump in magnetization behavior) and we can use this operation to adjust quantum gate time.

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