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Exploring Exchange Interactions in Two-Qubit System

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Abstract: We studied the effect of magnetic field and interdot distance on the exchange interaction in two systems of double qubits, one made of Si and the other made of GaAs. We found that the effect is the same for both systems, but the exchange value for Si qubits is smaller due to the larger effective mass of electrons. This study provides insights into the exchange interaction, which is essential for the development of quantum computers.

Keywords: Quantum computer, Qubit, quantum dot, exchange interaction

1 Introduction

Quantum computer is a device using quantum physics principals to store information and executes computations. To build quantum computer [1], it is required storage unit for information (qubit) and quantum logic gate. This qubit should be two level system with special criteria [2,3] some physical systems are suitable for qubits and quantum logic gate, but the best suitable system is semiconductor quantum dot [4] because of its long coherence time and scalability [5,6,7,8]. Qubit state is formed by superposition between two states of electron spin inside dot (spin up and spin down). According to Pauli Exclusion Principle and the Coulomb interaction, the ground state of two electrons is a spin singlet, while the first excited state is a spin triplet [9,10,11]. Quantum logic gate form from two qubits coupled by superposition and entanglement mechanisms, to investigate quantum logic gates operation, first, we calculate the unitary time evolution between spins in dots:

$$U_{12}(t) = \mathrm{e}^{\frac{-itH_S(t)}{\hbar}} \tag{1}$$

where H_s is given by $H_S(t) = J(t)S^i.S^j$ (J is the difference of energy between singlet and triplet state, S^i is the spin operator acting on electron i and S^j is the spin operator acting on electron j). So, the exchange coupling is the important parameter for quantum logic gate operation.

The spin of electron inside Silicon (Si) quantum dot and Gallim Arsenide (GaAs) quantum dot have long coherence time. Also, the Si and GaAs have a weak spin -orbit interaction, so GaAs and Si are the best suitable for qubits. Here we investigate two symmetry double quantum dots systems (each dot has one electron), one of them is GaAs double quantum dots and the other system is Si double quantum dots. we use the approximation models Hund-Mulliken and Heitler-London for calculation of exchange coupling between singlet and triplet state. We study the effect of external magnetic field and interdot distance on exchange interaction coupling for two systems.

2 Physical Model

We consider two symmetry double quantum dots systems as where one of them of GaAs quantum dot and the other from Si quantum dot. As shown in Fig. (1), in each center of the dot there is one electron of spin [maybe in up-state or in down-state] and the distance between each dot and origin is d. The effective mass of electron is $0.191\mathrm{m}_e$ for Si and 0.067 m_e for GaAs. The electron will allow to tunnel through the barrier between dots from one to another,

If we applied electric and magnetic fields on each system where electric field in x direction and magnetic

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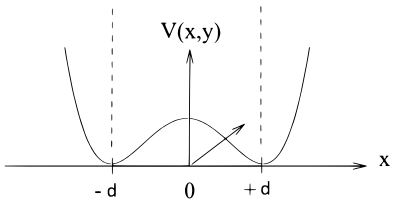

Fig. 1: Symmetry double quantum dot (for GaAs system and Si system) with inter dot distance is 2 d, one electron inside each dot. A magnetic field is applied in z axis.

field in z direction then we can write Hamiltonian as two terms:

$$H = H_1 + H_2 \tag{2}$$

where H_1 is summation of two particle energy and the potential between dots is given by:

$$H_1 = \sum_{i=1}^{2} \frac{1}{2m}(p_i - A(r_i))^2 + V(r_i) + V(x,y) \tag{3}$$

where $A(r_i)$ is the vector potential where is given by $A(r_i) = \frac{[B\times r_i]}{2} \rightarrow \frac{B}{2}(-y,x,0)$, $V(r_i)$ is the confined potential, the confinement potential for aligned double dots is the quartic potential is $V(x,y) = \frac{\omega_0\hbar}{2a_0^2}((\frac{x^2}{2a} - \frac{a}{2})^2 + y^2)$, and H_2 is summation of three terms:

$$H_2 = g_{eff}\mu_B \sum BS_Z^i + ex_iE + \frac{e^2}{\varepsilon r_{12}} \tag{4}$$

The first term is Zeeman energy where the g-factor is 0.44 for GaAs and 2 for Si and μ_B is the Boher magneton. The value of Zeeman effect for GaAs and Si is a small value, so we can neglect Zeeman energy for two systems. The second term is electric energy, and the third term is Coulomb interaction between two electrons, where ε is the dielectric constant (in GaAs $\varepsilon = 13.1$ and for Si=7.9), r_{12} is the distance between the two electrons. From the experimental researches, the potential of single dot is a harmonic oscillator potential [12,13,14], thus the potential between two quantum dots is chosen to be:

$$V(x,y) = \frac{m\omega_0^2}{2}(\frac{1}{4d^2}(x^2 - d^2)^2 + y^2) \tag{5}$$

These is the potential between two dots (two harmonic potential wells of frequency ω_0.

From experimental research the single quantum dot potential is harmonic oscillator. so, the electron ground state wave function $\phi(x,y)$ is given by:

$$\phi(x,y) = \sqrt{\frac{m\omega}{\pi\hbar}}\mathrm{e}^{\frac{-m\omega(x^2+y^2)}{2\hbar}} \tag{6}$$

where $\omega = \sqrt{\omega_0^2 + \omega_l^2}$ and $\omega_l$is the Larmor frequency (ω_l=$\frac{eB}{m^*}$), so the wave function of ground state electron inside dot is given by:

$$\phi_{\pm d}(x,y) = \exp(\pm\frac{iyd}{2l_B^2})\phi(x\mp d, y) \tag{7}$$

where $\exp(\pm\frac{iyd}{2l_B^2})$ is the magnetic field phase factor, ($l_B = \sqrt{\frac{\hbar c}{\omega_l m^*}}$) is the length of magnetic field, we choose the gauge described by the vector:

$$A = \frac{[B\times r]}{2} \rightarrow A_\pm = \frac{B}{2}(-y,x,0) \tag{8}$$

After this consideration, the two electrons Hamiltonian is:

$$H_{orb} = \frac{1}{2m}(p_1 - \frac{e}{c}A(r_1))^2 + \frac{1}{2m}(p_2 - \frac{e}{c}A(r_2))^2 + V(x,y) + \mathrm{e}^2/(\varepsilon r_{12}) \tag{9}$$

We can write the Hamiltonian of two quantum dots as:

$$H_{orb} = \sum_{i=1}^{2} \frac{((P_i - eA(r_i)/C))^2}{2m} + \frac{mw^2}{2}((x_i \mp d)^2 + {y_i}^2) + W + V_c \tag{10}$$

where $W(x,y) = V(x,y) - \frac{m\omega^2}{2}((x_1+d)^2 + (x_2-d)^2)$ and $V_c = \mathrm{e}^2/(\varepsilon r_{12})$.

Under magnetic field the two-electron spin have two spin state one of them is singlet state $(S=0)|S\rangle = \frac{1}{\sqrt{2}}|\uparrow\downarrow - \downarrow\uparrow\rangle$ and the other is triplet state $(S=1)|T_0\rangle = \frac{1}{\sqrt{2}}|\uparrow\downarrow + \downarrow\uparrow\rangle, |T_+\rangle = |\uparrow\uparrow\rangle, |T_-\rangle = |\downarrow\downarrow\rangle$, where the ground state is singlet and first excited state is triplet under condition $\hbar\omega_o \gg KT$. Exchange interaction is given by the difference between triplet and singlet state. So $J = E_T - E_S$ to calculate it we use this expectation equation:

$$J = \langle\psi_T \mid H_{orb} \mid \psi_T\rangle - \langle\psi_S \mid H_{orb} \mid \psi_S\rangle \tag{11}$$

Quantum dot is like an atom (artificial atom) so we can consider the two quantum dots as artificial molecule. Then, we can use the same approximation methods as Hund – Mulliken and Heitler – London models, under condition at zero magnetic field the ground state should be singlet (at $B = 0$ is $J > 0$).

3 Heitler-London model

Heitler-London model is the approximation method to evaluate the exchange interaction between two electrons

in molecule or in two quantum dots. It considers the single electron wave function as a basis and the system is two level one is singlet and the other is triplet state which is linear combination from basis. The accuracy of this method is related to the distance between two dots as larger as more accurate exchange value. The two-level system (singlet and triplet wave function) is:

$$\mid \psi_{ST}\rangle = \frac{\mid \phi_L(1)\phi_R(2) \pm \phi_L(2)\phi_R(1)\rangle}{\sqrt{(2(1 \pm p_{LR}^2))}} \times \frac{|\uparrow\downarrow \mp \downarrow\uparrow\rangle}{\sqrt{2}} \quad (12)$$

The first term is the orbital contribution, the spin wave function term can be neglected. The orbit wave function overlap is:

$$p = \int \phi_{+d}^*(r)\phi_{-d}(r)\mathrm{d}^2 r = \langle \phi_L \mid \phi_R\rangle = e^{(\frac{-m\omega d^2}{\hbar} - \frac{d^2\hbar}{4l_B^4 m\omega})} \quad (13)$$

From equations (7), (8), and (9) the exchange energy due to HL obtained by:

$$J_{HL} = \langle \psi_T \left| H_{orb} \right| \psi_T\rangle - \langle \psi_S \left| H_{orb} \right| \psi_S\rangle \quad (14)$$

This can be written as:

$$\begin{aligned} J_{HL} &= \frac{p^2}{1-p^4}(J_W + J_{V_c}) \\ &= \frac{p^2}{1-p^4}[\langle\phi_L(1)\phi_R(2)|w|\phi_L(1)\phi_R(2)\rangle \\ &\quad -\frac{1}{p^2}\langle\phi_L(1)\phi_R(2)|w|\phi_L(2)\phi_R(1)\rangle \\ &\quad +\langle\phi_L(1)\phi_R(2)|c|\phi_L(1)\phi_R(2)\rangle \\ &\quad -\frac{1}{p^2}\langle\phi_L(1)\phi_R(2)|c|\phi_L(2)\phi_R(1)\rangle] \end{aligned} \quad (15)$$

after calculation the exchange interaction by HL approximation method is given by:

$$\begin{aligned} J_{HL} &= \frac{\hbar\omega_0}{sinh[2d^2(2b-1/b)]}[\frac{b\alpha^2}{16\pi^2\omega}e^{-10b\alpha^2} \\ &\quad (1+e^{b\alpha^2(3-\frac{1}{b^2})}(\omega_0 - \frac{4\omega^2}{\omega_0} + 3\hbar\omega_0) \\ &\quad +\frac{(S\sqrt{b}Erf[2\sqrt{2b}d]}{8\pi^2}(e^{2ba^2} - e^{2(b-\frac{1}{b})d^2})] \end{aligned} \quad (16)$$

where Erf (error function) is given by $Erf(z) = \frac{2}{\sqrt{\pi}}\int_0^z e^{-t^2}dt$ *and* $s = \frac{1}{8\sqrt{2}\pi^{\frac{3}{2}}}\frac{\frac{e^2}{ka_0}}{\hbar\omega_o}$ is the ratio between Coulomb energy and confining energy, the b is the m is given by $b = \frac{\omega}{\omega_o} = \sqrt{1 + \frac{\omega_I^2}{\omega_0^2}}$ (magnetic factor), and α is the interdot distance to interatomic distance $\alpha = \frac{d}{a_o}$.

As shown in Fig. (2), the exchange energy J against the magnetic field is plotted for GaAs system. We note that J is positive at zero magnetic field, because the two electrons in singlet state. By increasing of magnetic field, the exchange coupling decreases until to be zero. The change from singlet to triplet state (sign change of J from positive to negative) occurs at B=1.3T (for $\hbar\omega_0 \approx$ 3meV,and d=0.7). Then by increasing the magnetic field J go to zero.

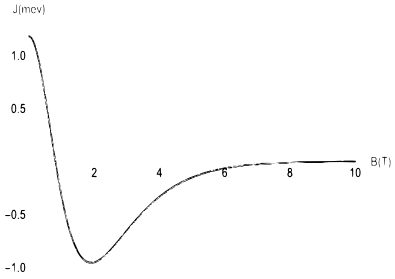

Fig. 2: For GaAs system: variation of exchange interaction with magnetic field at value 3 meV of confinement energy and the distance between dot is fixed (HL model).

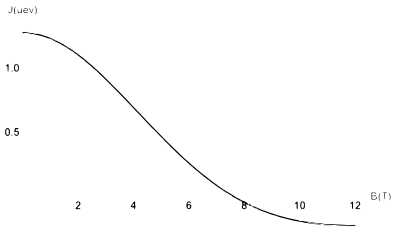

Fig. 3: For Si system, variation of exchange interaction with magnetic field at value 8 meV of confinement energy and the distance between dots is fixed (HL model).

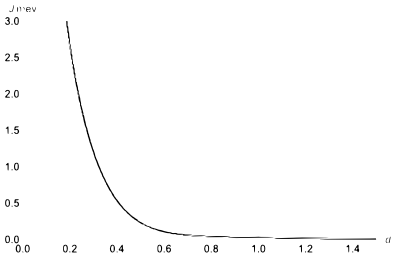

Fig. 4: Variation of J obtained from HL with inter dot distance d at zero magnetic field (B=0).

As shown in Fig. (3), the exchange energy J against the magnetic field is plotted for Si system. We note that J is positive at zero magnetic field, because the two electrons in singlet state. By increasing of magnetic field, the exchange coupling decreases, until to be zero. The change from singlet to triplet state (sign change of J from positive to negative) occurs at B=6.42T (for $\hbar\omega_0 \approx$ 8meV,and d=1.2).

As shown in Fig: (4) and (5) for Si and GaAs double quantum dots systems, it is clear that the J exhibits the same behavior for two systems, as the distance between two dots increases as the exchange interaction decreases where the distance between two dots is a measure the overlap between the wavefunction of two electrons.

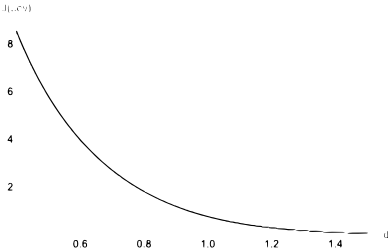

Fig. 5: For Si: the variation of J obtained from HL with inter dot distance d at zero magnetic field (B=0).

4 Hund-Mulliken method

Hund-Mullikan is approximate method which differ from Heitler-London model in the no. of states, here it include the doubly occupied states, where there are two doubly occupied states beside the Heitler-London singlets S(1,1) and triplet T(1,1). Where this states are linear combination from the same basis single electron wave function as in HL, the doubly occupied state should be singlet state according to Pauli principle. So, the two Hilbert space in HL become four Hilbert space in HM, the four wave functions are:

$$\psi_L^d = \Phi_L(r_1)\Phi_L(r_2) \tag{17}$$

$$\psi_R^d = \Phi_R(r_1)\Phi_R(r_2) \tag{18}$$

$$\begin{aligned}\psi_S &= \frac{\Phi_L(r_1)\Phi_R(r_2)+\Phi_L(r_2)\Phi_R(r_1)}{\sqrt{2}}\\ \psi_T &= \frac{\Phi_L(r_1)\Phi_R(r_2)-\Phi_L(r_2)\Phi_R(r_1)}{\sqrt{2}}\end{aligned} \tag{19}$$

The Hamiltonian operator according to HM wave functions is:

$$H_{orb} = \varepsilon_R + \varepsilon_L + \begin{pmatrix} U & X & \sqrt{2}t & 0 \\ X & U & \sqrt{2}t & 0 \\ \sqrt{2}t & \sqrt{2}t & V_s & 0 \\ 0 & 0 & 0 & V_T \end{pmatrix} \tag{20}$$

Then, we obtained the energy for states by:

$$E_T = \varepsilon_R + \varepsilon_L + V_T \tag{21}$$

$$E_{S0} = \varepsilon_R + \varepsilon_L + U - X \tag{22}$$

$$E_{S-} = \varepsilon_R + \varepsilon_L + \frac{U}{2} + \frac{V_S}{2} + \frac{X}{2} - \sqrt{\frac{(U-V_S+X)^2}{4} + 4t^2} \tag{23}$$

$$E_{S+} = \varepsilon_R + \varepsilon_L + \frac{U}{2} + \frac{V_S}{2} + \frac{X}{2} + \sqrt{\frac{(U-V_S+X)^2}{4} + 4t^2} \tag{24}$$

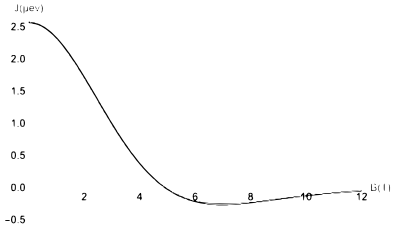

Fig. 6: For GaAs: The Hund-Mullikan exchange energy J as a function of magnetic field at a fixed inter-dot.

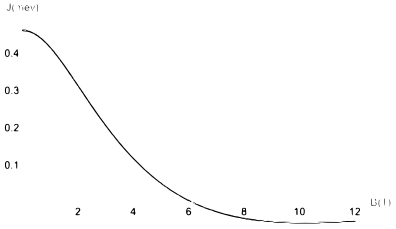

Fig. 7: For Si system: The Hund-Mullikan exchange energy J as a function of magnetic field at a fixed inter-dot.

where $\varepsilon_{R/L} = \langle \phi_{R/L} \mid k^0_{\pm d} \mid \phi_{R/L} \rangle$ are the single electron energy in the each dot, $U = \langle \psi^d_{L/R} \mid C \mid \psi^d_{L/R} \rangle$ is the coulomb reputation energy, $X = \langle \psi^d_{L/R} \mid C \mid \psi^d_{R/L} \rangle$ is Coulomb exchange energy, $V_s = \langle \psi_s \mid C \mid \psi_s \rangle$, $V_T = \langle \psi_T \mid C \mid \psi_T \rangle$ are the Coulomb energies for the singlet and triplet state for one electron inside each quantum dot $t = \langle \phi_{L/R} \mid k^0_{\mp d} \mid \phi_{R/L} \rangle + \frac{1}{\sqrt{2}} \langle \psi_s \mid C \mid \psi^d_{L/R} \rangle$ is tunneling energy matrix element. The orthonormal of basis (single electron wavefunction) is given by:

$$\Phi_{L/R} = \frac{\Phi_{L/R} - g\Phi_{R/L}}{\sqrt{1-2pg+g^2}} \tag{25}$$

where $g = \frac{(1-\sqrt{(1-p2)})}{p}$ and p is the overlap wavefunction between two electrons. We can obtain the exchange coupling J from diagonalizing of Hamiltonian, where J is the different between triplet state and singlet state so,

$$\begin{aligned}J_{HM} = E_{T-} = V_T - V_S - \tfrac{1}{2}(U - V_S + X) + \\ \tfrac{1}{2}\sqrt{(U-V_S+X)^2 + 16t^2}\end{aligned} \tag{26}$$

For Si and GaAs system, as shown in Fig. (6) and (7) exhibits the same behavior of HL, we can say that the result obtained from HM has a good agreement with that obtained by HL.

5 Conclusion

From our results, the effect of physical parameters as an interdot distance and external magnetic field parameter on exchange interaction for GaAs double quantum dots (GaAs qubits) is qualitatively the same for Si double quantum dots (Si qubits). The exchange interaction in Si is smaller than GaAs because of the smaller wave function overlap which due to large electron mass inside silicon. Also, the scalability is advantage for silicon qubits over other qubits types because of small size of silicon qubits.

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