Original article

Quantum Logic gate from Silicon quantum dots

N. K. Seadawy[1] – A. Khalaf [2,] A. M. Salem Shimaa[1] S. Abdelfattah[3]

[1]Physics Department, Basic Science Center, Misr University for Science and Technology, 6 October city, Almotamayz District, Egypt

[2]Physics Department, Faculty of Science, Al-Azhar University, (11884) Cairo, Egypt

[3]Physics Department, Faculty of Science, Al-Azhar University (Girl's Branch), (11754) Cairo, Egypt

ARTICLE INFO	ABSTRACT
	Quantum computer has a great attention all over the world, several attempts to construct them by supposing a theoretical or experimental model for qubit which is the basic unit of quantum computers. Qubit is formed from two-level physical systems, So, a semiconductor quantum dot is suitable for a qubit where a qubit state is formed from superposition between two spin states, silicon (Si) quantum dot is one of the suitable systems for qubit and quantum logic gate because of its long coherence time. In this work, we study the theoretical model of quantum dots from silicon (Si) which couple through superposition and entanglement mechanisms to form a quantum logic gate. we have investigated the magnetic field effect on exchange interaction by using two approximate methods Hund – Mullikan (HM) and Hitler – London (LH) for calculation and evaluation of the exchange interaction coupling, also studied the influence of inter – dots distance on the exchange coupling. From an investigation of exchange interaction, silicon quantum dots is the best suitable for quantum logic gate.

1. Introduction

Recently, nanotechnology has the principal role in all life fields and gives significant progress in all science directions, one of these areas is quantum computer. For establishing it, we need a unit for storge information and quantum logic gate. Quantum computers [1,2] depend on quantum mechanics such as superposition and entanglement which are two important mechanisms for quantum logic gates. There are quantum computer criteria as in [3,4]. There are many physical systems But the more suitable one for qubits is a quantum dot [5,6]. quantum dot is an example of a two-level system that achieve the idea of a qubit where the electron has two spin state (spin up or spin down), and the qubit state is a superposition between two levels. Quantum dot from Si is the best candidate for qubit because of the long coherence time and small size [7-9]. Quantum logic gates form from two qubits coupled by superposition and entanglement mechanism for example To calculate Quantum logic gates as we first the unitary time

evolution between spins in dots is important to calculate any quantum logic gate

$$U_{12}(t) = e^{-it\mathcal{H}_s(t)/\hbar}$$

Where $\mathcal{H}_s$ is given by $J_{12}(t)S_1 . S_2$ (where J_{12} is the difference of energy between singlet and triplet state), and S_i is the spin operator acting on electron i.

In our study, we investigate a model of Si double quantum dot as a quantum logic gate. We calculate the exchange interaction by two approximate methods Hund – Mullikan (HM) and Hitler – London (LH) [11-13]. Investigating the effect of physical parameters such as magnetic field and inter –dot distance on interaction coupling.

2. Theoretical model

Our model is two quantum dots from Si, in each center of the dot there is one electron of spin [may be in up state or in down state] and the distance between each dot and origin is d. The effective mass of an electron is $0.191 m_e$. The electron may be tunneled from a dot to another. To write the Hamiltonian of the system, first, to simplify the calculation suppose the two dots are the

∗ *Corresponding author*
E-mail address: shimaa.s.abdelfattah@gmail.com

Special issue "selected papers from the 2ⁿᵈ International Conference on Basic and Applied Science (2ⁿᵈ ICBAS-2023)"

same. In the z direction we applied a magnetic field and an electric field was applied in the x-axis, so Hamilton is

$$\mathcal{H} = \sum_{i=0}^{2} P_i + exE + \mathcal{H}_Z + F_{coul} + \mathcal{H}_{SO} + \mathcal{H}_S \qquad (1)$$

$$P_i = \frac{1}{2m}\left(p_i - \vec{A}(r_i)\right)^2 + V(r_i) \qquad (2)$$

Where P_i is the single particle energy,
is The vector potential where is given by:

$$\vec{A}(r_i) = \frac{[\vec{B} \times \vec{r_i}]}{2} \rightarrow A_{\pm}(r_i) = \frac{B}{2}(-y, x, 0) \qquad (3)$$

$\mathcal{H}_Z$ is zeeman term is given by:

$$\mathcal{H}_Z = g_{eff}\mu_B \sum B S_Z^i \qquad (4)$$

The zeman effect for silicon is small value, so we can neglect it from our calculation.

$\mathcal{H}_{SO}$ is the spin orbit coupling is:

$$H_{so} = \frac{\omega_o^2}{2mc^2} S.L \qquad (5)$$

(L is the election angular momentum inside the quantum dot in units of $\hbar$). The spin-orbit interaction has significant value for a system with few no. of electrons. Quantum computer is preferred qubit with weak spin-orbital coupling as semiconductor quantum dots [1] so, we can neglect it for Si quantum dots. The couloum energy between the electrons is:

$$F_{coul} = \frac{e^2}{\varepsilon\, r_{12}} \qquad (6)$$

Where ε is the constant of Si dialectic (Ɛ =7.9), r_{12} is two electrons distance, from experimental researches the quantum dot potential is a harmonic oscillator [4,7]
The potential between two dots should be quadratic potential

$$V(x,y) = \frac{\omega_0 \hbar}{2a_0^2}\left(\left(\frac{x^2}{2a} - \frac{a}{2}\right)^2 + y^2\right) \qquad (7)$$

Which separate double dots (*for x around* $\pm d$) into two harmonic wells of frequency ω_o, one for each dot, in the limit of large inter-dot distance, i.e. for $2d \gg 2d_B$, where a is half the distance between the centers of the dots, and the Boher radius of a single quantum dot as harmonic potential is $d_B = \sqrt{\hbar/m\omega_0}$ is a scale for wave function extension of an electron inside dots.
From the experimental the potential of a quantum dot is a harmonic oscillator, so, the wave function $\phi(x,y)$ of an electron in the ground state inside the quantum dot given by

$$\phi(x,y) = \sqrt{\frac{m\omega}{\pi\hbar}}\, e^{-m\frac{\omega(x^2+y^2)}{2\hbar}} \qquad (8)$$

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

$$\phi_{\pm d}(x,y) = \exp(\pm iyd/2\, l_B^2)\, \phi(x \mp d, y) \qquad (9)$$

Where $\exp(\pm iyd/2\, l_B^2)$ magnetic field phase factor [11], $l_B = \sqrt{\frac{\hbar c}{\omega_l m^*}}$ is the length of magnetic field, we choose the gauge described by the vector.

$$A = \frac{[B \times r]}{2} \rightarrow A_{\pm} = B(-y, x, 0) \qquad (10)$$

After this consideration, the two electrons Hamiltonian is.

$$\mathcal{H}_{orb} = \frac{1}{2m}\left(p_1 - \frac{e}{c}A(r_1)\right)^2$$
$$+ \frac{1}{2m}\left(p_2 - \frac{e}{c}A(r_2)\right)^2 \qquad (11)$$
$$+ V(x,y) + \frac{e^2}{\varepsilon\, r_{12}}$$

We can write the Hamiltonian of two quantum dots as:

$$\mathcal{H}_{orb} = \sum_{i=1}^{2} \frac{\left(P_i - e\frac{A(r_i)}{C}\right)^2}{2m}$$
$$+ \frac{mw^2}{2}((x_i \mp d)^2 \qquad (12)$$
$$+ y_i^2) + W + V_c$$

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

Under a magnetic field, the two electron spin have two spin states one of them is a singlet state (S = 0) $|S\rangle = \frac{1}{\sqrt{2}}|\uparrow\downarrow - \downarrow\uparrow\rangle$
and the other is triplet state (S = 1) $|T_o\rangle = \frac{1}{\sqrt{2}}|\uparrow\downarrow + \downarrow\uparrow\rangle$, $|T_+\rangle = |\uparrow\uparrow\rangle$, $|T_-\rangle = |\downarrow\downarrow\rangle$
where the ground state is a singlet and the first excited state is triplet under the condition $\hbar\omega_o \gg K T$. 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:

$$J = \langle\psi_T|\mathcal{H}_{orb}|\psi_T\rangle - \langle\psi_S|\mathcal{H}_{orb}|\psi_S\rangle \qquad (13)$$

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

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

$$|\psi_{S/T}\rangle = \frac{|\phi_L(1)\phi_R(2) \pm \phi_L(2)\phi_R(1)\rangle}{\sqrt{2(1 + p_{LR}^2)}}$$
$$\times \frac{|\uparrow\downarrow \mp \downarrow\uparrow\rangle}{\sqrt{2}} \qquad (14)$$

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

The orbit wave function overlap is:

$$\text{p} = \int \phi_{+d}^*(r)\phi_{-d}(r)\, d^2r = \langle \phi_L | \phi_R \rangle$$
$$= \exp\left(\frac{-m\omega d^2}{\hbar} - \frac{d^2\hbar}{4l_B m\omega} \right) \qquad (15)$$

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

$$J_{HL} = \langle \psi_T | \mathcal{H}_{orb} | \psi_T \rangle - \langle \psi_S | \mathcal{H}_{orb} | \psi_S \rangle \qquad (16)$$

This can be written as:

$$
\begin{aligned}
J_{HL} &= \frac{p^2}{1-p^4}\left(J_W + J_{V_c} \right) \\
&= \frac{p^2}{1-p^4}\Big[\langle \phi_L(1)\phi_R(2)|w|\phi_L(1)\phi_R(2)\rangle \\
&\quad - \frac{1}{p^2}\langle \phi_L(1)\phi_R(2)|w|\phi_L(2)\phi_R(1)\rangle \\
&\quad + \langle \phi_L(1)\phi_R(2)|c|\phi_L(1)\phi_R(2)\rangle \\
&\quad - \frac{1}{p^2}\langle \phi_L(1)\phi_R(2)|c|\phi_L(2)\phi_R(1)\rangle \Big]
\end{aligned} \qquad (17)
$$

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

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

Where Erf is the error function given by $\text{Erf}(z) = \frac{2}{\sqrt{\pi}}\int_0^z e^{-t^2}dt$, and $\boldsymbol{s} = \frac{1}{8\sqrt{2}\pi^{3/2}}\left(\frac{e^2}{ka_0}\right)/\hbar\boldsymbol{\omega_o}$ is Coulomb energy to confining energy, the b is the magnetic factor given by $\boldsymbol{b} = \frac{\omega}{\omega_o} = \sqrt{1 + \frac{\omega_l^2}{\omega_o^2}}$, and $\boldsymbol{\alpha} = \frac{d}{a_0}$ is the ratio between interdot distance and interatomic distance. As shown in Fig.(1), the exchange coupling **J (B)** against magnetic field. It is clear that at zero magnetic fields the exchange coupling is positive because the two electrons in a singlet state, as the magnetic field increases as J decreases until reaches zero at **B** = 6.25 T(for $\hbar\boldsymbol{\omega_o} \approx$ 8mev), then as the magnetic field increases as J decreases, means that the state changes from singlet to triplet state.

Hund-Mulliken method

Hund-Mullikan is an approximate method which differs from Heitler – London model in state number, it includes the doubly occupied states, where there are two doubly occupied states *beside the* Heitler – London singlets $S(1,1)$ and triplet $T(1,1)$. Of course, these states are linear combinations from the same basis single electron wave function as in HL the doubly occupied state should be a singlet state according to the Pauli principle. So the two Hilbert spaces in HL become four Hilbert spaces in HM, and the four-wave functions are:

$$\psi_L^d = \Phi_L(r_1)\Phi_L(r_2) \qquad (17)$$

$$\psi_R^d = \Phi_R(r_1)\Phi_R(r_2) \qquad (18)$$

$$\psi_S = \frac{\Phi_L(r_1)\Phi_R(r_2) + \Phi_L(r_2)\Phi_R(r_1)}{\sqrt{2}} \qquad (19)$$

$$\psi_T = \frac{\Phi_L(r_1)\Phi_R(r_2) - \Phi_L(r_2)\Phi_R(r_1)}{\sqrt{2}}$$

The Hamiltonian operator according to HM wavefunctions is:

$$
\mathcal{H}_{orb} = \epsilon_R + \epsilon_L + \begin{pmatrix} U & X & \sqrt{2}t & 0 \\ X & U & \sqrt{2}t & 0 \\ \sqrt{2}t & \sqrt{2}t & V_S & 0 \\ 0 & 0 & 0 & V_T \end{pmatrix} \qquad (20)
$$

Then, we obtained the energy for states by:

$$E_T = \epsilon_R + \epsilon_L + V_T \qquad (21)$$

$$E_{S0} = \epsilon_R + \epsilon_L + U - X \qquad (22)$$

$$
\begin{aligned}
E_{S_-} &= \epsilon_R + \epsilon_L + \frac{U}{2} + \frac{V_S}{2} + \frac{X}{2} \\
&\quad - \sqrt{\frac{(U-V_S+X)^2}{4} + 4t^2}
\end{aligned} \qquad (23)
$$

As in Figure [2], the distance between two dots increase as J decrease and that is physically true because wave function overlap decrease as the distance increase.

$$
\begin{aligned}
E_{S_+} &= \epsilon_R + \epsilon_L + \frac{U}{2} + \frac{V_S}{2} + \frac{X}{2} \\
&\quad + \sqrt{\frac{(U-V_S+X)^2}{4} + 4t^2}
\end{aligned} \qquad (24)
$$

Where

$\epsilon_{R/L} = \langle \Phi_{R/L}|k_{\pm d}^0|\Phi_{R/L}\rangle$ are the single electron energy in each dot, $U = \langle \psi_{L/R}^d|C|\psi_{L/R}^d\rangle$ is the coulomb reputation energy, $X = \langle \psi_{L/R}^d|C|\psi_{R/L}^d\rangle$ is Coulomb exchange energy, $V_S = \langle \psi_S|C|\psi_S\rangle$, $V_T = \langle \psi_T|C|\psi_T\rangle$ are the Coulomb energies for the singlet and triplet state for one electron inside each quantum dot. and $t = \langle \Phi_{\Phi_{L/R}}|k_{\mp d}^0|\Phi_{R/L}\rangle + \frac{1}{\sqrt{2}}\langle \psi_S|C|\psi_{L/R}^d\rangle$ as in [11], is a tunneling energy matrix element.
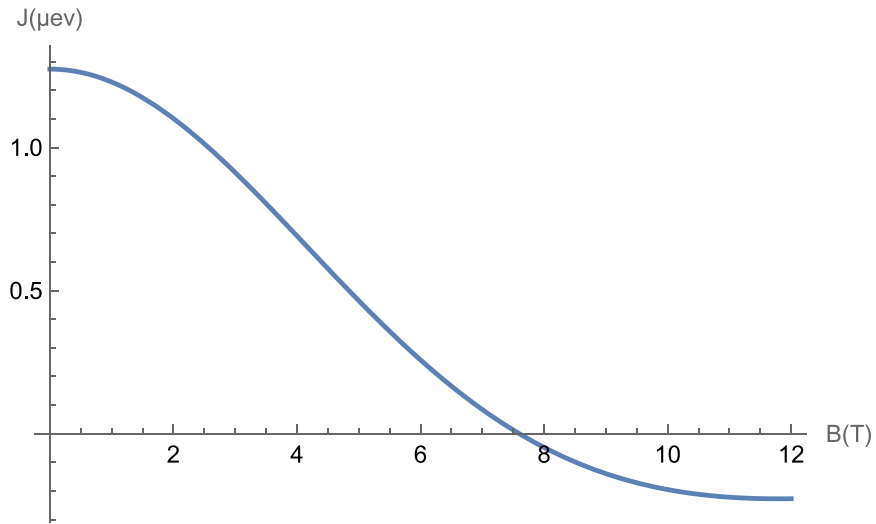
Figure (1). HL model, variation of exchange interaction with magnetic field at value 8 meV of confinement energy and 30.24nm for distance between dots.
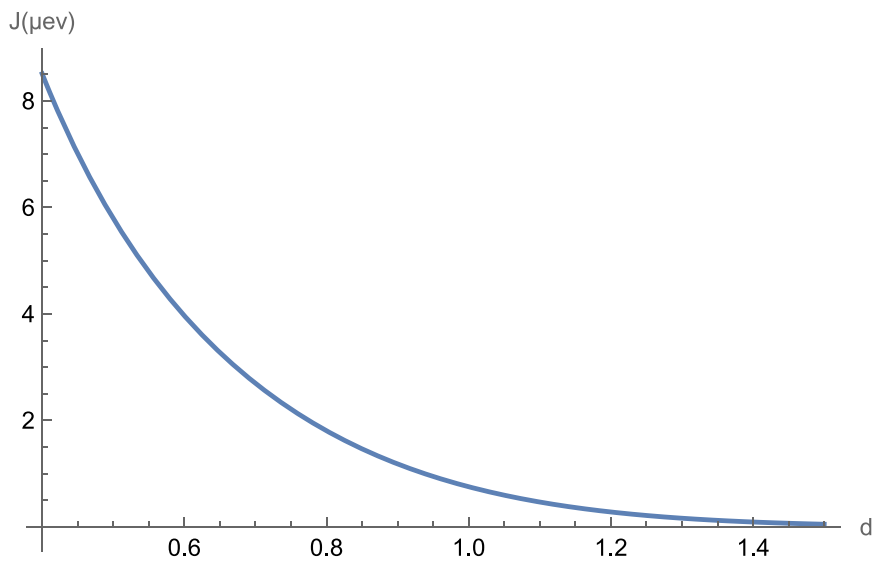

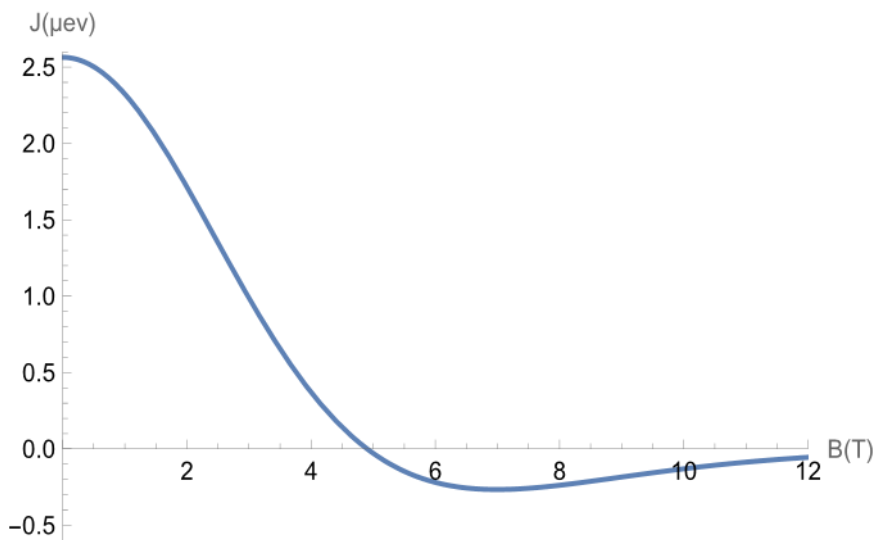Figure (2) the exchange coupling J with the distance between two dots (magnetic field is zero).

Fig.(3)The exchange coupling J against the magnetic field (the distance between two dots is fixed)

The orthonormal of basis (single electron wavefunction) is given by:

$$\Phi_{L/R} = (\phi_{L/R} - g\phi_{R/L})/\left(\sqrt{1 - 2\,p\,g + g^2}\right) \qquad (25)$$

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 difference between triplet state and singlet state

So,

$$J_{HM} = E_T -= V_T - V_S$$
$$-\frac{1}{2}(U - V_S + X)$$
$$+\frac{1}{2}\sqrt{(U - V_S + X)^2} \qquad (26)$$
$$+ 16t^2$$

As shown in Fig. (3), the HM gives qualitative agreement with HL behavior.

Conclusion

From our work, we investigate the exchange interaction which is the important parameter of the quantum logic gate from Si two quantum dots, we find the physical parameters as an interdot distance and external magnetic field parameter effect on exchange interaction and variation from singlet to triplet state. the calculation of the exchange interaction of double qubits Si is smaller than other semiconductor qubits on account of the electron mass inside Silicon which is large so the overlap is small which appears in the calculation. Besides our results, Si qubits have a small size which makes it the best suitable for quantum logic gate.

References

1. Di. Vincenzo, P. David "The Physical Implementation of Quantum Computation". Fortschritte der Physik. **48** (9–11): 771–783 (2000).
2. L. Platt "WKB Analysis of Tunnel Coupling in a Simple Model of a Double Quantum Dot", University of Waterloo, Ontario, Canada, (2008)
3. J. Adamowski, S. Bednarek, and B. Szafran, Schedae,vol. 14, (2005)
4. J. I. Cirac and P. Zoller, Phys. Rev. Lett. 74, 4091 (1995); C. Monroe, D. M. Meekhof, B. E. King, W. M. Itano, and D. J. Wineland, Phys. Rev. Lett. 75, 4714 (1995).
5. Q. A. Turchette, C. J. Hood, W. Lange, H. Mabuchi, and H. J. Kimble, Phys. Rev. Lett. 75, 4710 (1995).
6. I. L. Chuang, N. A. Gershenfeld, and M. Kubinec, Phys. Rev. Lett. 80, 3408. (1998)
7. J. A. Jones, M. Mosca, R. H. Hansen, Nature 393, 344 (1998).
8. G. Burkard, D. Ladd, Andrew Pan, M. Nichol, and R. Petta Rev. Mod. Phys. **95**, 025003 (2023)
9. Li. Qiuzi, Ł. Cywiński, D. Culcer, and S. Das Sarma, Phys. Rev. B 81, 085313 –(2010)
10. I. Tsiamis, "Quantum Transport through Single and Double Quantum Dots",(2013)
11. G. Burkard, D. Loss, and David P. DiVincenzo, Phys. Rev. B 59, 2070 (1999)
12. N. Golovach and D. Loss *Semicond. Sci. Technol.* 17 355 (2002)
13. R. de Wolf, Quantum Computing: Lecture Notes, University of Amsterdam, (2011)