JOURNAL OF KUFA–PHYSICS
journal.uokufa.edu.iq/index.php/jkp/index | ISSN: 2077–5830

Calculation of Exchange Energy in Double Quantum Dots Using COMSOL Wave Functions

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ARTICLE INF.

Article history:
Received: 5 JUL, 2024
Revised: 30 AUG., 2024
Accepted: 5 SEP., 2024
Available Online: 29 DEC. 2024

Keywords:

Double quantum dots
Exchange interaction
Quantum computing

ABSTRACT

Heitler-London(HL) and Hund-Mulliken(HM) approximations were applied in microscopic computations for double quantum dot (DQDs) spin qubits. The J- interaction between triplet and singlet states in a linked double quantum dot (DQD) at (Si/SiO2) interface using COMSOL Multiphysics wave functions was estimated. By evaluating different potential, this calculation is performed within a specified region of interest. We evaluated these findings in relation to a situation in which Fock-Darwin (FD) states are used and a precisely known solution of a one-dimensional Schrödinger equation exists. Our study reveals the effectiveness of the applied method and provides interesting investigation of the reliability and accuracy of the computational method used.

DOI: https://doi.org/10.31257/2018/JKP/2024/v16.i02.16833

حساب طاقة التبادل في النقاط الكمومية المزدوجة باستخدام دوال الموجات في COMSOL

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الـــخُـــلاصـــة

استخدمت تقريب هيتلر-لندن (HL) وتقريب هوند-مولكن (HM) في الحسابات المجهرية لنقطتي كيوبيات سبين الكمومية المزدوجة. تم تقدير تفاعل J بين حالات ثلاثية وثنائية في نقطة الكم المزدوجة (DQD) المرتبطة عند واجهة (Si/SiO2) باستخدام دوال الموجات لبرنامج COMSOL Multiphysics.من خلال تقييم الإمكانات المختلفة، تم إجراء هذا الحساب داخل منطقة اهتمام محددة.

الكلمات المفتاحية:

النقاط الكمومية
المزدوجة
تفاعل التبادل

قمنا بتقييم هذه النتائج فيما يتعلق بحالة استخدام حالات فوك-داروين (FD) وحل معروف بدقة لمعادلة شرودنجر أحادية البعد. يكشف دراستنا عن فعالية الطريقة المطبقة ويقدم تحقيقًا مثيرًا للاهتمام حول موثوقية ودقة الطريقة الحسابية المستخدمة.

الحوسبة الكمومية

1. INTRODUCTION

Highly interesting systems for investigating basic quantum physics and investigating uses in quantum electronics are double quantum dots (DQDs). They show great potential for application in the building of quantum computers[1-3]. These little objects have charge carriers restricted in three dimensions, which makes them occasionally compared to manufactured atoms[4].

Usually, it is used on a 2D electron gas (2DEG), the confinement is achieved by the means of electrical gating or etching processes. Research on conductance and spectroscopy has focused especially on quantum dots, which have diameters almost equal to the Fermi wavelength and show unusual energy levels.[5, 6]. Furthermore, measurements are carried out connected to the spectroscopy[7]. Starting from zero, one can have incremental control over the electron count in GaAs heterostructures by varying the dots[8, 9]. Fundamental in quantum computation, qubit encoding has been proposed using several approaches. Notably, semiconductor quantum dots hosting spin qubits are considered highly promising candidates due to their extended coherence time, high control fidelities[10-13], and scalability potential[14]. Design of spin-based quantum computers depends highly on the interaction between localized electrons. For instance, the first Loss-DiVincenzo (LDV) idea shows how to manipulate exchange interaction with electrical control to generate 2-qubit gates like SWAP and controlled NOT gates.[15].

The Kane proposal utilizes donor electron exchange to enable interactions between nuclear spins and generate two-qubit gates. On the other hand, the $|S\rangle$, $|T\rangle$ qubit proposal, as of late, utilizes controlled exchange splitting for single-qubit gates[14, 16]. Different qubit structures, such as the single-spin qubit and the exchange-only qubit, have been suggested, demonstrating the variety of techniques[15, 17-24]. Various qubit designs have been suggested, such as the single-spin qubit which is represented by the spin states of an electron[15, 17]. The ST_0 qubit employs $|S\rangle$,and $|T\rangle$ states of 2-electron configurations as the computational basis[10]. Furthermore, the

exchange(J) , only qubit[18-20] and its alternate counterpart, the resonance-exchange qubit[21, 25], can be realized by utilizing particular 3-electron states in triple quantum dots and hybrid qubits[22-24]. Silicon is becoming increasingly recognized as a highly promising material for hosting a spin quantum-information processor, as it possesses remarkable spin coherence qualities in its bulk[26, 27]. The native form of the substance consists of a limited number of nuclear spins (5% of ^{29}Si, with a spin of 1/2), which can be further purified isotopically.

The feeble hyperfine interaction between conduction electrons (or electrons attached to donors) and individual nuclei in silicon hinders electron-spin decoherence generated by hyperfine interaction[28], which is a major factor in III-V materials such as GaAs[29]. The silicon additionally demonstrates a negligible spin-orbit interaction[30] and does not possess piezoelectric interaction, which results in a delayed relaxation of electron spin caused by phonons. However, silicon's conduction band structure, which consists of six equivalent minima, poses a significant disadvantage[31]. The motivation for this research comes from recent progress in experimental development of spin qubits in (Si/SiO_2) [32-34]. Our calculations focus on determining the exchange interaction (J) and tunnel coupling of electrons in double quantum dot (DQD) structures within a silicon/silicon dioxide (Si/SiO_2) system. We would expect a more significant absolute value of J-interaction. Firstly, we utilize COMSOL Multiphysics to determine the wave functions by employing various potentials. Subsequently, we conduct a calculation of J-interaction by employing approximation techniques to determine the suitability of the HL and HM models in estimating exchange splitting in a silicon double dot. Afterwards, we will compare the results with the analytically solvable double-well potential solutions (CA) and the Fock-Darwin states (FD)[35, 36]. The structure of this document is as follows. In section 2, we employ the theoretical approach to determine the wave functions using the COMSOL Multiphysics tool. The calculation results are displayed in section 3, showcasing the J-interaction as a variable of inter-dot distance. This is achieved through the utilization of the HL and HM methods. Ultimately, we bring our paper to a close in section 4.

2.THEORETICAL FORMALISM

Let's examine a DQDs positioned at the interface between silicon (Si) and silicon oxide (SiO2), with its development direction aligned along the z-axis. The Hamiltonian describing the effective mass of two electrons in a double quantum dot (DQDs) that is given by [37]:

$$H = \sum_{i=1,2} h_i + \frac{e^2}{k r_{12}} \qquad (1)$$

where i=1,2 represent the labels for the two electrons, h_i refers to the single-particle Hamiltonian, k is the effective dielectric constant, which takes into account the image charge in the surrounding SiO_2 and is calculated as $k = (\varepsilon_{Si} + \varepsilon_{SiO2})/2$. r_{12} represents the distance between the two electrons. The Hamiltonian that describes the behavior of a single electron is:

$$\hat{h_i} = \hat{T_i} + V_{ri} + eEx_i + g_{eff}\mu_B BS_{iz} \quad (2)$$

$$\hat{T_i} = \frac{1}{2m}\left[p_i - \frac{e}{c} A(r_i)\right]^2 \qquad (3)$$

The effective mass in the traverse direction (z and −z direction) is denoted by m and has a value of $0.191m_e$ for Si/SiO_2 DQDs. The vector potential A(ri) corresponds to the magnetic field in the z direction. A is exactly the same as B, using the coordinates (-y, x, 0/2). However, our discussion will exclude the consideration of the vector potential because it is not applicable to solvable solutions, which are limited to one-dimensional situations. The electric field, represented by E, is oriented in the x-direction to shift the potential well in the z-direction. While "V(ri)" represents the potential confinement of electrons in the (DQDs), the final term in equation (2), g_{eff}, corresponds to the effective g-factor, which is, μ_B Bohr magneton.

They examine a configuration comprising of two quantum dots connected horizontally, where each dot houses a single electron in the conduction band. The localization of electrons in (DQDs) system can be precisely determined using a two-dimensional potential function, primarily responsible for the intense confinement in the z-direction [38]. Nevertheless, the existence of solvable double-well potential solutions is restricted to 1D solutions [36, 39-43] and has not yet been extended to 2D solutions. Hence, in this study, we will utilize the approach proposed by Caticha [36], to solve the 1D double-well potential Schrödinger equation.

$$V^{CA}(x) = -2\frac{(a^2-b^2)[a^2\cosh^2(bx)+b^2\sinh^2(ax)}{[a\cosh(ax)\cosh(bx)-b\sinh(ax)\sinh(bx)]^2} \quad . \qquad (4)$$

While the Fock-Darwin states do not precisely fulfill the Schrödinger equation for the double well potential function, they are commonly used to describe the state of a single electron in (DQDs). This is based on the assumption that the potential function can be estimated as bi-quadratic when the electron is in the ground energy state and is close to the bottom of the well. [38].

$$V^{BQ}(x) = \frac{1}{2}m\omega_0^2(\min[(x-d)^2,(x+d)^2]) \qquad (5)$$

The energy difference between $|T_0\rangle$ and $|S\rangle$ state is the essential physical parameter that allows for quantum computing in the ST_0 qubit architecture. The J- interaction refers to the phenomenon of energy splitting. $J = E_{T0} - E_S$. If the DQD contains two electrons and their interaction is limited to the Coulomb interaction there will be four spin eigenstates in a uniform magnetic field. These states are $|S\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$ with a total spin of S = 0) and ($|T_{0,+,-}\rangle = \frac{1}{2}\ |\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle, |\uparrow\uparrow\rangle, |\downarrow\downarrow\rangle$ with a total spin of S = 1.

The study will provide a detailed explanation of the two approaches, HL and HM , that can be employed for calculating the J- interaction.

$$|S/T_0\rangle = \frac{|\psi_L(1)\psi_R(2)\rangle \pm \psi_L(1)\psi_R(2)\rangle\rangle}{\sqrt{2(1\pm\ell^2)}} \qquad (6)$$

A. Heitler-London Approach

Considering only the states with a single occupant, namely $|S\ (1,\ 1)\ \rangle$ and $|T_0(1,\ 1)\rangle$, and assuming the existence of a doubly occupied singlet state, the HL technique provides the most direct calculation of the exchange interaction. By considering our system as a pair of artificial atoms that exhibit behavior like hydrogen, we can use the Heitler-London approach, also known as the valence orbit approximation, to calculate the exchange energy component. $|S\rangle$ and $|T_0\rangle$ states are indicated by[44].

The overlap between the left $|\psi_L\rangle$ and right $|\psi_R\rangle$ dot single electron states is denoted by ℓ and is defined as the inner product of the state $\ell = \langle\psi_L|\psi_R\rangle$. J_{HL} which refers to the energy difference

between |S⟩ and |T_0⟩ state, can be represented by

$$J_{HL} = \langle T_0|\hat{H}|T_0\rangle - \langle S|\hat{H}|S\rangle \quad (7)$$

which can be rewritten in a simpler form as follows:

$$J_{HL} = \frac{2\ell^2}{1-\ell^4}(W_v + D_0 - \frac{1}{\ell}E_0) \quad (8)$$

The explicit form of each element in eq. (8) can be shown as follows :

Wv is the kinetic energy gain of the singlet state.

$$W_v = (u - \frac{w}{\ell}) \quad (9)$$

$$u = V_{qL}^{LL} + V_{qR}^{RR} = \langle \psi_L|V_q - V_L\,|\psi_L\rangle + \langle \psi_R|V_q - V_R\,|\psi_R\rangle \quad (10)$$

$$w = V_{qL}^{RL} + V_{qR}^{LR} = \langle \psi_R|V_q - V_L\,|\psi_L\rangle + \langle \psi_L|V_q - V_R\,|\psi_R\rangle \quad (11)$$

$$D_0 = \langle \psi_L(1)\psi_R(2)|\hat{C}\,|\psi_L(1)\psi_R(2)\rangle \quad (12)$$

$$E_0 = \langle \psi_L(1)\psi_R(2)|\hat{C}\,|\psi_R(1)\psi_L(2)\rangle \quad (13)$$

D_0 represents the Coulomb interaction contribution, while E_0 represents the exchange Coulomb interaction. It is evident that when the precise solutions and their matching potential functions are utilized in any scenario.

B. Hund-Mulliken Approach

Let us now examine the HM method for molecular orbitals[45]. This extends the HL method by incorporating the 2 doubly occupied states, which are characterized by their spin singlet nature. This results in the presence of four dimensions within the orbital Hilbert space. Consequently, two additional states, |S (2, 0) ⟩ and |S (0, 2)⟩, which are doubly occupied, are incorporated into the Hamiltonian *H*. As a result, a matrix of size 4 × 4 is obtained. The HM approach, with its more rigorous estimation, has been proven to provide a more accurate estimation of the J- interaction [37, 38]. Firstly, it is necessary to perform the orthonormalization of the wave function for a single electron. This involves using two functions.

$$\phi_L = L(x) \quad (14a)$$

$$\phi_R = \frac{1}{\sqrt{1-\ell^2}}\big(R(x) - \ell\, L(x)\big) \quad (14b)$$

The DQDs has two-electron states with orthonormalized wave functions representing single electron states. These states consist of two doubly occupied singlets, denoted as |S (2, 0) ⟩. It is feasible to generate the (1,1) , |T(1, 1)⟩, the (1,1) , |S (1, 1)⟩, and |S (0, 2)⟩. The spatial wave functions for the three

singlet and the (1, 1) triplet can be expressed as follows:

$$\psi^{d}_{L/R}(r_1, r_2) = \phi_{L/R}(r_1)\phi_{L/R}(r_2) \quad , \tag{15}$$

$$\psi^{(1,1)}_{S/T}(r_1, r_2) = \frac{1}{\sqrt{2}}[\phi_L(r_1)\phi_R(r_2) \pm \phi_L(r_2)\phi_R(r_1)] \quad . \tag{16}$$

The states that are occupied by two particles are denoted by the superscript. The Hamiltonian expressed in the S(2, 0), S(0, 2), S(1, 1), T (1, 1) basis can be represented as follows

$$H = \begin{bmatrix} 2\varepsilon_L + U & X & W & 0 \\ X & 2\varepsilon_R + U & W & 0 \\ W & W & V_s & 0 \\ 0 & 0 & 0 & V_T \end{bmatrix} \quad , \tag{17}$$

Where

$$\varepsilon = \varepsilon_R - \varepsilon_L \tag{18}$$

$$\varepsilon_R = \langle\phi_R|h_0|\phi_R\rangle \quad , \qquad \varepsilon_L = \langle\phi_L|h_0|\phi_L\rangle \tag{19}$$

where h_0 the single particle Hamiltonian.

$$X = \left\langle\psi^{d}_{L/R}\middle|\hat{C}\middle|\psi^{d}_{R/L}\right\rangle \tag{20}$$

$$U = \left\langle\psi^{d}_{L/R}\middle|\hat{C}\middle|\psi^{d}_{L/R}\right\rangle \quad , \tag{21}$$

$$W = \frac{1}{\sqrt{2}}\left\langle\psi^{d}_{L/R}\middle|\hat{C}\middle|\psi^{(1,1)}_{s}\right\rangle , \tag{22}$$

$$V_s = \left[\varepsilon + \frac{1}{2}\left\langle\psi^{(1,1)}_{s}\middle|\hat{C}\middle|\psi^{(1,1)}_{s}\right\rangle\right] \tag{23}$$

$$V_T = \left[\frac{1}{2}\left\langle\psi^{(1,1)}_{T}\middle|\hat{C}\middle|\psi^{(1,1)}_{T}\right\rangle\right] \tag{24}$$

The energy of individual particles in the left(L) and right(R)dots in the previous matrix are denoted by ε_L and ε_R , respectively. The difference between them in ε which serves as the detuning parameter. U represents the Coulomb repulsion that occurs on-site. V_S and V_T are the Coulomb energies associated with the |S⟩ and |T⟩ states of (1,1) respectively. $\psi^{(1,1)}_{T/S}$ is formed by using orthogonalized single-electron orbitals. X can be likened to an interdot Coulomb exchange integral and a W Coulomb matrix element. All these

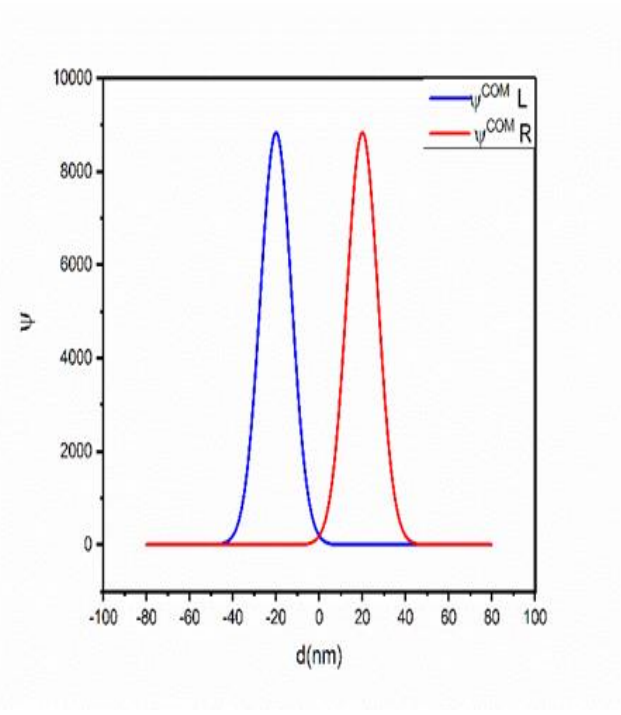
quantities can be represented in terms of the corresponding matrix elements between the initial, non-orthogonal, L, and R orbitals $\phi_{L/R}$. These matrix elements, referred to as D_0, E_0, X, etc., represent the naked orbital interactions. The energy diagram for the 2-dot system can be produced by extracting the eigenvalues and eigenvectors from the 4×4 Hamiltonian matrix (eq. (17)). The energy value of the state eigenvector is directly related to each corresponding eigenvalue. A mixed state can be represented by a state vector that has distinct probabilities associated with different bases. Alternatively, it can also be a pure basis state. Calculating the numerical values for every matrix element allows one to approximate the energy of every electron state by considering variables including potential well separation and detuning strength. One can deduct the energy value of |T⟩ state from that |S⟩ state to determine the (J_{HM}) between the $|S\rangle$ and $|T_0\rangle$ state.

Integrations using FD states can sometimes yield analytical solutions for both the Coulomb and kinetic terms. Nevertheless, the immense intricacy of the wave functions represented by Caticha[36], which are totally solvable, renders analytic solutions unachievable. Consequently, numerical integration methods were employed as an alternative. By utilizing COMSOL Multiphysics, we conducted a study on the exchange coupling in the ST_0 qubit architecture. Through this investigation, we successfully determined the wave functions for both the left $\boldsymbol{\psi_L^{COM}}$, and right $\boldsymbol{\psi_{R,}^{COM}}$ states, and subsequently performed calculations on the exchange reactions ,considering both the potential of V^{BQ} nature and V^{CA}. This study involved a comparison between the COMSOL Multiphysics wave functions approach and the Fock-Darwin states as represented by equation (5). Furthermore, the V^{CA} can be solved exactly, as shown in equation (4).

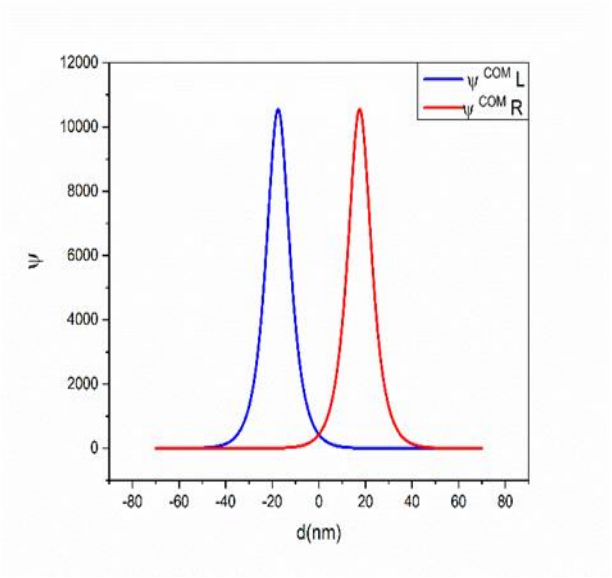
3. RESULTS AND DISCUSSION

We calculate the J-interaction between the $|T$ and $|S\rangle$ states in a linked DQDs near a (Si/SiO_2) interface, by of the COMSOL Multiphysics wave functions in the specific domain. Maintaining the same spacing between dots, the well depth and possible barrier of the V^{BQ} were tuned to match the V^{CA}. Our estimates have been done using dot sizes that are practically feasible in tests. We study the effects on exchange in symmetric DQDs of confinement energy and inter-dot distance.

Additionally, the impact of inter-dot distance on the J-interaction is determined using the HL and HM approaches. Lastly, the influence of different types of potentials on the exchange coupling is discussed**.** This section displays the wave function employed by the COM program to compute the exchange interaction(*J*) for this project under two distinct potentials, namely V^{BQ} and V^{CA}. It also compares this solution with the FD states and the analytically solvable wave function proposed by Caticha[36]. The exchange interaction (*J*)is determined as a function of the inter -dot distance (d) between the dots while keeping the well depth constant. The well depth and potential barrier are selected to have similar magnitudes as the V^{BQ} employed for FD states (with $\hbar\omega_0 = 7.658meV$). The COMSOL wave functions $\psi_L^{COM}, \psi_{R,}^{COM}$, in Fig 1. Fig 1 (b) illustrates that the wave functions CA was most focused at the interdot region compared to FD's. Consequently, one would anticipate a robust interdot Coulomb interaction over extended distances and a high likelihood of interdot hopping. The presence of a dense concentration of probability at the interdot area was deemed a typical in cellular automata due to two specific reasons. The wave functions were expected to display symmetry because of the symmetric characteristics of both the left(L) and right(R) wells. In addition, the V^{CA} exhibited a greater degree of confinement compared to the V^{BQ}, although having identical barrier height and interdot distance. However, this attribute can be clarified by the existence of a neighboring secondary potential well. This allows the particle located in one well to experience quantum tunneling across the potential barrier and appear in the adjacent well.



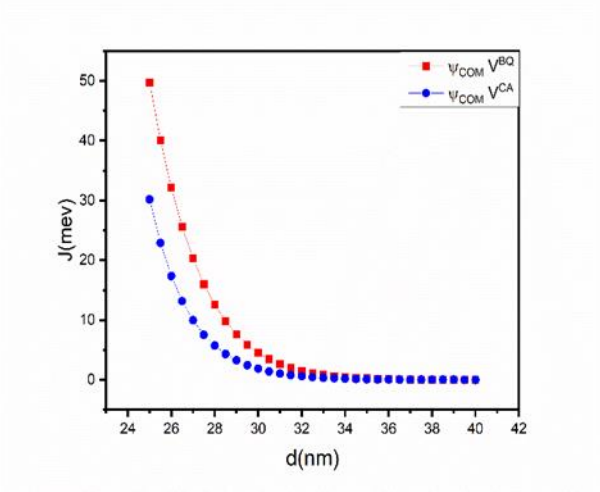
(a)



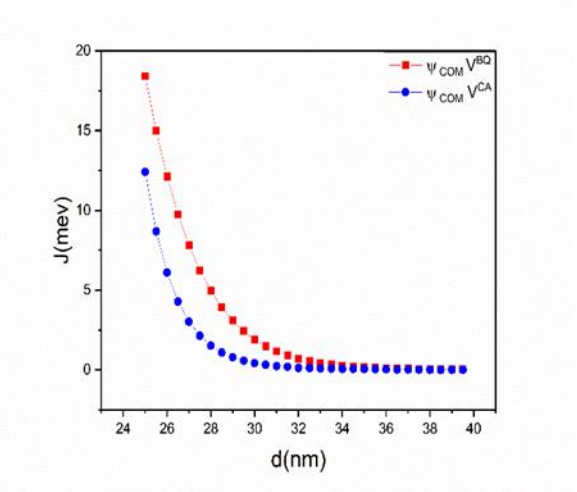
(b)

Fig 1: COMSOL wave functions ψ_L^{COM}, $\psi_{R,}^{COM}$, (a) corresponding to bi-quadratic potential V^{BQ} , (b) corresponding to CA potential.

In Fig 2, the most prominent observation is the estimated exchange interaction(J) as determined by the COMSOL Multiphysics wave function when applied. The V^{CA} exhibited a notably greater magnitude compared to that calculated by FD states with V^{BQ}, owing to two main factors: (i) the elevated concentration of $\psi_L^{COM}, \psi_{R,}^{COM}$ achieved through the utilization of the CA potential V^{CA} (Fig 1 (b)) derived from the V^{BQ} (Fig1(a)), and (ii) the more overlap resulting from the V^{CA} function, which surpasses that of the V^{BQ} with equivalent barrier height and inter-dot distance. Furthermore, Fig.2 demonstrates that as the distance between the dots increased, the level of interaction between them decreased. Dot degree of overlap between the wave functions of the left and right dots (Ψ_L , Ψ_R)clarifies the obtained result. Reduced overlap between the left(L) and right(R) dot resulting from increased spacing between the dots reduced Coulomb interaction and inter-dot hopping, therefore weakening the J-interaction at last.



(a)



(b)

Fig 2: Calculated exchange interaction vs. inter-dot distance (d) by sing COMSOL Multiphysics

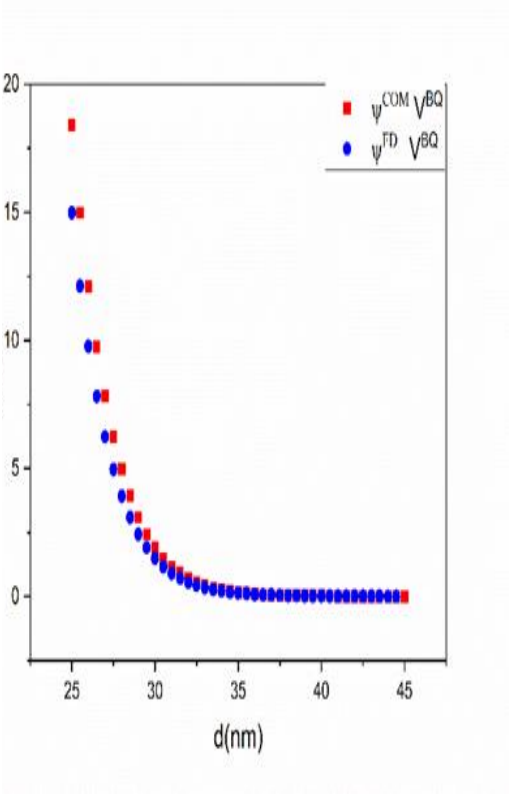
wave functions for bi-quadratic potential V^{BQ} and Caticha's potential V^{CA} (a) HL approach, (b) HM approach.

Furthermore, due to the limited scope of the HL approach, which only considered the |S (1, 1) ⟩ and |T_0⟩ states, the omission of the |S (2, 0) ⟩ and |S (0, 2) ⟩ states may have introduced some level of error in the calculation of the J-interaction. Consequently, the HM technique yielded a more precise outcome for the J- interaction due to the inclusion of the |S (2, 0)⟩ and the |S (0, 2)⟩ states in the Hamiltonian H. Fig 2 (b) demonstrates that the (*J*)predicted by the HL approach was at least one times greater than that predicted by the HM approach, while observed in previous studies the HL approach was larger by at least five times than that predicted by the HM approach .

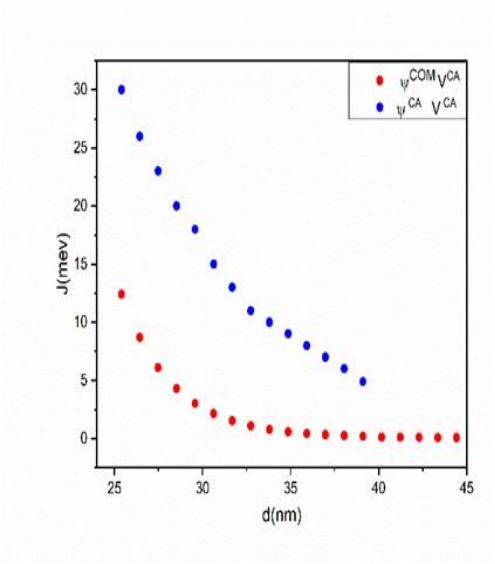
Due to our utilization of COMSOL Multiphysics wave functions and the mathematical approach employed to determine the components of the 4×4 Hamiltonian matrix, this indicates that incorporating the doubly occupied state in the HM method has a substantial impact on the magnitude of the (J_{HM}) provided a significantly more precise estimation of (J_{HL}) compared to the HL model.

Specifically, the exponential decay occurs when the interdot distance d is large, regardless of whether the HL or HM techniques are used. Nevertheless, we notice a significant and rapid growth in the J- interaction when the distance (d) reached *25 nm* in both the HL and HM approximations. This phenomenon was unrealistic according to previous studies [34, 35]. Upon further examination, it was observed that the exponential increase mentioned earlier was less prominent in the HM approximation compared to the HL approximation. This suggests that the HM approximation yields a most accurate result, especially when the distance between the dots is small. Furthermore, it was noted that the (*J*) obtained was within the *meV* range, rather than the μ *eV* range commonly reported in earlier investigations [34, 35]. The conflicting outcomes can be ascribed to the utilization of the one-dimensional wavefunction instead of the two-dimensional wavefunction when characterizing the single electron state in DQD in the proposed methodology. Nevertheless, the J-interaction with the COMSOL Multiphysics wave function produced distinct qualitative outcomes in both HL and HM approaches. This is evident when comparing the acquired findings with those from previous investigations, which utilized the

identical potential and quantum dot sizes, as depicted in Fig 3, Fig 4. In Fig 3 a, the J- interaction exhibited similar characteristics in both our calculations using the HL approach and the Fock Darwin states. This similarity can be attributed to the equal overlap between the COMSOL states and FD states. Nevertheless, a discrepancy arose when employing Caticha's wave function, as depicted in Fig 3b. Similarly, the Hand-Millikan technique yielded consistent results with the Fock Darwin examples, as depicted in Fig 4 a.



(a)



(b)

Fig 3: Comparison between exchange coupling by using COMSOL states , FD states and, Caticha's wave function .(a)The solid blue line corresponds to (*J*) calculated by FD states ψ^{FD} , The O-red line corresponds to the $\psi_L^{COM}, \psi_{R,}^{COM}$ along with V^{BQ}. (b)The O- blue line corresponds to (*J*) calculated by Caticha's wave function ψ^{CA} , The solid red line corresponds to the $\psi_L^{COM}, \psi_{R,}^{COM}$ along with V^{CA}

4. CONCLUSION

From the Coulombic interactions among the system's electrons, one gets the interaction J. Using the Hitler-London and Hand-Millikan approximation, we have determined the exchange coupling between two electrons in double quantum dot configurations within a Si/SiO2 heterostructure. The J- interaction for the singlet-triplets qubit ST_0 was computed using the wave functions produced by COMSOL Multiphysics. This computation considered several possible values including $V^{CA}$and V^{BQ}. When

compared to results provided from conventional methods, the J-interaction acquired from the states of COMSOL shows some interesting properties. These comprise a non-monotonic curve of (J) as well as a significant size of (J) resulting from a high interdot probability density. When comparing the findings of standard techniques using finite difference (FD) states with a V^{BQ} with the V^{CA}, one finds notable differences.

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