Universal set of quantum gates for double-dot exchange-only spin qubits with intradot coupling

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Abstract
We present a universal set of quantum gate operations based on exchange-only spin qubits in a double quantum dot, where each qubit is obtained by three electrons in the (2,1) filling. Gate operations are addressed by modulating electrostatically the tunneling barrier and the energy offset between the two dots, singly and doubly occupied respectively. We propose explicit gate sequences of single qubit operations for arbitrary rotations, and the two-qubit controlled NOT gate, to complete the universal set. The unswitchable interaction between the two electrons of the doubly occupied quantum dot is taken into account. Short gate times are obtained by employing spin density functional theory simulations.

Keywords: spin qubit, quantum dots, universal set, quantum gates

(Some figures may appear in colour only in the online journal)
spins removes the need for an inhomogeneous field as interactions between adjacent electron spins suffice for all one and two qubit operations [4, 10]. A compact variant of the three spin qubit in (1,1,1) states of three QDs proposed by DiVincenzo [10] has been recently developed for (2,1) states in double QDs, with total spin states belonging to the subspace $S = 1/2$ and $S_z = \pm 1/2$ [11–13] and it was experimentally demonstrated in [14, 15]. Differently from the (1,1,1) system, the (2,1) system offers the advantages of higher protection from hyperfine interactions of the singlet and triplet state in one of the two dots [7], and compact fabrication —only two dots instead of three [16, 17]. A possible drawback consists of more constrained interactions, as it is not possible to tune separately the exchange of the two electrons sharing the same site with the third electron spin. In addition, exchange interaction between the electrons in the doubly occupied dot cannot be effectively turned off. While a case limited to the first aspect has been considered in the past [11], the demonstration of a universal set of quantum logic gates when the inescapable intra-dot interaction of a realistic QD is included, is still lacking. The single qubit operations proposed in [11] for extending the ports are incorrect (see appendix A). Universal quantum computation in an alternative scheme, where spin and valley degrees of freedom of two electrons in two QDs are exploited, has been proposed [18].

Here, we report on a universal set of gates for two exchange-only qubits in double QDs with fixed intradot exchange, generated by single qubit rotations along $X$ axis ($R_X(\phi)$ gate) and $Z$ axis ($R_Z(\theta)$ gate), and a controlled-NOT (CNOT) gate based on two qubits. For each gate interaction, sequences supplied with operation times are calculated by employing a genetic algorithms which takes into account the intradot interaction of the electrons in the doubly occupied QD. One and two qubits systems are modeled by effective Hamiltonians and a dynamical evolution operator is used to find the overall effect of the interactions. We developed and used a search algorithm to find the interactions sequences. A spin density functional theory (SDFT) simulator is used to estimate the parameters of the effective Hamiltonians, revealing short gate times for high performances.

1. The three-electrons in a double quantum dot exchange-only spin qubit

The qubit is composed of a double QD with two electrons in one QD (left) and one electron in the other QD (right) and its energy landscape is shown in figure 1. Let us now define the logical basis, enumerating the possible transitions between the three electrons spin states that can be induced by manipulations which preserve total spin angular momentum. The Hilbert space of three electron spins has eight possible spin states: the total spin eigenstates form indeed a quadruplet with $S = 3/2$ and $S_z = \pm 3/2$, $\pm 1/2$ and two doublets each with $S = 1/2$ and $S_z = \pm 1/2$, where the square of the total spin is $\hbar^2S(S + 1)$ and the $z$-component of the
total spin is $\hbar S_z$. The logical qubit space is chosen to be in the two-dimensional subspace with $S = 1/2$, $S_z = -1/2$. We point out that only states with the same $S$ and $S_z$ can be coupled by spin independent terms in the Hamiltonian. The value of the total angular momentum operator $S$ specifies whether the decoherence free subsystem qubit has leaked; $S = 1/2$ is unleaked while $S = 3/2$ is leaked. The logical basis $\{|0\rangle, |1\rangle\}$ written via Clebsch–Gordan coefficients is given by

$$
|0\rangle \equiv |S\rangle \downarrow, \quad |1\rangle \equiv \frac{1}{\sqrt{3}} \left| T_0 \right\rangle \downarrow \uparrow, \quad \frac{2}{\sqrt{3}} \left| T_- \right\rangle \downarrow \uparrow,
$$

where $|S\rangle$, $|T_0\rangle$ and $|T_-\rangle$ are respectively the singlet and triplet states of the pair in the left dot, in combination with the angular momentum state of the electron spin localized in the right dot.

The double quantum dot exchange-only spin qubit is described by an Hubbard-like model that, following the Schieffer–Wolff projection operator method, could be recast in a spin Hamiltonian [13]. The effective Hamiltonian is expressed as a sum of exchange interactions between each pair of electron spins

$$
H_{\text{eff}} \approx J_{13} \mathbf{S}_1 \cdot \mathbf{S}_3 + J_{23} \mathbf{S}_2 \cdot \mathbf{S}_3 + J_{12} \mathbf{S}_1 \cdot \mathbf{S}_2
$$

with exchange interactions

$$
J_{13} \approx \frac{1}{E_{(012)} - E_{(111)}} 4 \left( t_{13} - J_{13}^1 \right)^2 - 2 J_{13}^3,
$$

$$
J_{23} \approx \frac{1}{E_{(102)} - E_{(111)}} 4 \left( t_{23} - J_{23}^1 \right)^2 - 2 J_{23}^3,
$$

$$
J_{12} \approx \left( \frac{1}{E_{(201)} - E_{(111)}} + \frac{1}{E_{(021)} - E_{(111)}} \right) 4 \left( J_{12}^1 \right)^2 - 2 J_{12}^3,
$$

where $E_{(a b)}$ are the energies with $a$ ($b$) electrons in the ground state (first excited) of the left dot and $c$ electrons in the second dot. The parameters $t_{ij}$ are the tunneling rates, $J_{ij}^c$ account for the occupation-modulated hoppings, $J_{ij}^m$ are the spin-exchange terms from the energy level $i$ to $j$ as defined in [19].

Differently from inter-QD interactions governed by tunable $J_{13}$ and $J_{23}$, the intra-QD interaction $J_{12}$ can not be effectively controlled. In fact $J_{12}$ does not depend on the tunneling rates (see equation (3)) whose values can span several order of magnitudes and strongly control $J_{13}$ and $J_{23}$. We assumed max ($J_{12}$) = max ($J_{13}$) = $J_{\text{max}}$ and we set a realistic value for $J_{12} = J_{\text{max}}/2$ to model the control ineffectiveness. The exchange interactions $J_{13}(t)$ and $J_{23}(t)$ are assumed to have instantaneous turn-on and turn-off as in [11]. Actual electronic instrumentation can assure switching times of gate potentials in the hundreds of picoseconds range thus producing exchange interaction switching times in the same range.

In order to clarify how tunneling rates $t_{ij}$ and the energy detuning potential $\varepsilon$ between the two QDs can control the qubit, the simplified Hamiltonian for a double quantum dot exchange-only spin qubit as a function of the inter-QD tunneling rates and of the inter-QD energy detuning reported in [13] is used, by formally providing the results previously suggested only heuristically in [12]. We consider a basis with an intermediated state $|E\rangle \equiv |1\rangle |S\rangle$ in addition to the logical states $|0\rangle$ and $|1\rangle$. The state $|E\rangle$, with one electron in the left dot and two electrons in the right dot featuring the same total angular momentum $S^2$ and $S_z$ of $|0\rangle$ and $|1\rangle$, is directly involved in the physical process that leads to transitions between the two logical states. Equation (4) reports the effective Hamiltonian in the basis
where the inter-QD detuning $\varepsilon$ is introduced

$$
\varepsilon = -\varepsilon_1 - \varepsilon_2 + \varepsilon_3 + \varepsilon_4.
$$

The matrix representation of $H^{3\times 3}$ is given by

$$
H^{3\times 3} = \begin{pmatrix}
-\frac{3}{4} J_{12} & -\frac{\sqrt{3}}{4} (J_{13} - J_{23}) & \frac{3}{8} (J_{23} - J_{13} + J_{12}) \\
-\frac{\sqrt{3}}{4} (J_{13} - J_{23}) & \frac{1}{4} J_{12} - \frac{1}{2} (J_{13} + J_{23}) & -\frac{\sqrt{3}}{8} (J_{13} + 3J_{23} - J_{12}) \\
\frac{3}{8} (J_{23} - J_{13} + J_{12}) & -\frac{\sqrt{3}}{8} (J_{13} + 3J_{23} - J_{12}) & -\frac{3}{4} J_{12} - \varepsilon
\end{pmatrix}.
$$

$H^{3\times 3}$ eigenvalues are reported in figure 2 as a function of $\varepsilon$ in three different cases: both tunneling rates are zero; $t_{13}$ is on and $t_{23}$ is off; $t_{13}$ is on and $t_{23}$ is off. Transitions from logical state $|0\rangle$ to $|1\rangle$ can be induced by first setting $\varepsilon$ to the avoided crossing between $|0\rangle$ and $|E\rangle$ when $t_{13}$ is switched on (solid red curves in the right box) and then switching $t_{13}$ off and on. Then, changing $\varepsilon$ to the avoided crossing between $|E\rangle$ and $|1\rangle$ when $t_{23}$ is on (dashed blue lines in the left box) and pulsing $t_{23}$ on and off. The same argument can be applied to induce transition conversely from logical state $|1\rangle$ to $|0\rangle$.

2. Gate sequences for a single qubit gate generating arbitrary rotations

In the following the qubit sequences are calculated under the assumption that a sufficiently high number of external inputs (electrostatic gates) are available to finely control the band structure of the double QDs, producing a perfect control of $J_{13}$ and $J_{23}$.

A single qubit gate which performs arbitrary rotations in the subspace $\{|0\rangle, |1\rangle, |E\rangle\}$ can be found by using the Euler angle method, if rotations by arbitrary angles about two orthogonal axes are available. Here we present two single-qubit gates performing rotations along $Z$ and $X$ axes.

The first single-qubit gate $R_Z(\theta)$, which generates rotations by $\theta$ along the $Z$ axis, has a matrix representation reported in figure 3. The $R_Z(\theta)$ is implemented by a three-step sequence (see figure 3) where the first step of the sequence features $J_{13} = J_{12} = J_{23} = J_{13}^\text{max}$ for $t_{13}$ time, the second one $J_{23} = J_{12} = J_{13}^\text{max}$ for $t_{23}$ time and the third one $J_{12} = J_{13}^\text{max}$ for $t_{12}$ time.
The unitary evolution matrix of each step is

$$U_{ij}(t_{ij}) = \exp\left( -i2\pi H^{2\times2}(J_{ij}) t_{ij}/\hbar \right),$$

where $H^{2\times2}(J_{ij})$ corresponds to the first two rows and columns of the effective Hamiltonian reported in equation (4). The product between the unitary evolution matrix of each step, i.e. $U_{12}(t_{12})U_{23}(t_{23})U_{13}(t_{13})$, is the evolution matrix of the entire sequence. By imposing

$$U_{12}(t_{12})U_{23}(t_{23})U_{13}(t_{13}) = R_Z(\theta)$$

and the non-negativeness of $t_{13}$, $t_{23}$ and $t_{12}$, the analytical expressions for minimum step times $t_{13}$, $t_{23}$ and $t_{12}$ are (see derivation in appendix B)

$$t_{13}(\theta) = t_{23}(\theta) = \begin{cases} \frac{3\theta}{10\pi} + \frac{1}{5} & \text{with } 0 < \theta < \frac{2\pi}{3}, \\ \frac{3\theta}{10\pi} - \frac{1}{5} & \text{with } \frac{2\pi}{3} < \theta < 2\pi, \end{cases}$$

$$t_{12}(\theta) = 2 - \frac{\theta}{\pi} \quad \text{for } 0 < \theta < 2\pi$$

in units of $\hbar/J_{\max}$. The resulting total time $t_{R_Z}(\theta)$ for a $R_Z(\theta)$ gate is:

$$t_{R_Z}(\theta) = t_{13} + t_{23} + t_{12} = \begin{cases} \frac{2}{5} \left( 6 - \frac{\theta}{\pi} \right) & \text{for } 0 < \theta < \frac{2\pi}{3}, \\ \frac{2}{5} \left( 4 - \frac{\theta}{\pi} \right) & \text{for } \frac{2\pi}{3} < \theta < 2\pi, \end{cases}$$

which depends on $\theta$.

The second single-qubit gate $R_X(\phi)$, which generates rotations by $\phi$ along the $X$ axis, has a matrix representation and it is implemented by a two-step sequence reported in figure 4. For the $R_X(\phi)$ gate we have to impose
\[ R_X(\phi) = \begin{pmatrix} \cos(\phi/2) & -i \sin(\phi/2) \\ -i \sin(\phi/2) & \cos(\phi/2) \end{pmatrix} \]

and, following the same approach used to derive the sequence for \( R_Z(\theta) \), the resulting analytical expressions of minimum \( t_{13} \) and \( t_{23} \) are

\[ t_{13}(\phi) = \frac{4}{5} - \frac{1}{\sqrt{3}} \frac{\phi}{2\pi} , \]
\[ t_{23}(\phi) = \frac{4}{5} + \frac{1}{\sqrt{3}} \frac{\phi}{2\pi} \]

with \( 0 < \phi < 2\pi \). The total time \( t_{RX} \) of an \( R_X(\phi) \) gate is

\[ t_{RX} = t_{13} + t_{23} = \frac{8}{5} \]

which does not depend on \( \phi \).

3. Gate sequences for an exact CNOT

When considering two qubit operations, the two most significant configurations, where the number of inter-qubit connections is maximized, are reported in figure 5. Dropping the \( \text{eff} \) superscripts, the effective Hamiltonian of the couple of qubits in the \( K \) configuration is:

\[ H_{ab}^K = H_a + H_b + H_{int}^K \]

(for \( K = A, B \)), where \( H_a, H_b \) are the effective Hamiltonians of the single qubits \( a \) and \( b \), respectively (see equation (2)), and \( H_{int}^K \) is the interaction Hamiltonian. When configuration \( A \) is considered

\[ H_{int}^A = \sum_{i=1}^{2} J_{3a_i} S_{3a_i} \cdot S_{b_i} , \]

\[ \text{Figure 4. Matrix representation and exchange sequence implementing an } R_X(\phi) \text{ gate.} \]
whereas when $K = B$

$$H_{\text{int}}^B = \sum_{i=1}^{2} J_{i} \cdot S_i \cdot S_i.$$ (14)

The detailed derivation of the two qubit Hamiltonians is reported in appendix C. In order to obtain the exchange interaction sequences for the CNOT gates, we developed a search algorithm similar to the one described in [20], which is a combination of a simplex-based and a genetic algorithms. At each iteration of the search algorithm sequences become closer to the global minimum, featuring a reduced number of exchange steps and minimum interaction time per step. The qubit gate sequences for exact CNOT gates with fixed $J_{12} = J_{\text{max}}/2$ in both qubits for the configurations $A$ and $B$ are presented in figure 6. These sequences differs from those reported in [11] because ours account for ineffectively controlled interactions $J_{12}$ and because we provide exacts CNOTs instead of locally equivalent ones only. Note that the CNOT sequence for configuration $B$ reported in [11] provides only a correct locally equivalent CNOT because the corresponding single qubit operations needed to transform a locally equivalent CNOT to an exact CNOT are incorrect (see appendix A).

Moreover, dynamical corrected gates have been an actively investigated topic in the quantum dot spin qubits community [21–23] and such types of gates for double quantum dot exchange-only spin qubits will be considered in future works.

Figure 5. Couple of double quantum dot exchange-only spin qubits: configurations $A$ and $B$. Configurations differ for the orientation of qubit $a$ and, consequentially, for the inter-qubit connections.
$CNOT = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ \hfill (15)

**Figure 6.** Matrix representation and exchange sequence for an exact CNOT operation (up to a global phase) with fixed $J_{x,x} = J_{y,y} = J^{\text{max}}/2$ as a function of time $t$ for both configurations $A$ and $B$. 
4. Gate performances

Sequence times are evaluated for each gate by estimating $J^{\text{max}}$ through a simulator based on spin density functional theory (SDFT) [24]. For each couple of valleys of silicon [25] along $\Delta$ crystallographic directions, the simulator solves the Kohn–Sham equations in the effective mass approximation with anisotropic effective masses for both spin down and spin up populations [26]. When the eigenstates are obtained, the spin density concentrations are calculated and the effective potentials, namely the Hartree and the exchange-correlation potentials, are derived. For the exchange-correlation potential a local density approximation is assumed by using the parametrization presented in [27]. The total potential is then calculated self-consistently by solving the Poisson equation with the applied potentials from the external. The simulation ends when the error between the potential of the current iteration and that of the previous one is under a given tolerance.

To exemplify a realistic condition, we consider a double QD created in a Si nanowire featuring a rectangular section with a thickness $T_{\text{Si}} = 15$ nm and width $W = 60$ nm on a thick layer of SiO$_2$ as pictured in Figure 7. An Al$_2$O$_3$ layer with thickness $T_{\text{Al}_2\text{O}_3} = 40$ nm is deposited on the nanowire, and Al gates placed orthogonally to the nanowire direction and separated by $d_{\text{interGate}}$ are used to electrostatically confine electrons and control the inter-QD tunneling rates in the underlying silicon. In order to exploit quantum states from a single $\Delta$ valley, the valley splitting $\Delta E_{\text{v}}$ is enhanced to $\Delta E_{\text{v}} \sim 500 \mu$eV by increasing the electric field at the Si/Al$_2$O$_3$ interface by polarizing negatively the back gate. Simulations show that, when $d_{\text{interQD}} \equiv 2d_{\text{interGate}} = 40$ nm, the maximum effective interaction $J^{\text{max}} = 7.2 \mu$eV, providing for $R_X(\phi)$ an operation time of $t_{R_X} = 0.92$ ns irrespectively of $\phi$ and for $R_Z(\theta)$ times $t_{R_Z} \leq 1.38$ ns depending on $\theta$. Calculated CNOT gate times are $t_{\text{CNOT}} = 7.40$ ns and $t_{\text{CNOT}} = 10.9$ ns for two qubit configurations $A$ and $B$, respectively. Effects of charge and spin noise on the double quantum dot exchange-only spin qubit decoherence in natural silicon with DC pulsed gating scheme are reported in [28] where a fidelity of 99.995% for the $z$-rotations and 83% for the $x$-rotation have been estimated.

5. Summary

To conclude, we derived a universal set of quantum gates for double quantum dot exchange-only spin qubits with realistic non-vanishing intradot interaction, composed by arbitrary rotation gates and CNOT gates. Feasible interaction sequences have been reported for each
gate by taking into account not switchable interactions between the two electrons confined inside the same quantum dot. The two principal configurations have been studied by coupling two qubits. Under such conditions, we obtain the exact CNOT sequences for realistic qubits in both configurations, including single qubit operations. CNOT gate operation times in the range of 10 ns are predicted by employing SDFT simulations.

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Appendix A. Incorrect sequence presented in [11]

In the following, we explicitly evaluate the time evolution generated by the sequence of exchange operations proposed in [11] for configuration B, in which a locally equivalent CNOT gate is presented equipped with single-qubit operations to obtain an exact CNOT. In figure A1, we represent graphically the modulus and phase of the final transformation matrix quantified in the supplemental material of [11] for the configuration B. It includes the sequence to obtain a locally equivalent CNOT and single-qubit operations to obtain exactly a CNOT gate. While the locally equivalent CNOT presented in the supplemental material of [11] is correct, when the single-qubit operations proposed are applied before and after the central sequence, the 4 × 4 block for |00⟩, |01⟩, |10⟩ and |11⟩ states of figure A1, contrarily to the claim, does not match the matrix representation of an exact CNOT gate (see equation (15)).

Appendix B. Details of the derivation of equation (10)

We present the derivation of the equation (10). Considering the three-step sequence reported in figure 3, the resulting matrix is \( U_{12}(t_{12})U_{23}(t_{23})U_{13}(t_{13}) \) which must match \( R_z(\theta) \). After carrying out the calculations in equation (5) for each step of the sequence, it is found that
\[
U_{12} U_{23} U_{13} = \begin{pmatrix} \alpha \cos (\gamma) & i\alpha \sin (\gamma) \\ i\beta \sin (\gamma) & \beta \cos (\gamma) \end{pmatrix}
\]

where
\[
\alpha = \exp \left( i\frac{5\pi (t_{13} + t_{23} + t_{12})}{4} \right),
\beta = \exp \left( i\frac{4(t_{13} + 5t_{23} + t_{12})}{4} \right),
\gamma = \frac{\sqrt{3}\pi (t_{13} - t_{23})}{2}.
\]

By imposing
\[
\begin{pmatrix} \alpha \cos (\gamma) & i\alpha \sin (\gamma) \\ i\beta \sin (\gamma) & \beta \cos (\gamma) \end{pmatrix} = \begin{pmatrix} e^{-i\theta/2} & 0 \\ 0 & e^{i\theta/2} \end{pmatrix}
\]

it derives that
\[
\sin (\gamma) = 0 \Rightarrow t_{13} = t_{23}
\]

and substituting this result in equations (B.2) one obtains
\[
U_{12} U_{23} U_{13} = \begin{pmatrix} \alpha (t_{13} = t_{23}) & 0 \\ 0 & \beta (t_{13} = t_{23}) \end{pmatrix}
\]

By imposing \(\alpha (t_{13} = t_{23}) = e^{-i\theta/2}\) and \(\beta (t_{13} = t_{23}) = e^{i\theta/2}\) it is straightforward to find
\[
t_{13} = t_{23} = \frac{3\theta}{10\pi} - \frac{2}{5} + n,
\]
\[
t_{12} = 2(2 - n) - \frac{\theta}{\pi},
\]
\[
n = \left\lfloor 1 - \frac{\theta}{2\pi} \right\rfloor
\]

with \(n\) integer parameter. Moreover, \(t_{13}, \ t_{23}\) and \(t_{12}\) must be non-negative and as short as possible. The resulting step times are
\[
t_{13}(\theta) = t_{23}(\theta) = \begin{cases} \frac{3\theta}{10\pi} + \frac{1}{5} & \text{for } 0 < \theta < \frac{2\pi}{3}, \\ \frac{3\theta}{10\pi} - \frac{1}{5} & \text{for } \frac{2\pi}{3} < \theta < 2\pi, \end{cases}
\]
\[
t_{12}(\theta) = 2 - \frac{\theta}{\pi} & \text{for } 0 < \theta < 2\pi
\]

in units of \(\hbar/J_{\text{max}}\).

Appendix C. Derivation of the effective Hamiltonians for two interacting qubits

We present the explicit expressions of the effective Hamiltonian models of two interacting qubits. The total Hamiltonian model is composed by two free terms describing the two qubits and by an interaction part between the two.
The free Hamiltonians of the two qubits $a$ and $b$, written in terms of the creation and annihilation fermionic operators $c^\dagger_k$ and $c_k$ respectively are given for $q \equiv a, b$ by

$$H_q = H_{q_1} + H_{q_2} + H_{q_3} + H_{q_4},$$ (C.1)

where terms on the right-hand side are reported in equations (C.2)–(C.6) for every pair of spins considered.

$$H_{q_1} = \sum_{k=1}^{3} \varepsilon_k c^\dagger_k c_k \quad \text{with} \quad \sigma = \uparrow, \downarrow, \quad \text{(C.2)}$$

$$H_{q_2} = n_{1,\sigma} \sum_{\sigma} \left( c^\dagger_{1,\sigma} c_{3,\sigma} + \text{h.c.} \right) + t_{2,\sigma} \sum_{\sigma} \left( c^\dagger_{2,\sigma} c_{3,\sigma} + \text{h.c.} \right), \quad \text{(C.3)}$$

$$H_{q_3} = \sum_{k=1}^{3} U_k n_{1,k} n_{k,\uparrow} + U_{1,2,3} \left( n_{1,1} + n_{1,\downarrow} \right) \left( n_{2,1} + n_{2,\downarrow} \right) + U_{1,3,2} \left( n_{1,\uparrow} + n_{1,\downarrow} \right) \left( n_{3,1} + n_{3,\downarrow} \right) + U_{2,3,1} \left( n_{2,\uparrow} + n_{2,\downarrow} \right) \left( n_{3,1} + n_{3,\downarrow} \right), \quad \text{(C.4)}$$

$$H_{q_4} = H^{(1,3,1)} + H^{(2,3,1)} + H^{(1,2,3)}, \quad \text{(C.5)}$$

$$H^{(1,3,1)} = -J^{(1,3,1)} \left( n_{1,\uparrow} n_{1,\downarrow} + n_{1,\downarrow} n_{1,\uparrow} \right) - \sum_{\sigma} \left( J^{(1,1,\sigma)} c^\dagger_{1,\sigma} c^\dagger_{1,\sigma} c_{1,\sigma} c_{1,\sigma} + \text{h.c.} \right) + \sum_{k,\sigma} \left( J^{(1,1,\sigma)} n_{k,\sigma} c^\dagger_{1,\sigma} c_{1,\sigma} + \text{h.c.} \right). \quad \text{(C.6)}$$

$H_{q_1}$ and $H_{q_2}$ describe respectively the single electron energy level of each dot and the tunneling energy. The last two terms $H_{q_3}$ and $H_{q_4}$ constitute the intra-dot and inter-dot Coulomb interactions. $J^{(1,3,1)}$ is the spin exchange term, $J^{(1,2,3)}$ the pair-hopping term and $J^{(1,1,\sigma)}$ the occupation-modulated one.

Regarding the configuration $A$ the interaction Hamiltonian is given by the sum of the following terms

$$H_i = t_{1,1,1} \sum_{\sigma} \left( c^\dagger_{1,\sigma} c_{1,\sigma} + \text{h.c.} \right) + t_{3,2,3} \sum_{\sigma} \left( c^\dagger_{3,\sigma} c_{2,\sigma} + \text{h.c.} \right),$$

$$H_U = U_{1,1,1} \left( n_{1,\uparrow} + n_{1,\downarrow} \right) \left( n_{1,\uparrow} + n_{1,\downarrow} \right) + U_{3,2,3} \left( n_{3,\uparrow} + n_{3,\downarrow} \right) \left( n_{2,\uparrow} + n_{2,\downarrow} \right),$$

$$H_J = H^{(1,1,1)} + H^{(3,2,3)},$$

where $H_J$ is defined as in equation (C.6).
Following the same procedure reported in [13], we calculate the projected Hamiltonian using an appropriate operator. The effective Hamiltonian, concerning the low energy excitation, appears as the sum of all the exchange interactions between pairs of spins

\[
H^{\text{eff}} = \sum_{q=a,b} \left( J_{1,q,3} S_q \cdot S_{3,q} + J_{2,q,4} S_{2,q} \cdot S_{4,q} \right) + J_{3,1a} S_{1a} \cdot S_{3a} + J_{3,2b} S_{1b} \cdot S_{2b},
\]

(C.7)

The effective coupling constants, considering that intra-dot Coulomb energies are larger than all the other contributions are finally given by

\[
\begin{align*}
J_{1,3} & \approx \frac{1}{\Delta E_1} 4 \left( E_{1,3} - J_1^{(1,3)} \right)^2 - 2 J_1^{(1,3)}, \\
J_{2,3} & \approx \frac{1}{\Delta E_2} 4 \left( E_{2,3} - J_2^{(2,3)} \right)^2 - 2 J_2^{(2,3)}, \\
J_{1,2} & = \left( \frac{1}{\Delta E_3} + \frac{1}{\Delta E_4} \right) 4 \left( E_{1,2} - 2 J_3^{(1,2)} \right)^2 - 2 J_3^{(1,2)}, \\
J_{3,1} & \approx \frac{1}{\Delta E_5} 4 \left( E_{3,1} - J_4^{(3,1)} \right)^2 - 2 J_4^{(3,1)}, \\
J_{3,2} & \approx \frac{1}{\Delta E_6} 4 \left( E_{3,2} - J_5^{(3,2)} \right)^2 - 2 J_5^{(3,2)}, \\
\end{align*}
\]

where the energy differences for qubits a and b are

\[
\begin{align*}
\Delta E_{1,4} & = E_{(012,111)} - E_{(111,111)}, \\
\Delta E_{2,5} & = E_{(012,111)} - E_{(111,111)}, \\
\Delta E_{3,6} & = E_{(012,111)} - E_{(111,111)}, \\
\Delta E_{4,7} & = E_{(012,111)} - E_{(111,111)}, \\
\Delta E_{5,8} & = E_{(110,111)} - E_{(111,111)}, \\
\Delta E_{6,9} & = E_{(110,111)} - E_{(111,111)}, \\
\end{align*}
\]

with the different terms defined in equations (C.8)–(C.10) where we point out that the first (last) three indices inside parenthesis, 0 \leq i \neq j \neq k \leq 2, assuming only integer values, denote the number of electrons in each level for qubit a (b)

\[
E_{ijk,111} = i \varepsilon_1 + j \varepsilon_2 + k \varepsilon_3 + ijU_{1,2,e} + ikU_{1,3,e} + kju_{2,3} + \delta_{12} U_{1a} + \delta_{12} U_{2b} + \delta_{22} U_{3b} + \varepsilon_{1a} + \varepsilon_{2a} + \varepsilon_{3a} + U_{1,2a} + U_{1,3a} + U_{2,3b} + kU_{3,1b} + kU_{3,2b},
\]

(C.8)
For the second configuration $B$ under study we assume that the energy detuning between the double occupied QDs is small enough so terms of the Hamiltonian containing tunnelling rates and exchange interactions between energy levels in different QDs with different indexes (i.e. $1_a 2_b$, $2_a 1_b$) are negligible. The interaction Hamiltonian terms are finally given by

$$H_i = n_{l,1_a} \sum_{\sigma} \left(c_{1_a \sigma}^\dagger c_{1_a \sigma} + \text{h.c.}\right) + n_{l,2_b} \sum_{\sigma} \left(c_{2_b \sigma}^\dagger c_{2_b \sigma} + \text{h.c.}\right),$$

$$H_U = U_{1_a,1_b} \left(n_{l,1} + n_{l,1}\right) \left(n_{l,1} + n_{l,1}\right) + U_{1_a,2_b} \left(n_{l,2} + n_{l,1}\right) \left(n_{l,2} + n_{l,2}\right) + U_{2_a,1_b} \left(n_{l,2} + n_{l,2}\right) \left(n_{l,1} + n_{l,1}\right) + U_{2_a,2_b} \left(n_{l,2} + n_{l,2}\right) \left(n_{l,2} + n_{l,2}\right),$$

$$H_J = H_{J^{1,1}} + H_{J^{2,2}},$$

where $H_J$ is defined as in equation (C.6).

Analogously to the previous case, the effective Hamiltonian appears as the sum of exchange interactions:

$$H_{\text{eff}} = \sum_{q=a,b} \left(J_{1_q,3_q} S_{1_q} \cdot S_{3_q} + J_{2_q,3_q} S_{2_q} \cdot S_{3_q}\right) + J_{1_q,2_q} S_{1_q} \cdot S_{2_q} + J_{1_q,1_q} S_{1_q} \cdot S_{1_q} + J_{2_q,1_q} S_{2_q} \cdot S_{1_q} + J_{2_q,2_q} S_{2_q} \cdot S_{2_q},$$

(C.11)

The effective coupling constants, under the assumption of larger intra-dot energies with respect to inter-dot ones are finally given by

$$J_{1_q,3_q} \approx \frac{1}{\Delta E_{1_q}} \left(f_{1_q,3_q} - f_{1_q,3_q}\right)^2 - 2f_{1_q,3_q},$$

$$J_{2_q,3_q} \approx \frac{1}{\Delta E_{2_q}} \left(f_{2_q,3_q} - f_{2_q,3_q}\right)^2 - 2f_{2_q,3_q},$$

(C.12)
\[ J_{1,2_e} = \left( \frac{1}{\Delta E_{\nu}} + \frac{1}{\Delta E_{\delta}} \right) 4J_{1}^{(1,2_{\nu})} - 2J_{2}^{(1,2_{\delta})}, \]

\[ J_{1,1_p} \approx -2J_{1}^{(1,1_{\nu})}, \]

\[ J_{1,2_p} = 0, \]

\[ J_{2,1_p} = 0, \]

\[ J_{2,2_p} \approx -2J_{2}^{(2,2_{\nu})}. \]

where

\[ \Delta E_{i(ab)} = E_{(012,111)}(E_{(111,012)}) - E_{(111,111)}, \]

\[ \Delta E_{2(a,b)} = E_{(102,111)}(E_{(111,012)}) - E_{(111,111)}, \]

\[ \Delta E_{3(a,b)} = E_{(201,111)}(E_{(111,012)}) - E_{(111,111)}, \]

\[ \Delta E_{4(a,b)} = E_{(021,111)}(E_{(111,012)}) - E_{(111,111)} \]

with the different terms defined in equations (C.12)–(C.14)

\[ E_{(ijk,111)} = ie_{1s} + je_{2s} + ke_{3s} + ijU_{1s,2s} + ikU_{1s,3s} \]

\[ + kU_{2s,3s} + \delta_{12}U_{1s} + \delta_{13}U_{2s} + \delta_{23}U_{3s} \]

\[ + \epsilon_{1s} + \epsilon_{2s} + \epsilon_{3s} + U_{1s,2s} + U_{1s,3s} + U_{2s,3s} \]

\[ + iU_{1s,1s} + iU_{2s,2s} + jU_{3s,1s} + jU_{3s,2s}, \]  \hspace{1cm} (C.12)

\[ E_{(111,ijk)} = \epsilon_{1s} + \epsilon_{2s} + \epsilon_{3s} + U_{1s,2s} + U_{1s,3s} + U_{2s,3s} \]

\[ + ie_{1s} + je_{2s} + ke_{3s} + ijU_{1s,2s} + ikU_{1s,3s} \]

\[ + kU_{2s,3s} + \delta_{12}U_{1s} + \delta_{13}U_{2s} + \delta_{23}U_{3s}, \]

\[ + iU_{1s,1s} + iU_{2s,2s} + iU_{3s,1s} + jU_{3s,2s}, \]  \hspace{1cm} (C.13)

\[ E_{(111,111)} = \epsilon_{1s} + \epsilon_{2s} + \epsilon_{3s} + U_{1s,2s} + U_{1s,3s} + U_{2s,3s} \]

\[ + \epsilon_{1s} + \epsilon_{2s} + \epsilon_{3s} + U_{1s,2s} + U_{1s,3s} + U_{2s,3s}, \]

\[ + U_{1s,1s} + U_{2s,2s} + U_{2s,2s}. \]  \hspace{1cm} (C.14)

References

[1] Koppens F H L, Buizert C, Tielrooij K J, Vink I T, Nowack K C, Meunier T, Kouwenhoven L P and Vandersypen L M K 2006 Driven coherent oscillations of a single electron spin in a quantum dot Nature 442 766–71

[2] Morello A et al 2010 Single-shot readout of an electron spin in silicon Nature 467 687–91

[3] Maune B M et al 2010 Coherent singlet-triplet oscillations in a silicon-based double quantum dot Nature 481 344–7

[4] Medford J, Beil J, Taylor J M, Bartlett S D, Doherty A C, Rashba E I, DiVincenzo D P, Lu H, Gossard A C and Marcus C M 2013 Self-consistent measurement and state tomography of an exchange-only spin qubit Nat. Nanotechnology 8 654–9

[5] Loss D and DiVincenzo D P 1998 Quantum computation with quantum dots Phys. Rev. A 57 120
[6] Vrijen R, Yablonovitch E, Wang K, Wen Jiang H, Balandin A, Roychowdhury V, Mor T and DiVincenzo D 2000 Electron-spin-resonance transistors for quantum computing in silicon–germanium heterostructures Phys. Rev. A 62 012306

[7] Levy J 2002 Universal quantum computation with spin-1/2 pairs and Heisenberg exchange Phys. Rev. Lett. 89 147902

[8] Petta J R, Johnson A C, Taylor J M, Laird E A, Yacoby A, Lukin M D, Marcus C M, Hanson M P and Gossard A C 2005 Coherent manipulation of coupled electron spins in semiconductor quantum dots Science 309 2180–4

[9] Taylor J M, Engel H-A, Dur W, Yacoby A, Marcus C M, Zoller P and Lukin M D 2005 Fault-tolerant architecture for quantum computation using electrically controlled semiconductor spins Nat. Phys. 1 177

[10] DiVincenzo D P, Bacon D, Kempe J, Burkard G and Whaley K 2000 Universal quantum computation with the exchange interaction Nature 408 339

[11] Shi Z et al 2012 Fast hybrid silicon double-quantum-dot qubit Phys. Rev. Lett. 108 140503

[12] Koh T S, Gamble J K, Friesen M, Eriksson M A and Coppersmith S N 2012 Pulse-gated quantum-dot hybrid qubit Phys. Rev. Lett. 109 250503

[13] Ferraro E, De Michielis M, Mazzeo G, Fanciulli M and Prati E 2014 Effective Hamiltonian for the hybrid double quantum dot qubit Quantum Inf. Process. 13 1155–73

[14] Shi Z et al 2014 Fast coherent manipulation of three-electron states in a double quantum dot Nat. Commun. 5 3020

[15] Kim D et al 2014 Quantum control and process tomography of a semiconductor quantum dot hybrid qubit Nature 511 70–74

[16] Prati E et al 2012 Few electron limit of n-type metal oxide semiconductor single electron transistors Nanotechnology 23 215204

[17] Pierre M, Wacquez R, Roche B, Jehl X, Sanquer M, Vinet M, Prati E, Belli M and Fanciulli M 2009 Compact silicon double and triple dots realized with only two gates Appl. Phys. Lett. 95 242107

[18] Rohling N and Burkard G 2012 Universal quantum computing with spin and valley states New J. Phys. 14 083008

[19] Jefferson J H and Häusler W 1996 Effective charge-spin models for quantum dots Phys. Rev. B 54 4936–47

[20] Fong B H and Wandzura S M 2011 Universal quantum computation and leakage reduction in the 3-qubit decoherence free subsystem Quantum Inf. Comput. 11–12 1003–18

[21] Hickman G T, Wang X, Kestner J P and das Sarma S 2013 Dynamically corrected gates for an exchange-only qubit Phys. Rev. B 88 161303

[22] Setiawan F, Hui H-Y, Kestner J P, Wang X and Das Sarma S 2014 Robust two-qubit gates for exchange-coupled qubits Phys. Rev. B 89 085314

[23] Kosut R L, Grace M D and Brif C 2013 Robust control of quantum gates via sequential convex programming Phys. Rev. A 88 052326

[24] von Barth U and Hedin L 1972 A local exchange-correlation potential for the spin polarized case: I J. Phys. C: Solid State Phys. 5 1629–42

[25] Prati E 2011 Valley blockade quantum switching in silicon nanostructures J. Nanosci. Nanotechnol. 11 8522–6

[26] De Michielis M, Prati E, Fanciulli M, Fiori G and Iannaccone G 2012 Geometrical effects on valley-orbital filling patterns in silicon quantum dots for robust qubit implementation Appl. Phys. Express 5 124001

[27] Perdew J P and Wang Y 1992 Accurate and simple analytic representation of the electron–gas correlation energy Phys. Rev. B 45 13244–9

[28] Koh T S, Coppersmith S N and Friesen M 2013 High fidelity gates in quantum dot spin qubits Proc. Natl Acad. Sci. 110 19695