Two-Qubit Couplings of Singlet-Triplet Qubits Mediated by One Quantum State

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We describe high-fidelity entangling gates between singlet-triplet qubits (STQs) which are coupled via one quantum state (QS). The QS can be provided by a quantum dot itself or by another confined system. The orbital energies of the QS are tunable using an electric gate close to the QS, which changes the interactions between the STQs independent of their single-qubit parameters. Short gating sequences exist for CNOT operations.

A spin-based quantum computer can be realized using singlet-triplet qubits (STQs). One qubit is encoded in the spin subspaces of two singly-occupied quantum dots (QDs). Single-qubit control is provided by the exchange interaction between the electrons on the two QDs and a magnetic field gradient over the double quantum dot (DQD). The magnitude of the exchange interaction can be tuned rapidly using electric gates near the QDs. Single-qubit control of a STQ is extremely successful for gate-defined QDs in GaAs and Si; low-frequency noise is successfully eliminated in decoupling experiments.

Two-qubit gates are more demanding for STQs. Two approaches have been suggested. Electrostatic couplings between STQs allow one to make use of the exchange interaction between the electrons on the two QDs. However, electrostatic couplings are usually weak, which makes these operations slow. Alternatively, direct exchange interactions between the DQDs can be used. This approach was originally introduced for single-electron spin qubits. The realization of direct exchange gates between STQs has not been successful so far. The DQDs must be close to each other to allow an overlap of the electrons’ wave functions.

In this paper we explore indirect exchange interactions between STQs via one quantum state (QS). This approach was already proposed in passing in Ref. [17]. We explore the rich opportunities of mediated couplings while considering all possible charge configurations of the QS. The QS can be empty, singly-occupied, or filled with two electrons. Each charge configuration permits entangling operations for STQs. We describe entangling gate sequences which are shorter than all earlier proposals for direct exchange interactions and do not require the interaction strength to be raised to unrealistically large values. Our gate sequences are high fidelity even if the interactions between the STQs are not strongly coupled. The possibility to tune two-qubit interactions directly using a gate close to the QS makes mediated exchange gates superior to direct exchange gates.

The main findings of this paper are explicit, simple two-qubit gate sequences for STQs, which are mediated by one QS. A single QS can be provided by one QD itself or by another confined system. We also provide expressions for the resulting mediated exchange coupling. The magnetic field gradients are fixed at a constant value and have magnitudes similar to the mediated exchange interactions. For empty or a doubly-occupied QS, the two-qubit entangling operations via the QS are needed only once if the magnetic field gradients are identical across the DQDs. Such a one-step entangling gate through exchange interactions has never been described before. Two entangling operations together with one single-qubit operation create a CNOT for magnetic field gradients of opposite signs. A singly-occupied QS allows a CNOT operation with two/three entangling operations with the QS together with single-qubit gates for equal/opposite magnetic field gradients across the DQDs. These gate sequences realize high-fidelity entangling operations for STQs encoded in GaAs and Si QDs.

Model – We consider an array of four singly-occupied QDs (QD₁, QD₄); two QD pairs are coupled by one QS [cf. Fig. 1(a)]. QD₁ and QD₂ encode one STQ, which we call STQL (QD₃ and QD₄ encode STQR). A large global magnetic field splits the energies of the s₂ = 0 and s₂ = ±1 subspaces of a DQD. We identify the computational subspace with the electron configurations \{ | ↑ \rangle_{L,R}, | ↓ \rangle_{L,R} \} on STQL,R as the logical qubit states \{ | 1 \rangle_{L,R}, | 0 \rangle_{L,R} \}. The electron configurations \{ | ↑ \rangle, | ↓ \rangle \} on the DQDs represent leakage states. Energy P is needed to fill a QD with one electron, Q for the second electron. For the QS, energy U is needed to add one electron, and Δ for a second electron [cf. Fig. 1(b)].

We assume ideal single-qubit gates: phase evolutions are generated by the Hamiltonian \( \tau_Z = | 1 \rangle \langle 1 | - | 0 \rangle \langle 0 | \); \( \tau_x = | 1 \rangle \langle 0 | + | 0 \rangle \langle 1 | \) creates transitions between the qubit states. A magnetic field gradient \( \Delta B_L \) over STQL causes, through \( \Delta B_L (\sigma_1 - \sigma_2^z) \), a phase evolution...
Figure 1. Coupling of two STQs via one QS. (a) Four gate-defined QDs, which are shown in red, define two STQs. Each QD is filled with one electron. A global magnetic field acts on all QDs. There is a static, small magnetic field gradient across the left/right QD, \( \Delta B_{L/R} \). We assume identical magnetic field gradients \( \Delta B = \Delta B_L = \pm \Delta B_R \); magnetic fields are equal at the QS and averaged across the QDQDs. Exchange interactions together with \( \Delta B_L \) and \( \Delta B_R \) are sufficient to control the \( s_z = 0 \) subspace. One QS, which can be provided by another QS, couples STQL and STQR. (b) Orbital energy levels of the QDs and the QS: Adding one electron at the QS requires the energy \( P \), the second electron \( Q \). The first electron at the QS costs the energy \( U \), the second electron \( \Delta \). Adding one electron to the QDs requires the energy \( Q \). The magnitudes of \( U \) and \( \Delta \) can be tuned using an electric gate close to the QS.

\[
\Delta B_L \tau_z, \quad \sigma_i^{\pi/2,\pi/2} \text{ are the Pauli matrices at } QD_i. \text{ Exchange interactions } J_{12} \tau_z \text{ generate qubit rotations } J_{12} \tau_z. \quad \sigma_i \text{ is the vector of Pauli matrices on } QD_i, \quad 1 \text{ is the identity operation, and } J_{12} \text{ is the exchange coefficient between electrons on } QD_1 \text{ and } QD_2. \text{ We label exchange gates by } X_{\frac{\pi}{2}} = e^{-i\frac{\pi}{2} (\sigma_z, \sigma_z)}, \text{ and phase gates by } Z_{\frac{\pi}{2}} = e^{-i\frac{\pi}{2} (\sigma_z, \sigma_z)}, \text{ with } \beta = \Delta B_{L/R}. \text{ Equivalent descriptions apply for STQR.}

Empty or doubly-occupied QS – A non-trivial two-qubit interaction between STQL and STQR can be mediated by an empty or a doubly-occupied QS. The configuration with four electrons and an empty QS, which we denote \((1,1,0,1,0,1)\), is the ground state. If the Fermi energy \( E_F \) fulfills \( E_F \gtrsim 4P \) and \( E_F < (3P + U, 2P + U + \Delta, 3P + Q) \). The ground-state is \((1,1,2,1,1)\) with six electrons and a doubly-occupied QS if \( E_F \gtrsim 4P + U + \Delta \) and \( E_F < (4P + U + Q, 4P + 2Q, 3P + Q + U + \Delta) \).

Virtual couplings of the STQs with the QS cause an effective exchange interaction between \( QD_2 \) and \( QD_3 \):

\[
\mathcal{H}_{eff} = \frac{J_{eff}}{2} (\sigma_2 \cdot \sigma_3 - 1). \tag{1}
\]

The exchange coefficient \( J_{eff} \) can be derived: \( J_{eff}^0 = \sqrt{\frac{2t^4}{(U - P)^2} \left( \frac{2}{U + \Delta - 2P} + \frac{1}{Q - P} \right)} \) for an empty QS and \( J_{eff}^2 = \frac{2t^4}{(U - P)^2} \left( \frac{2}{U + \Delta - 2P} + \frac{1}{Q - P} \right) \) for a doubly-occupied QS \([21]\). The tunnel coupling \( t \) describes the transfer of electrons between \( QD_2 \) or \( QD_3 \) to the QS. \( t \) is much smaller than any orbital energy differences, which allows us to derive effective low-energy Hamiltonians using Schrieffer-Wolff (SW) perturbation theory \([22,23]\). Spin effects are relevant in fourth-order lower. Adding two electrons to a quantum level is only permitted in the singlet configuration, making the singlet energy lower. We assume that we can tune \( J_{eff} \) in Eq. (1) to magnitudes similar to \( \Delta B_{L/R} \) and restrict \( \Delta B = \Delta B_L = \pm \Delta B_R \). The average magnetic fields across each QD and at the QS are also taken to be identical. The time evolution is described by:

\[
U_{\epsilon, \beta}^z = e^{-i2\pi \left[ \frac{\beta}{2}(\sigma_2 \cdot \sigma_3 - 1) + \frac{\epsilon}{2}(\sigma_1 \cdot \sigma_1) \right]},
\]

with \( \beta = \frac{\Delta B_R}{h}, \epsilon = \frac{J_{eff}}{h} \).

There exists a perfect entangler, which is equivalent to a CNOT operation, with only one exchange operation for \( \Delta B_L = \Delta B_R; U_{1/4, \sqrt{3}/4}^x [\text{Fig. 2(a)]}. \text{ Leakage from the computational subspace is absent. One can prove easily that } U_{1/4, \sqrt{3}/4}^x \text{ is maximally entangling by calculating the Makhlin invariants \([21,24]\). The entangling gate uses the exchange operations only once. In previous studies exchange gates were described that needed the exchange interactions twice \([11,18]\). Even though these studies relate to direct exchange interactions between STQs, our gate can be used without change in these setups.}

The values \((\epsilon, \beta) = \left\{ \frac{\pi}{4}, \sqrt{3} \right\} \) are not the only possible parameters which describe a CNOT. Evaluating \( U_{\epsilon, \beta}^z \) from Eq. (4) on the \( s_z = 0 \) subspace shows that leakage out of the computational subspace is proportional to \( 2 \sqrt{\beta^2 + \epsilon^2} \): leakage is absent for \( 2 \sqrt{\beta^2 + \epsilon^2} \in \mathbb{N} \).

The Makhlin invariants are \( G_1 = \cos^2 (2\pi \epsilon), G_2 = 1 + 2G_1 \) under this condition. We obtain a CNOT operation with \( G_1 = 0, G_2 = 1 \) for \( 2\epsilon \in (2N + 1)/2 \).

Magnetic field gradients of opposite signs \( \Delta B_L = -\Delta B_R \) also permit entangling operations. There is no entangling operation with one coupling to the QS: gates without leakage from the computational subspace have the Makhlin invariants \( G_1 = 1, G_2 = 3 \) and are equivalent to single-qubit operations \([24]\). Up to local unitaries, \( \text{CNOT} \) is constructed by \( U_{\epsilon, \beta}^z \mathcal{U}_{n, \beta}^+ \mathcal{U}_{n, \beta}^-, \text{ with } n = (2N + 1)/8 \text{ and finite } \beta \) [Fig. 2(b)]. The entangling properties of this sequence are untouched by the value of \( \beta \), which means that this operation is independent of the ratio of \( \Delta B \) and \( J_{eff} \). Levy proposed an equivalent gate sequence for direct exchange interactions between STQs without any magnetic field gradients during the entangling operation \([11]\).

Singly-occupied QS – Constructing two-qubit gates for STQs mediated by a singly-occupied QS is more challenging, because this setup involves more leakage states.
with $\beta = \frac{\Delta B}{h}$, $\epsilon = \frac{\mu_i t}{h}$.

There is an entangling gate for $\Delta B_L = \Delta B_R$ that uses $U_3^{+\sqrt{31}/10/31}$ twice together with one single-qubit rotation. The operation $U_3^{+\sqrt{31}/10/31}$ does not cause leakage from the computational subspace and describes the time evolution
diag $\left(e^{2\pi i (4-4\sqrt{3})/\sqrt{31}}, e^{8\pi i/\sqrt{31}}, 1, e^{2\pi i (4+4\sqrt{3})/\sqrt{31}}\right)$

Figure 2. Entangling gates that are equivalent to a CNOT up to single-qubit operations for two STQs coded on QD_{1,2} and QD_{3,4}. We denote the configurations by the electron numbers at (QD_1, QD_2, QS, QD_3, QD_4). The DQDs are coupled via one QS (cf. Fig. 1). Entangling operations between two STQs mediated by an empty or a doubly-occupied QS for equal (a) and opposite (b) magnetic field gradients. The CNOT operation requires one/two entangling operation according to Eq. (2). Entangling operations mediated by a singly-occupied QS for equal (c) and opposite (d) magnetic field gradients. This setup requires two/three entangling operations according to Eq. (3). All gate sequences and parameters ($\beta, \phi, \psi_{1-4}$) are discussed in the text.

The (1, 1, 1, 1) configuration is the ground state for $E_F > 4P + U$ and $E_F < (4P + Q, 3P + U + \Delta)$. The mediated interactions between QD_{2,3} and QD_3 can be described by the exchange interactions with the QS:

$$H_{\text{eff}} = \frac{J_{\text{eff}}}{2} \left[(\sigma_2 \cdot \sigma_{QS} - 1) + (\sigma_{QS} \cdot \sigma_3 - 1)\right].$$

$J_{\text{eff}}$ describes direct exchange interactions between QD_{2,3} and the QS. The couplings between QD_{2,3} and the QS are identical. Global magnetic fields are sufficiently strong to consider only one $s_z$ subspace of all five electrons (we choose $s_z = \frac{1}{2}$). Besides the computational subspace, which is spanned by $|\uparrow\downarrow\uparrow\downarrow\downarrow\rangle, |\downarrow\uparrow\uparrow\downarrow\downarrow\rangle, |\downarrow\uparrow\downarrow\uparrow\downarrow\rangle, |\uparrow\downarrow\downarrow\uparrow\downarrow\rangle$ on QD_{1-4} coupled to $\uparrow$ on the QS, there are six leakage states in the same $s_z$ subspace. We take the magnetic field gradients on STQ_L and STQ_R to be identical $\Delta B = \Delta B_L = \pm \Delta B_R$. Average magnetic fields across each DQD and at the QS are taken to be equal; each cross DQD and is described by:

$$U_{\epsilon, \beta} = e^{-2\pi i \left[\frac{1}{2}((\sigma_2 \cdot \sigma_{QS} - 1) + (\sigma_{QS} \cdot \sigma_3 - 1) + \frac{1}{2}((\sigma_1^z - \sigma_2^z) \pm (\sigma_1^z - \sigma_3^z))\right]},$$

with $\beta = \frac{\Delta B}{h}$, $\epsilon = \frac{\mu_i t}{h}$.

Gate performance and noise properties – Entangling two STQs via one QS has advantages compared to direct exchange couplings between STQs. The state energies of the QS are directly tunable using electric gates without affecting the DQDs. It has turned out in experiments that manipulating state energies is easier (cf. especially Ref. [3]) than tuning tunnel couplings [17]. Consequently, the setup with a mediating QS also simplifies the realization of entangling operations for weak tunnel couplings $t$. Magnitudes of $t$ are on the order of 20 $\mu$eV and the addition energy $Q$ reaches a few meV for single-qubit operations [3]. Exchange operations are possible with megahertz frequencies: $\nu = (t^2/Q)/h \approx 100$ MHz. Reaching large $t$ is very critical for two-qubit gates. DQDs are preferably some distance apart from each other; $t$ decreases exponentially with this distance. One can raise the mediated interaction for small $t$ by significantly lowering $U$ and $\Delta$, and completely turn it off for large $U$ and $\Delta$. It should be possible to raise $J_{\text{eff}}$ to magnitudes similar to $\Delta B$. Manipulation frequencies of 100 MHz are sufficient for fast gate operations; experiments with magnetic field gradients with this order of magnitude have been carried out [3, 14]. Note, that two-qubit interactions are tunable independent of the single-qubit parameters.

A real system may not fulfill all restrictions of the pro-
posed setup due to fabrication errors: 1) in our gate constructions, the magnetic field gradients have the same magnitude across the DQDs while only the sign is allowed to differ. The average magnetic field across each DQD is equal to the field at the QS. In reality, only the local magnetic fields at $QD_2$, $QD_3$, and the QS matter for the proposed gate sequences. $QD_1$ and $QD_4$ are decoupled during the entangling operations. Shifts in their local magnetic fields can be corrected by single-qubit operations. Local magnetic field shifts at the QS are only critical when the QS is singly-occupied. In the case of an empty and a doubly-occupied QS, states with an unpaired electron at the QS are only virtually occupied. 2) All QDs are identical in the model for the entangling gates, especially $QD_2$ and $QD_3$ have equal couplings to the QS. In the case of an empty and a doubly-occupied QS, the same gate sequences can be used if $QD_2$ and $QD_3$ differ. Eq. (1) remains valid with a modified exchange constant (cf. [21]). In the case of a singly-occupied QS, unequal qubit parameters disturb the entangling gates. In addition to the interactions from Eq. (3), there is a term $\frac{\delta J}{2} (\sigma_2 \cdot \sigma_{QS} - \sigma_{QS} \cdot \sigma_3)$. The coupling between $QD_2$ and the QS differs from $J_{eff}^{12}$ between the QS and $QD_3$. Only strong asymmetries of $\delta J/J_{eff}^{12} > 2\%$ generate gate infidelities of more than 1% for the sequences of Fig. 2 (c)-(d) (cf. [21]).

Hyperfine interactions generate fluctuating magnetic fields locally at the positions of the QDs and the QS. Fluctuations of the nuclear spins are low frequency; they can be treated as static during one entangling operation and only have different distributions for subsequent measurements [26]. A random component $\delta B^z$ parallel to the external magnetic field gives the main contribution for strong global magnetic fields. For uncorrected nuclear baths, typical values for $\delta B^z$ are 100 neV (5 mT) in GaAs QDs [3] and 3 neV (25 $\mu$T) for Si QDs [27]. $\delta B^z$ was suppressed to 10 neV (0.5 mT) in GaAs QDs by preparing the nuclear spin-bath in a narrowed state with smaller fluctuations [4]. We use these values as the root mean square of a Gaussian distribution for $\delta B_i^z$ at each QD and at the QS [3]. The gate sequences in Fig. 2 (a)-(d) have infidelities of several percent for GaAs QDs with uncorrected nuclear baths, but the errors are suppressed by two orders of magnitude when using a narrowed nuclear spin distribution. The infidelities are below 0.1% for Si QDs (cf. [21]). $\delta B^z$ can be suppressed by one order of magnitude in isotopically purified Si compared to natural Si; these heterostructures contain fewer finite-spin nuclei ($^{29}$Si). Additionally, one can decrease $\delta B^z$ by measuring the local hyperfine fields and adjusting the gate sequences in a feedback loop.

Spin-orbit interactions (SOIs) cause additional errors. The spin rotates slightly when an electron is transferred between localized states. SOIs renormalize the exchange constants weakly. Anisotropic exchange terms introduce errors [21, 28, 29]. The gate sequences in [15] were constructed to be optimal with respect to the Dzyaloshinskii-Moriya interaction, which is one part of the anisotropic exchange terms. Our fidelity analysis shows, however, that SOIs have only a minor effect on the gate sequences in Fig. 2 (cf. [21]). In the worst case, gate infidelities reach a few percent for GaAs QDs. The errors are several orders of magnitudes lower for Si QDs. SOIs are less critical if the external magnetic field is perpendicular to the SO field. In this case, SOIs couple states of different $s_z$, which have a large energy difference [18].

Charge traps induce energy fluctuations between states of different charge character [30,32]. Charge noise is critical for small $t$ (cf. [21]). The occupation of energy levels different from the initial charge configuration is higher to reach large $J_{eff}$ for small $t$. Entangling operations via an empty and a doubly-occupied QS are more susceptible to charge noise than the operations with a singly-occupied QS. $J_{eff}^1$ and $J_{eff}^2$ require a larger population of the excited energy levels to reach magnitudes similar to $J_{eff}^1$.

**Conclusion** – We have shown that exchange-based entangling operations for two STQs are possible through mediated exchange couplings with one QS. One additional QD or another confined system can provide this QS. The strength of the mediated interactions can be tuned to magnitudes similar to the static magnetic field gradients across the DQDs. It can be controlled independent of the STQs. If the QS is empty or doubly-occupied, one needs to use interactions of the QS and the STQs only once if the magnetic field gradients across the DQDs have the same sign. The entangling operations are needed twice for STQs with magnetic field gradients of opposite signs. These gating sequences are also applicable for direct exchange interactions between STQs. A singly-occupied QS has slightly lower entangling ability. One needs two operations with the QS if $\Delta B_L$ and $\Delta B_R$ are equal, but three if they are opposite to each other. Note that another possibility to couple spin qubits via a mediating QD was proposed recently [33]. However, the entangling mechanism is distinct from our approach; it uses two QWs of a multi-electron QD.

Hyperfine interactions introduce major errors if the mediated interactions are of the same size as the uncertainty of the hyperfine fields. Hyperfine interactions can be critical for GaAs QDs; narrowing the nuclear spin distributions for GaAs QDs or choosing Si QDs greatly improves the gate fidelities. Other noise sources and small fabrication errors are less important. Entangling STQs through mediated exchange interactions is very promising, especially since larger arrays of QWs are currently becoming available [34,37]. Using multi-electron QDs for the mediated coupling is also beneficial. The addition energies in these systems are suppressed. Multi-electron QDs were successfully explored recently [38]. High-fidelity two-qubit gate operations with excellent control should justify the effort of fabricating one QS between the DQDs, rather than coupling them directly.
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See Supplemental Material at [URL will be inserted by publisher] for further information about the effective Hamiltonians and the gate sequences. Numerical values for $\psi_i$, $i = 1, \ldots, 4$ are given. We introduce a complete description of spin-orbit interactions for the mediated interactions. The supplement provides additional data for the fidelity analysis of fabrication errors, hyperfine interactions, SOIs, and charge noise.

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Supplemental Material to Two-Qubit Couplings of Singlet-Triplet Qubits Mediated by One Quantum State

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I. GATE DESCRIPTION

A. Characterization of Entangling Gates

The Makhlin invariants [1, 2] characterize the entangling properties of a gate. The values

\[ G_1 = \text{tr}^2(m) / (16 \det(m)) \in \mathbb{C}, \]
\[ G_2 = (\text{tr}^2(m) - \text{tr}(m^2)) / (4 \det(m)) \in \mathbb{R} \]

fully characterize two-qubit operations, independent of additional single-qubit operations before and after the gate. \( m = M_B^2 M_B \), where \( M_B \) is the representation of the gate in the Bell-basis. A gate is a perfect entangler if it creates a maximally entangled state from a separable state. It needs to fulfill \( \sin^2(\gamma) \leq 4|G_1| \leq 1 \) and \( \cos(\gamma) (\cos(\gamma) - G_2) \geq 0 \) for \( G_1 = |G_1| e^{i\gamma} \). One example is a controlled-NOT operation (CNOT), which is characterized by \( G_1 = 0 \) and \( G_2 = 1 \). We also searched for the square root of SWAP gate, with \( G_1 = i/4 \) and \( G_2 = 0 \). The sequences we found for \( \sqrt{\text{SWAP}} \) required more entangling operations with the QS than for the CNOT.

B. Fidelity Analysis

A disturbed operation \( U_d \) is characterized by the entanglement fidelity [3, 4]:

\[ F = \text{tr} \left[ \rho^{RS} 1_R \otimes (U_i^{-1} U_d)_S \rho^{RS} 1_R \otimes (U_d^{-1} U_i)_S \right]. \quad (3) \]

\( U_i \) describes the ideal time evolution. We double the state space to two identical Hilbert spaces \( R \) and \( S \). \( \rho^{RS} = |\psi \rangle \langle \psi| \) represents a maximally entangled state on the larger Hilbert space, e.g. \( |\psi \rangle = (|0000\rangle + |0110\rangle + |1001\rangle + |1111\rangle) / 2 \). \( F \) reaches unity for perfect gates. This definition captures also leakage errors of the qubit.

\( U_d \) differs from \( U_i \) through systematic or random errors. We describe random errors with a parameter \( \xi \) that modifies \( U_d(\xi) \) between different runs of the experiment and obeys a classical probability distribution \( f(\xi) \). The fidelity \( F \) is calculated by averaging Eq. (3) over many instances of \( U_d(\xi) \) giving \( F = \int d\xi \ f(\xi) \ F(\xi) \).

II. ORBITAL HAMILTONIAN

Our description of the system uses the orbital energies of the charge configurations and the transition matrix elements between them. We include in this study \( QD_2, QD_3 \), and the QS while considering one orbital at each position (cf. Fig. 1 of the main text). Each energy level can be empty, singly occupied, or doubly occupied. This treatment corresponds to a Hund-Mulliken approximation [5]. We describe the electron configurations by the electron numbers on the QDs and the QS: \( (n_{QD_2}, n_{QS}, n_{QD_3}) \). Electron transfer between the QDs and the QS is described by the spin-conserving hopping...
Hamiltonian:

\[ H_t = t \sum_{i \in \{2,3\}, \sigma} \left( c_{i\sigma}^\dagger c_{Q\sigma} + \text{h.c.} \right). \]  \hspace{1cm} (4)

\( c_{i\sigma}^{(1)} \) is the annihilation (creation) operator of an electron at position \( i \) with spin \( \sigma \), h.c. is the hermitian conjugate of the preceding term, and \( t \in \mathbb{R} \) is the tunnel coupling.

Adding one electron to a QD requires energy \( P \), the second electron \( Q \). One electron at the QS requires energy \( U \), a second electron \( \Delta \) (cf. Fig. 1 (b) of the main text). We disregard global magnetic fields as we consider a global \( s_z \) subspace in the study of the main text. We assume that energy shifts from local magnetic fields are small compared to the orbital energy scales, especially the magnetic field gradients across the DQDs fulfill \( \Delta B \ll (P, Q, U, \Delta) \). \( \Delta B \) are typically on the order of 2 meV (100 mT) \([6, 7]\), which corresponds to the manipulation frequency \( \Delta B/h \approx 500 \text{ MHz} \) for GaAs nanostructures. The orbital energy scales are usually on the order of few meV \([8]\). Similar considerations are valid for Si QDs. Note that \( QD_1 \) and \( QD_4 \) are omitted in the following discussion, because they are decoupled during the entangling operations. \( QD_1 \) and \( QD_4 \) are always singly-occupied and add the energies \( 2P \) to all electron configurations considered in the main text.

### A. Empty QS

The electron configurations can be tuned to \((1,0,1)\) with an empty QS. The Fermi energy fulfills \( E_F \gtrsim 2P \) and \( E_F \ll (P+U, U+\Delta, P+Q) \). One can reach the electron configurations \((1,1,0)\) and \((0,1,1)\) after one electron transfer. \((2,0,0), (0,2,0), \) and \((0,0,2)\) are reached after two hopping events. \( H_t \) from Eq. (4) couples states of the same number of spin-up and spin-down electrons on \( QD_2, QD_3 \), and the QS. The problem can be separated into different \( s_z \) subspaces \( N_{s_z} = N_{QD_2,QS,QD_3}^\dagger - N_{QD_2,QS,QD_4}^\dagger \) when deriving effective Hamiltonians.

The discussions of the \( N_{s_z} = \pm 2 \) subspaces are equivalent. We show only the \( N_{s_z} = 2 \) subspace. The state notation is fixed to \( |QD_2 \uparrow, QD_2 \downarrow, QS \uparrow, QS \downarrow, QD_3 \uparrow, QD_3 \downarrow \rangle \). We obtain in the basis \(|1,0,0,0,1,0\rangle, |1,0,1,0,1,0\rangle, \) and \(|0,0,1,0,0,0\rangle, |0,0,1,0,1,0\rangle\) the Hamiltonian:

\[ H_{N_{s_z}=2} = \begin{pmatrix} 2P & -t & -t \\ -t & P+U & 0 \\ -t & 0 & P+U \end{pmatrix}. \]  \hspace{1cm} (5)

\( H_{N_{s_z}=2} \) provides a perfect example where Schrieffer-Wolff (SW) perturbation theory can be used \([9, 10]\). It describes two energetically separated subspaces, which are weakly coupled. The ground-state subspace \( P \) consists of the state \(|1,0,0,0,1,0\rangle \). All other states are part of the excited subspace \( Q \). The effective Hamiltonian on \( P \) in fourth-order SW perturbation theory \([10]\) describes an energy shift: \( \text{shift} = \frac{2t^2 \Delta B}{(U-P)^2} + \frac{2t^2}{U-P} \).

We use the basis \(|1,0,0,0,1,0\rangle, |0,1,0,1,1,0\rangle, |1,0,1,0,0,0\rangle, |0,1,1,0,0,0\rangle, |0,0,0,1,1,0\rangle, |0,0,1,1,0,0\rangle, |1,1,0,0,0,0\rangle, |0,0,0,0,1,1\rangle \) for \( N_{s_z} = 0 \). The total Hamiltonian, splits into two weakly coupled subspaces \( P \) (at zero energy) and \( Q \) (at higher energy). We derive again an effective Hamiltonian on \( P \) in fourth-order SW perturbation theory:

\[ \tilde{H}_P \approx \text{shift} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}. \]  \hspace{1cm} (7)
which includes the same energy shift as for $N_z = \pm 2$.

We introduced $J_{eff}^0 = \frac{2t_4^2}{(U-\Delta-P)^2} \left( \frac{2}{U-\Delta-P} + \frac{1}{Q-\rho} \right)$.

The total low-energy Hamiltonian on the subspace spanned by the states $\{1,0,0,0,1,0\}$, $\{1,0,0,0,0,1\}$, $\{0,1,0,0,1,0\}$, and $\{0,1,0,0,0,1\}$ is:

$$\tilde{H}_t \approx \frac{J_{eff}^0}{2} (\sigma_2 \cdot \sigma_3 - 1).$$

The effective exchange interaction $J_{eff}^0$ lowers only the singlet energy, while it keeps all triplet states untouched. Note that the constant energy shift is neglected in Eq. (8).

### B. Singly-Occupied QS

The low-energy subspace of a singly-occupied QS consists of the states with the electron configurations $(1,1,1)$. We reach it for $E_F \geq 2P + U$ and $E_F < (2P + F, P + U + \Delta)$. The interaction between $QD_2$ and the QS can be separated from the interaction between $QD_3$ and the QS, because couplings to excited states are weak. $\tilde{H}_t$ from (4) introduces exchange interactions on the low-energy subspace. No couplings are possible for $(n_{QD_2}, n_{QS}) = (1,1)$ in the $|\uparrow, \uparrow\rangle / |\downarrow, \downarrow\rangle$ configurations. Singlet pairing lowers the energy of the singlet configuration on $QD_2$ and QS. $\tilde{H}_t$ couples to the singlets in $(1,1), (2,0)$ and (0,2). It is straightforward to derive an effective Hamiltonian in second-order SW perturbation theory:

$$\tilde{H}_t \approx \frac{J_{eff}^1}{2} (\sigma_2 \cdot \sigma_{QS} - 1),$$

with $J_{eff}^1 = t_2^2 \left( \frac{1}{Q-U} + \frac{1}{Q-\rho} \right)$. The same result holds for the coupling of the QS to $QD_3$.

### C. Doubly-Occupied QS

The last possible case is one doubly-occupied QS. The electron configuration $(1,2,1)$ is the ground state for $E_F \geq 2P + U + \Delta$ and $E_F < (2P + U + Q, 2P + Q, P + Q + U + \Delta)$. From the $(1,2,1)$ configuration, one can reach, with the transfer of one electron, the $(2,1,1)$ and $(1,1,2)$ configurations. After a second electron transfer, one can reach the configurations $(2,2,0), (0,2,2), (2,0,2)$. Deriving an effective Hamiltonian is equivalent to the case of an empty QS. In fourth order SW, we obtain an effective exchange Hamiltonian between $QD_2$ and $QD_3$:

$$\tilde{H}_t \approx \frac{J_{eff}^2}{2} (\sigma_2 \cdot \sigma_3 - 1),$$

with $J_{eff}^2 = \frac{2t_4^2}{(Q-\Delta)^2} \left( \frac{2}{Q-\Delta} + \frac{1}{Q-P} \right)$. This effect explains the antiferromagnetism of many materials; it is called superexchange in the field of magnetism [11, 12].

### III. FABRICATION ERRORS:UNEQUAL QDS

**Empty/Doubly-Occupied QS** – In fourth-order SW perturbation theory, there is only a modification of the existing exchange term if $QD_2$ differs from $QD_3$:

$$J_{eff}^0 = \sum_{i=1,2} \frac{t_{i1}^2 t_{i0}^2}{(U-P_i)^2} \left( Q_{2i-1} - P_i \right) + \frac{t_{i1}^2 t_{i2}^2}{(U+\Delta-S_{i1})^2} \left( Q_{1i} - P_i \right) + \frac{t_{i2}^2 t_{i0}^2}{(U+\Delta-S_{i0})^2} \left( Q_{0i} - P_i \right),$$

$$J_{eff}^1 = \sum_{i=1,2} \frac{t_{i1}^2 t_{i0}^2}{(U-P_i)^2} \left( 2 \prod_{i=1,2} \frac{1}{(U-P_i)} + \sum_{i=1,2} \frac{1}{(U-P_i)^2} \right),$$

$$J_{eff}^2 = \sum_{i=1,2} \frac{t_{i1}^2 t_{i0}^2}{(U+\Delta-S_{i1})^2} \left( 2 \prod_{i=1,2} \frac{1}{(Q_{1i} - P_i)} + \sum_{i=1,2} \frac{1}{(Q_{1i} - P_i)^2} \right) \cdot$$

$t_{i1,2}$ is the tunnel coupling between $QD_{2,3}$ and the QS. $P_{i1,2}$ is the addition energy for an electron to $QD_{2,3}$, the second electron costs $Q_{i1,2}$.

**Singly-Occupied QS** – Differences in the fabrication of $QD_2$ and $QD_3$ matter for the entangling operations of Fig. 2 (c)-(d) of the main text. The exchange coupling between $QD_2$ and the QS then differs from $J_{eff}^1$ between $QD_3$ and the QS. We use a total exchange Hamiltonian:

$$\tilde{H}_t = \frac{J_{eff}^1}{2} (\sigma_2 \cdot \sigma_{QS} - \sigma_{QS} \cdot \sigma_3),$$

where $\delta J$ is the difference in the exchange constants and $\overline{J_{eff}^1}$ is their average value. Fig. 1 shows the gate infidelities as a function of $\delta J/\overline{J_{eff}^1}$.

### IV. HYPERFINE INTERACTIONS

We model hyperfine interactions by a random component of the local magnetic fields at the positions of the QDs and at the QS. We average 1000 nuclear distributions with a random $\frac{\delta B_z}{2} \sigma_{z}^i$ at each QD and the QS. $\delta B_z$ is the root mean square of a Gaussian distribution, single-qubit gates are ideal. Typical values for $\delta B_z$ are 100 neV (5 mT) in GaAs QDs [8] and 3 neV (25 mT) for Si QDs [13] for uncorrected nuclear spins. $\delta B_z$ was suppressed to 10 neV (0.5 mT) in GaAs QDs by narrowing the nuclear spin distribution [14]. Fig. 2 shows the gate infidelities $1 - F$ of the gate sequences from Fig. 2 (a)-(d) of the main text as a function of $\delta B_z/\overline{J_{eff}^1}$. 
Figure 1. Gate infidelities $1 - F$ of the entangling gates of Fig. 2 (c)-(d) of the main text for unequal exchange couplings $J_{eff}^i$ of QD$_2$ with the QS and QD$_3$ with the QS. The difference of the exchange constants $\delta J$ to their average value $J_{eff}$ is varied in Eq. (13).

\[
\sigma = (\sigma_x, \sigma_y, \sigma_z)^T \text{ is a vector of Pauli matrices. } iS \text{ describes transition matrix element between localized states generated by SOI. It has been shown that } S \text{ can be represented by a real vector } |16\rangle. S \text{ defines the direction of the spin-orbit (SO) field. There is a common approximation for localized states which are the distance } d \text{ apart: } S = |S| \approx t \xi, \text{ with } \xi = \frac{d}{l_{so}} \text{ and } l_{so} \text{ is the spin-precession length } |16–18\rangle. \xi \ll 1 \text{ for common GaAs and Si QD pairs.}
\]

V. SPIN-ORBIT INTERACTIONS

Spin-orbit interactions (SOIs) cause spin rotations when an electron moves between localized states. We assume a linear QD arrangement (cf. Fig. 1 (a) of the main text) and describe the influence of SOIs by \cite{15}:

\[
\mathcal{H}_{so} = iS \cdot \sum_{\sigma \sigma'} \left( c_{2\sigma}^\dagger \sigma_\sigma c_{Q\sigma} + c_{Q\sigma}^\dagger \sigma_\sigma' c_{3\sigma'} + h.c. \right).
\]

(14)

A. Effective Hamiltonians

The low-energy Hamiltonian becomes anisotropic when we include, in addition to $\mathcal{H}_s$ in Eq. (4), the SOIs through $\mathcal{H}_{so}$ from Eq. (14). We obtain in fourth-order SW perturbation theory additional terms:

- empty QS

\[
\mathcal{H}_{so}^0 = \frac{1}{U - P} \left( \frac{2}{U + \Delta - 2P} + \frac{1}{Q - P} \right) \cdot \left\{ - S^2 \left[ (6t^2 - S^2) \sigma_2 \cdot \sigma_3 + (2t^2 + S^2) \right] \right. \\
\left. + 4t (t^2 - S^2) S \cdot (\sigma_2 \times \sigma_3) \right. \\
\left. + 8t^2 (S \cdot \sigma_2) (S \cdot \sigma_3) \right\}.
\]

(15)

- singly-occupied QS

\[
\mathcal{H}_{so}^1 \approx \left( \frac{1}{Q - U} + \frac{1}{\Delta - P} \right) \cdot \left\{ - \frac{S^2}{2} \left[ (\sigma_2 \cdot \sigma_{QS} + 1) + (\sigma_{QS} \cdot \sigma_3 + 1) \right] \right. \\
\left. + iS \cdot \left[ (\sigma_2 \times \sigma_{QS}) + (\sigma_{QS} \times \sigma_3) \right] \right. \\
\left. + (S \cdot \sigma_2) (S \cdot \sigma_{QS}) + (S \cdot \sigma_{QS}) (S \cdot \sigma_3) \right\}.
\]

(16)

- doubly-occupied QS

\[
\mathcal{H}_{so}^2 \approx \frac{1}{(Q - \Delta)^2} \left( \frac{2}{2Q - (U + \Delta)} + \frac{1}{Q - P} \right) \cdot \left\{ - S^2 \left[ (6t^2 - S^2) \sigma_2 \cdot \sigma_3 + (2t^2 + S^2) \right] \right. \\
\left. + 4t (t^2 - S^2) S \cdot (\sigma_2 \times \sigma_3) \right. \\
\left. + 8t^2 (S \cdot \sigma_2) (S \cdot \sigma_3) \right\}.
\]

(17)

For all charge configurations of the QS, SOIs influence the low-energy subspace similarly. The first term renormalizes the exchange constant. The last two terms describe an anisotropic (super-) exchange interaction. The second term is the dominant contribution, as it scales linearly with $S$ for $S \ll t$. This term is called Dzyaloshinskii-Moriya interaction in literature \cite{19–21}. We simplify the expressions in Eq. (15)-(17) for $S \ll t$, while we ignore the small renormalization of the exchange

\[
\mathcal{H}_{so} = iS \cdot \sum_{\sigma \sigma'} \left( c_{2\sigma}^\dagger \sigma_\sigma c_{Q\sigma} + c_{Q\sigma}^\dagger \sigma_\sigma' c_{3\sigma'} + h.c. \right).
\]
constant:
\[
\tilde{\mathcal{H}}_{so}^0 \approx J_{eff}^0 \left[ 2\xi eS \cdot (\sigma_2 \times \sigma_3) + 4\xi^2 (eS \cdot \sigma_2)(eS \cdot \sigma_3) \right],
\]
(18)
\[
\tilde{\mathcal{H}}_{so}^1 \approx J_{eff}^1 \left\{ (\xi eS \cdot (\sigma_2 \times \sigma_{QS}) + (\sigma_{QS} \times \sigma_3) \right\},
\]
(19)
\[
+ \xi^2 \left[ (eS \cdot \sigma_2)(eS \cdot \sigma_{QS}) + (eS \cdot \sigma_{QS})(eS \cdot \sigma_3) \right],
\]
\[
\tilde{\mathcal{H}}_{so}^2 \approx J_{eff}^2 \left[ 2\xi eS \cdot (\sigma_2 \times \sigma_3) + 4\xi^2 (eS \cdot \sigma_2)(eS \cdot \sigma_3) \right].
\]
(20)
e_S is the unit vector pointing along the SO field.

B. Fidelity Analysis

We assume that the magnetic field is oriented in the plane of the QDs, so that the SO field is also restricted to this plane. The effective mediated exchange constant \( J_{eff} \) is chosen to be 100 MHz and the external global external magnetic field is fixed to 500 MHz. The magnetic field strength corresponds to 100 mT in GaAs and 25 mT in Si. \( d \approx 200 \) nm is a typical distance between localized states. Larger values of \( d \) increase the influence of SOIs, but decrease the tunnel couplings between localized states. We introduce common SOI parameters [22, 23]: typical SO lengths are around \( l_{so} \approx 2 \) \( \mu \)m in GaAs samples. Note that experimentally measured values for \( l_{so} \) in GaAs QDs can be much larger [24, 25] and are strongly probe dependent [22]. The effective mass in Si heterostructures is nearly three times larger than in GaAs; nanostructures in Si are about two times smaller than in GaAs, while \( l_{so} \) is approximately one order of magnitude larger. We use \( d = 100 \) nm and \( l_{so} = 10 \) \( \mu \)m for Si QDs. The gate infidelities \( 1 - F \) for the sequences of Fig. 2 (a)-(d) of the main text are shown in Fig. 3. We assume ideal single-qubit operations.

VI. CHARGE NOISE

Charge traps of the substrate are uncontrollably filled and unfilled with electrons. These fluctuations, called charge noise, create low-frequency fluctuations of the electric fields at the the position of the QDs. We model the dominant effect of charge noise through a zero-frequency fluctuation \( \delta \epsilon(t) \) of the energy difference \( C \) between different charge configurations. \( J_{eff} \) is also controlled by \( C \):

\[
J_{eff}^0 \approx J_{eff}^2 \approx \frac{2t^4}{[C + \delta \epsilon(t)]^3},
\]
(21)
\[
J_{eff}^1 \approx \frac{t^2}{C + \delta \epsilon(t)}.
\]
(22)

We disregard, for the case of an empty QS, occupations of states with two electrons at the QS and approximate \( C \approx U - P \approx \frac{U + \Delta}{2} - P \). For a doubly-occupied QS, we disregard all states other than in \( (1, 2, 1, 1), (1, 1, 2, 1), \) and \( (1, 2, 0, 2, 1) \). We approximate \( C \approx Q - \Delta \approx \frac{2\Delta(U + \Delta)}{2} \). Fig. 4 shows the influence of charge noise for exchange gates of \( J_{eff}/\hbar = 100 \) MHz. Charge noise is introduced through the random variable \( \delta \epsilon(t) \) of a Gaussian distribution with root mean square \( \delta \epsilon \); the fidelity is averaged over 1000 random values of \( \delta \epsilon(t) \). Energy fluctuations in GaAs charge qubits were measured at few \( \mu \)eV [26, 27]. Charge noise in Si QDs may be assumed to be of the same order of magnitude.
We use a numerical gate search algorithm (cf. Ref. [28]), which works similar to the algorithm described by Fong and Wandzura [29]. We define an objective function $f$, that describes the deviation of a gate sequence from an ideal gate. The ideal gate is reached at $f = 0$. An example is the construction of a $CNOT$ on the computational subspace $P$. The unitary operation on the leakage subspace $Q$ is arbitrary, but the matrix elements between $P$ and $Q$ must vanish. We can search for a $CNOT$ up to local unitary gates. These gate sequences have the Makhlin invariants $G_1 = 0$ and $G_2 = 1$. We construct the objective function $f = \|G_1(U_{PP})\| + \|G_2(U_{PP}) - 1\| + \|U_{PQ}\| \geq 0$, where $\|\ldots\|$ describes a matrix norm and $U_{ij}$ is the projected gate sequence $P_i U_{ij} P_j$. $f = 0$ for ideal gates.

A gate operation is defined by a sequence of single-qubit and two-qubit gates. $X$ and $Z$ rotations, which construct a universal set of single-qubit gates, are characterized by one parameter (cf. description in the main text). The two-qubit gates considered require two parameters. The numerical gate search is constructed in a three-step program:

1. Initialization: A large number of possible gates is constructed with arbitrary parameters for the single and the two-qubit gates.

2. Gate Optimization: All gate sequences are optimized. We minimize the objective function $f$. We minimize randomly one, two, or all gates. Most of the time the minimization procedure does not converge.

3. Gate Selection: We analyze the sequences created in 2. If the ideal gate is not reached to some accuracy by one gate sequence, we go back to 2. We keep a collection of gate sequences which are closest to $f = 0$ and drop sequences which are far away from the ideal gate.

The obtained gate can usually be simplified. One may especially remove some single-qubit operations from the sequence.

VIII. GATE SEQUENCES

A. Full Gate Sequences for CNOT Operations

We describe the gate sequences to construct a $CNOT$ operation on the computational subspace in the basis $\{|\uparrow, \downarrow, \uparrow, \downarrow, |\uparrow, \downarrow, \downarrow, \downarrow, |\downarrow, \uparrow, \uparrow, \downarrow, |\downarrow, \downarrow, \downarrow, \downarrow\}$ using one (for an empty/doubly-occupied QS) and two (for a singly-occupied QS) entangling operations with the QS.

- empty/doubly-occupied QS, $\Delta B_L = \Delta B_R$:

$$C PHASE = Z_L^{(3-\sqrt{3})/8} Z_R^{(3-\sqrt{3})/8} U_{1/4}^+ \sqrt{3/4}$$

$$C NOT = I \otimes H \cdot C PHASE \cdot I \otimes H$$

$$1 \otimes H = X_R^{1/8} Z_R^{1/8} X_R^{1/8}$$

- singly-occupied QS, $\Delta B_L = \Delta B_R$:

$$C NOT = U_{E} \cdot U_{\phi_1}^{+} \sqrt{3/\sqrt{31}} X_{\phi_1}^{L} U_{\phi_2}^{+} \cdot U_{\phi_2}$$

$$U_{E} = X_{\phi_1}^{L} Z_{\phi_2}^{L} X_{\phi_2}^{R} Z_{\phi_2}^{R} X_{\phi_1}^{1/8}$$

$$U_{I} = X_{\phi_1}^{L} Z_{\phi_2}^{L} X_{\phi_2}^{R} Z_{\phi_2}^{R} X_{\phi_1}^{1/8}$$
**B. Numerical Values**

The numerical values for the gate sequence of Fig. 2 (d) of the main text and Eq. (27)-(28) of the supplement are:

\[
\begin{align*}
\phi_1 &= 0.29863890926183401 \\
\phi_2 &= 0.39562438490324259 \\
\phi_3 &= 0.44782756169938542 \\
\phi_4 &= 0.97098194934834639
\end{align*}
\]

\[
\begin{align*}
\phi_5 &= 0.30231205192017918 \\
\phi_6 &= 0.34055840199539983 \\
\psi_1 &= 0.25112650148258442 \\
\psi_2 &= 0.63771948242765397 \\
\psi_3 &= 0.93365278621170444 \\
\psi_4 &= 0.22651273139644371
\end{align*}
\]

---

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